

MOX-Report No. 09/2023

Gauss-Newton oriented greedy algorithms for the reconstruction of operators in nonlinear dynamics

Buchwald, S.; Ciaramella, G.; Salomon, J.

MOX, Dipartimento di Matematica Politecnico di Milano, Via Bonardi 9 - 20133 Milano (Italy)

mox-dmat@polimi.it

https://mox.polimi.it

1 GAUSS-NEWTON ORIENTED GREEDY ALGORITHMS FOR THE 2 RECONSTRUCTION OF OPERATORS IN NONLINEAR DYNAMICS

3

S. BUCHWALD^{*}, G. CIARAMELLA[†], AND J. SALOMON[‡]

Abstract. This paper is devoted to the development and convergence analysis of greedy recon-4 struction algorithms based on the strategy presented in [Y. Maday and J. Salomon, Joint Proceedings 5 6 of the 48th IEEE Conference on Decision and Control and the 28th Chinese Control Conference, 2009, 7 pp. 375–379]. These procedures allow the design of a sequence of control functions that ease the 8 identification of unknown operators in nonlinear dynamical systems. The original strategy of greedy reconstruction algorithms is based on an offline/online decomposition of the reconstruction process 9 10 and on an ansatz for the unknown operator obtained by an a priori chosen set of linearly independent matrices. In the previous work [S. Buchwald, G. Ciaramella and J. Salomon, SIAM J. Control 11 Optim., 59(6), pp. 4511-4537], convergence results were obtained in the case of linear identification 12 13 problems. We tackle here the more general case of nonlinear systems. More precisely, we show that 14 the controls obtained with the greedy algorithm on the corresponding linearized system lead to the local convergence of the classical Gauss-Newton method applied to the online nonlinear identification 15 problem. We then extend this result to the controls obtained on nonlinear systems where a local 1617 convergence result is also obtained. The main convergence results are obtained for the reconstruction 18 of drift operators in linear and bilinear dynamical systems.

19 **Key words.** Gauss-Newton method, operator reconstruction, Hamiltonian identification, quan-20 tum control problems, inverse problems, greedy reconstruction algorithm, control theory

21 **AMS subject classifications.** 65K10, 65K05, 81Q93, 34A55, 49N45, 34H05, 93B05, 93B07

1. Introduction. This paper is concerned with the development and the anal-22 vsis of a new class of numerical methods for the reconstruction of nonlinear operators 23 24 in controlled differential systems. The identification of unknown operators and parameters characterizing dynamical systems is a typical problem in several fields of 25applied science. In general, this is understood as an inverse problem, where the goal 26 27is to best fit simulated and experimental data. However, when a system is affected by input forces that can be controlled by an external user, the data used in the fitting 28 29process can be manipulated. If the input forces are not properly chosen, the fitting process can result in a very poor quality of the reconstructed parameters or operators. 30 Thus, it is natural to look for a set of such input forces that allows one to generate 31 good data allowing the best possible reconstruction. This is a typical case in the field 32 33 Hamiltonian identification in quantum mechanics [5, 9, 17–21, 29, 33, 34, 36–39], or in engineering in the context of state space realization [16, 22, 25, 32] and optimal design 34 35 of experiments [1, 4, 7].

In this paper, we focus on the analysis and development of a class of greedy-36 type reconstruction algorithms (GR) that were introduced in [30] for Hamiltonian identification problems, further developed and analyzed in [11], and later adapted to 38 the identification of probability distributions for parameters in the context of quantum 39 systems in [13]. This approach decomposes the identification process into offline phase, 40 where the control functions are computed by a GR algorithm, and online phase, where 41 the controls are used to generate experimental data to be used in an inverse problem 42for the final reconstruct of the unknown operator. In [11], a first detailed convergence 43 analysis of this strategy was provided for the identification of the control matrix in 44 45 a linear input/output system. Based on this analysis, the authors developed a new

^{*}Universität Konstanz, Germany (simon.buchwald@uni-konstanz.de).

[†]MOX, Dipartimento di Matematica, Politecnico di Milano (gabriele.ciaramella@polimi.it).

[‡]INRIA Paris, France (julien.salomon@inria.fr).

46 more efficient and robust numerical variant of the standard greedy reconstruction 47 algorithm. It was then shown in [13] that this strategy is also able to reconstruct 48 the probability distribution of control inhomogeneities for a spin ensemble in Nuclear

49 Magnetic Resonance; see, e.g., [10, 23, 28].

The goal of this paper is to further develop the work [11] by considering nonlinear systems, and to relate the greedy-reconstruction procedure to the Gauss-Newton method (GN), which is one of the most famous methods for solving inverse problems [26]. In particular, we assume that the inverse problem in the online phase is solved by GN, and study the effect of the control functions generated by GR algorithms on the convergence of GN. This is achieved in two steps, which represent the main novelties of this manuscript.

57 First, we introduce a new greedy-type reconstruction approach. In particular, rather than applying GR directly to the nonlinear identification problem, we use it on 58its linearization. This corresponds to using GR for designing control functions that make the GN matrix, namely the Jacobian of the nonlinear residual, full rank in a 60 neighborhood of the solution, which is a sufficient condition for local convergence of 61 GN. We refer to this strategy as linearized greedy reconstruction algorithm (LGR), 62 and provide a corresponding detailed analysis for two classes of problems: the recon-63 struction of the drift matrix in linear input/output systems and the reconstruction 64 of an Hamiltonian matrix in skew-symmetric bilinear systems. Both cases represent 65 nonlinear problems, since the unknown operators act on the states of the systems. 66 Notice that the analysis that we are going to presented for the drift matrix is also 68 valid in the case of the reconstruction of the control matrix in a linear input/output systems, as considered in [11, Section 5]. Thus, this part of the present work is a 69 substantial extension of the results of [11]. 70

The second novelty of this work is to provide a first analysis of the original GR algorithm applied to nonlinear systems. This is achieved by relating the behavior of GR (applied to the original nonlinear problem) and LGR: under appropriate controllability and observability assumptions, we show that the controls generated by GR are suitable also for LGR and thus make the GN Jacobian matrix full rank.

The two GR and LGR approaches are compared by direct numerical experiments. These show that GR and LGR are comparable when working locally near the solution. However, the GR applied directly to the original nonlinear system is superior when only poor information about the solution is available.

The paper is organized as follows. In Section 2, the notation used throughout 80 this work is fixed. Section 3 describes how GN can be used to solve general recon-81 struction problems. In order to guarantee convergence of GN, the LGR algorithm 82 is introduced in Section 4. In sections 5 and 6, we present analyses of LGR for the 83 reconstruction of linear drift matrices in linear systems and an Hamiltonian matrix in 84 bilinear systems, respectively. Section 7 focuses on GR for nonlinear problems, and 85 a corresponding analysis is provided in section 7.1. Within section 7.2, we recall and 86 extend an optimized greedy reconstruction (OGR) algorithm introduced in [11]. The 87 LGR, GR and OGR algorithms are then tested numerically in section 8. Finally, our 88 89 conclusions are drawn in Section 9.

2. Notation. Consider a positive natural number N. We denote by $\langle \mathbf{v}, \mathbf{w} \rangle :=$ 91 $\mathbf{v}^{\top}\mathbf{w}$, for any $\mathbf{v}, \mathbf{w} \in \mathbb{R}^N$, the usual real scalar product on \mathbb{R}^N , and by $\|\cdot\|_2$ the 92 corresponding norm. For any $A \in \mathbb{R}^{N \times N}$, $[A]_{j,k}$ is the j, k (with $j, k \leq N$) entry of 93 A, and the notation $A_{[1:k,1:j]}$ indicates the upper left submatrix of A of size $k \times j$, 94 namely, $[A_{[1:k,1:j]}]_{\ell,m} := [A]_{\ell,m}$ for $\ell = 1, \ldots, k$ and $m = 1, \ldots, j$. Similarly, $A_{[1:k,i]}$ denotes the column vector in \mathbb{R}^k corresponding to the first k elements of the column *j* of A. Additionally, im(A) is the image of A, and ker(A) its kernel. We indicate by $\mathfrak{so}(N)$ the space of skew-symmetric matrices in $\mathbb{R}^{N \times N}$. Moreover, when talking about symmetric matrices, PD and PSD stand for positive definite and semidefinite, respectively. By (A, B, C) we denote the input/output dynamical system

100 (2.1)
$$\boldsymbol{x}(t) = C\boldsymbol{y}(t), \quad \dot{\boldsymbol{y}}(t) = A\boldsymbol{y}(t) + B\boldsymbol{\epsilon}(t), \quad \boldsymbol{y}(0) = \boldsymbol{y}^0$$

101 For an interval $X \subset \mathbb{R}$, the notation $\phi : X \Rightarrow \mathbb{R}^N$ indicates that ϕ is a set-valued 102 correspondence, i.e. $\phi(x) \subset \mathbb{R}^N$ is a set for $x \in X$. Finally, we denote by $\mathcal{B}_r^N(x) \subset \mathbb{R}^N$ 103 the *N*-dimensional ball with radius r > 0 and center $x \in \mathbb{R}^N$.

104 **3.** Gauss-Newton method (GN) for reconstruction problems. Consider 105 a state $\boldsymbol{y}(t) \in \mathbb{R}^N, N \in \mathbb{N}$, whose time evolution is governed by the system of ordinary 106 differential equations (ODE)

107 (3.1)
$$\dot{\boldsymbol{y}}(t) = f(A_{\star}, \boldsymbol{y}(t), \boldsymbol{\epsilon}(t)), \ t \in (0, T], \quad \boldsymbol{y}(0) = \boldsymbol{y}^{0},$$

where $\boldsymbol{y}^0 \in \mathbb{R}^N$ is the initial state and $\boldsymbol{\epsilon} \in E_{ad}$ denotes a control function belonging to E_{ad} , a non-empty and weakly compact subset of some Hilbert space of control functions from [0,T] to \mathbb{R}^M , $M \in \mathbb{N}$ (e.g., $E_{ad} \subset L^2(0,T;\mathbb{R}^M)$). The operator A_{\star} is unknown and assumed to lie in the space spanned by a finite-dimensional set $\mathcal{A} =$ $\{A_1,\ldots,A_K\}, K \in \mathbb{N}$, and we write $A_{\star} = \sum_{j=1}^K \boldsymbol{\alpha}_{\star,j} A_j =: A(\boldsymbol{\alpha}_{\star})$. We assume that $f: \operatorname{span}(\mathcal{A}) \times \mathbb{R}^N \times \mathbb{R}^M \to \mathbb{R}^N, (A, \boldsymbol{y}, \boldsymbol{\epsilon}) \mapsto f(A, \boldsymbol{y}, \boldsymbol{\epsilon})$ is differentiable in A and \boldsymbol{y} .

114 To identify the unknown operator A_{\star} one uses a set of control functions $(\boldsymbol{\epsilon}^m)_{m=1}^K \subset$ 115 E_{ad} to perform K laboratory experiments and obtain the experimental data

116 (3.2)
$$\boldsymbol{\varphi}_{data}^{\star}(\boldsymbol{\epsilon}^{m}) := C\boldsymbol{y}(A_{\star}, \boldsymbol{\epsilon}^{m}; T), \text{ for } m = 1, \dots, K.$$

117 Here, $\boldsymbol{y}(A_{\star}, \boldsymbol{\epsilon}; T)$ denotes the solution to (3.1) at time T > 0, corresponding to the 118 operator A_{\star} and a control function $\boldsymbol{\epsilon}$. The matrix $C \in \mathbb{R}^{P \times N}$ $(P \leq N)$ is a given 119 observer matrix. The measurements are assumed not to be affected by noise.

Using the set $(\boldsymbol{\epsilon}^m)_{m=1}^K$ and the data $(\boldsymbol{\varphi}_{data}^{\star}(\boldsymbol{\epsilon}^m))_{m=1}^K \subset \mathbb{R}^P$, the unknown vector *a* is obtained by solving the least-squares problem

122 (3.3)
$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{K}} \frac{1}{2} \sum_{m=1}^{K} \|\boldsymbol{\varphi}_{data}^{\star}(\boldsymbol{\epsilon}^{m}) - C\boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^{m}; T)\|_{2}^{2}.$$

GN is a typical iterative strategy to solve (3.3), and its process is initialized by a vector which we will call $\boldsymbol{\alpha}_{o} \in \mathbb{R}^{K}$. We denote by $\boldsymbol{\alpha}_{c} \in \mathbb{R}^{K}$ the GN iterate, and define $f_{m}(\boldsymbol{\alpha}) := \frac{1}{2} \sum_{i=1}^{P} ||(R_{m}(\boldsymbol{\alpha}))_{i}||_{2}^{2} = \frac{1}{2} R_{m}(\boldsymbol{\alpha})^{\top} R_{m}(\boldsymbol{\alpha})$, where

$$\mathbb{E}_{127}^{126} \quad (3.4) \qquad \qquad R_m(\boldsymbol{\alpha}) := C\boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^m; T) - \boldsymbol{\varphi}_{data}^{\star}(\boldsymbol{\epsilon}^m),$$

128 for $m \in \{1, \ldots, K\}$. Thus, the identification problem (3.3) is equivalent to

129 (3.5)
$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^K} \sum_{m=1}^K f_m(\boldsymbol{\alpha}).$$

130 Given an iterate $\boldsymbol{\alpha}_c$, GN computes the new iterate by solving a problem of the form

131 (3.6)
$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{K}} \sum_{m=1}^{K} \| R'_{m}(\boldsymbol{\alpha}_{c})(\boldsymbol{\alpha} - \boldsymbol{\alpha}_{c}) - R_{m}(\boldsymbol{\alpha}_{c}) \|_{2}^{2},$$

where $R'_m(\boldsymbol{\alpha}_c) \in \mathbb{R}^{P \times K}$ denotes the Jacobian of R_m at $\boldsymbol{\alpha}_c \in \mathbb{R}^K$. The first-order optimality condition of (3.6) is

134 (3.7)
$$\sum_{m=1}^{K} \left(R'_m(\boldsymbol{\alpha}_c)^{\top} R'_m(\boldsymbol{\alpha}_c) \right) \boldsymbol{\alpha} = \sum_{m=1}^{K} R'_m(\boldsymbol{\alpha}_c)^{\top} R_m(\boldsymbol{\alpha}_c),$$

where $\sum_{m=1}^{K} R'_m(\boldsymbol{\alpha}_c)^{\top} R'_m(\boldsymbol{\alpha}_c) =: \widehat{W}_c \in \mathbb{R}^{K \times K}$ is symmetric PSD. Now, we recall the following convergence result from [27, Theorem 2.4.1] (for a proof see also the supplementary material [12]).

138 LEMMA 3.1 (local convergence of GN). Consider a problem of the form (3.5). 139 Let $\boldsymbol{\alpha}_{\star}$ be a minimizer of (3.5) such that for all $m \in \{1, \ldots, K\}$ the function R_m is 140 Lipschitz continuously differentiable near $\boldsymbol{\alpha}_{\star}$ and $R_m(\boldsymbol{\alpha}_{\star}) = 0$. If the initialization 141 vector $\boldsymbol{\alpha}_{\circ} \in \mathbb{R}^K$ is sufficiently close to $\boldsymbol{\alpha}_{\star}$, and \widehat{W}_c is PD for all iterates $\boldsymbol{\alpha}_c \in \mathbb{R}^K$, 142 then GN converges quadratically to $\boldsymbol{\alpha}_{\star}$.

143 Lemma 3.1 implies that, given an initialization vector $\boldsymbol{\alpha}_{\circ}$ sufficiently close to the 144 solution $\boldsymbol{\alpha}_{\star}$, the functions $(\boldsymbol{\epsilon}^{m})_{m=1}^{K}$ should be chosen such that the GN matrix $\widehat{W}_{c} =$ 145 $\sum_{m=1}^{K} R'_{\boldsymbol{\epsilon}^{m}}(\boldsymbol{\alpha}_{c})^{\top} R'_{\boldsymbol{\epsilon}^{m}}(\boldsymbol{\alpha}_{c})$ is PD for all $\boldsymbol{\alpha}_{c} \in \mathbb{R}^{K}$ in a neighborhood of $\boldsymbol{\alpha}_{\star}$. Notice that 146 \widehat{W}_{c} being PD is equivalent to (3.6)-(3.7) being uniquely solvable. Using (3.4), we can 147 write (3.6) more explicitly. For a direction $\delta \boldsymbol{\alpha} \in \mathbb{R}^{K}$, we have

148 (3.8)
$$R'_{m}(\boldsymbol{\alpha}_{c})(\delta\boldsymbol{\alpha}) = C\delta\boldsymbol{y}_{c}(A(\delta\boldsymbol{\alpha}),\boldsymbol{\epsilon}^{m};T),$$

149 where $\delta \boldsymbol{y}_c(A(\delta \boldsymbol{\alpha}), \boldsymbol{\epsilon}^m; T)$ denotes the solution at time T to the linearized state equation

150 (3.9)
$$\begin{cases} \delta \dot{\boldsymbol{y}}_c = \partial_{\boldsymbol{y}} f(A(\boldsymbol{\alpha}_c), \boldsymbol{y}_c, \boldsymbol{\epsilon}) \delta \boldsymbol{y}_c + \sum_{j=1}^K \delta \boldsymbol{\alpha}_j \Big(\partial_A f(A(\boldsymbol{\alpha}_c), \boldsymbol{y}_c, \boldsymbol{\epsilon})(A_j) \Big), \ \delta \boldsymbol{y}_c(0) = 0, \\ \dot{\boldsymbol{y}}_c = f(A(\boldsymbol{\alpha}_c), \boldsymbol{y}_c, \boldsymbol{\epsilon}), \quad \boldsymbol{y}_c(0) = \boldsymbol{y}^0. \end{cases}$$

151 Hence, problem (3.6) can be written as

152 (3.10)
$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{K}} \sum_{m=1}^{K} \| C \delta \boldsymbol{y}_{c}(A(\boldsymbol{\alpha} - \boldsymbol{\alpha}_{c}), \boldsymbol{\epsilon}^{m}; T) - R_{m}(\boldsymbol{\alpha}_{c}) \|_{2}^{2}.$$

Notice that the vectors $R_m(\boldsymbol{\alpha}_c) \in \mathbb{R}^P$ are independent of $\boldsymbol{\alpha}$ and can therefore be considered as fixed data when solving (3.10). Now, we recall that the GR algorithm, introduced in [30] and further analyzed in [11], was designed specifically to generate control functions $(\boldsymbol{\epsilon}^m)_{m=1}^K$ that make problems of the form (3.10) uniquely solvable.

4. A linearized GR algorithm (LGR). Let us assume to be provided with an initialization vector $\boldsymbol{\alpha}_{\circ}$ for GN that is sufficiently close to $\boldsymbol{\alpha}_{\star}$. Further, let $\delta \boldsymbol{y}_{\circ}(A(\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\circ}), \boldsymbol{\epsilon}^{m}; T)$ denote solution at time T to

160 (4.1)
$$\begin{cases} \delta \dot{\boldsymbol{y}}_{\circ} = \partial_{\boldsymbol{y}} f(A(\boldsymbol{\alpha}_{\circ}), \boldsymbol{y}_{\circ}, \boldsymbol{\epsilon}) \delta \boldsymbol{y}_{\circ} + \sum_{j=1}^{K} (\boldsymbol{\alpha}_{j} - \boldsymbol{\alpha}_{\circ, j}) \Big(\partial_{A} f(A(\boldsymbol{\alpha}_{\circ}), \boldsymbol{y}_{\circ}, \boldsymbol{\epsilon})(A_{j}) \Big), \ \delta \boldsymbol{y}_{\circ}(0) = 0, \\ \dot{\boldsymbol{y}}_{\circ} = f(A(\boldsymbol{\alpha}_{\circ}), \boldsymbol{y}_{\circ}, \boldsymbol{\epsilon}), \ \boldsymbol{y}_{\circ}(0) = \boldsymbol{y}^{0}. \end{cases}$$

161 The goal is to generate control functions $(\boldsymbol{\epsilon}^m)_{m=1}^K$ such that (3.10) in $\boldsymbol{\alpha}_{\circ}$, that is

162 (4.2)
$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{K}} \sum_{m=1}^{K} \| C \delta \boldsymbol{y}_{\circ}(A(\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\circ}), \boldsymbol{\epsilon}^{m}; T) - R_{m}(\boldsymbol{\alpha}_{\circ}) \|_{2}^{2},$$

Algorithm 4.1 Linearized Greedy Reconstruction Algorithm (LGR)

Require: A set of linearly independent operators $\mathcal{A} = \{A_1, \dots, A_K\}$. Recall that $\delta \boldsymbol{y}_{\circ}(A, \boldsymbol{\epsilon}; T)$ solves (4.1).

1: Compute the control ϵ^1 by solving

(4.3)
$$\max_{\boldsymbol{\epsilon} \in E_{ad}} \|C \delta \boldsymbol{y}_{\circ}(A_1, \boldsymbol{\epsilon}; T)\|_2^2$$

- 2: for k = 1, ..., K 1 do
- $\underline{\text{Fitting step:}} \quad \text{Let } A^{(k)}(\boldsymbol{\beta}) := \sum_{j=1}^k \boldsymbol{\beta}_j A_j, \text{ find } \boldsymbol{\beta}^k = (\boldsymbol{\beta}_j^k)_{j=1,\ldots,k} \text{ that solves}$ 3:

(4.4)
$$\min_{\boldsymbol{\beta} \in \mathbb{R}^k} \sum_{m=1}^k \left\| C \delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}), \boldsymbol{\epsilon}^m; T) - C \delta \boldsymbol{y}_{\circ}(A_{k+1}, \boldsymbol{\epsilon}^m; T) \right\|_2^2.$$

Splitting step: Find $\boldsymbol{\epsilon}^{k+1}$ that solves 4:

(4.5)
$$\max_{\boldsymbol{\epsilon}\in E_{ad}} \left\| C\delta\boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}),\boldsymbol{\epsilon};T) - C\delta\boldsymbol{y}_{\circ}(A_{k+1},\boldsymbol{\epsilon};T) \right\|_{2}^{2}.$$

5: end for

1

is uniquely solvable. Then, in Section 5.2, we show that if (4.2) is uniquely solvable, 163 the same holds for (3.10) at all iterates $\boldsymbol{\alpha}_c$ of GN. 164

The set $(\boldsymbol{\epsilon}^m)_{m=1}^K$ is computed by the LGR Algorithm 4.1, which is the original 165GR algorithm from [30] applied to (4.2). Our goal is to prove that the set $(\boldsymbol{\epsilon}^m)_{m=1}^K$ 166 makes $\widehat{W}_{\circ} := \sum_{m=1}^{K} R'_m(\boldsymbol{\alpha}_{\circ})^{\top} R'_m(\boldsymbol{\alpha}_{\circ})$ PD, and thus (4.2) uniquely solvable. From (4.1), we have that $\delta \boldsymbol{y}_{\circ}$ is linear in $\boldsymbol{\alpha}$. Thus, $R'_m(\boldsymbol{\alpha}_{\circ})(\delta \boldsymbol{\alpha}) = \delta \boldsymbol{y}_{\circ}(A(\delta \boldsymbol{\alpha}), \boldsymbol{\epsilon}^m; T) = \sum_{j=1}^{K} \delta \boldsymbol{\alpha}_j C \delta \boldsymbol{y}_{\circ}(A_j, \boldsymbol{\epsilon}^m; T)$. Hence, $R'_m(\boldsymbol{\alpha}_{\circ})$ is a matrix with columns $R'_m(\boldsymbol{\alpha}_{\circ})_j = C \delta \boldsymbol{y}_{\circ}(A_j, \boldsymbol{\epsilon}^m; T)$ for $j = 1, \ldots, K$, and hence 167168169170

171 (4.6)
$$[\widehat{W}_{\circ}]_{i,j} = \sum_{m=1}^{K} \langle C \delta \boldsymbol{y}_{\circ}(A_i, \boldsymbol{\epsilon}^m; T), C \delta \boldsymbol{y}_{\circ}(A_j, \boldsymbol{\epsilon}^m; T) \rangle, \quad i, j \in \{1, \dots, K\}.$$

- Using (4.6), we can rewrite (4.3), (4.4) and (4.5) in a matrix form. 172
- LEMMA 4.1 (Algorithm 4.1 in matrix form). Consider Algorithm 4.1. Then: 173• The initialization problem (4.3) is equivalent to 174

175 (4.7)
$$\max_{\boldsymbol{\epsilon}\in E_{ad}} [W_{\circ}(\boldsymbol{\epsilon})]_{1,1}$$

176
$$where [W_{\circ}(\boldsymbol{\epsilon})]_{i,j} := \langle C\delta \boldsymbol{y}_{\circ}(A_i, \boldsymbol{\epsilon}; T), C\delta \boldsymbol{y}_{\circ}(A_j, \boldsymbol{\epsilon}; T) \rangle \text{ for } i, j \in \{1, \dots, K\}$$

• Let
$$W_{\circ}^{(\kappa)} := \sum_{m=1}^{\kappa} W_{\circ}(\boldsymbol{\epsilon}^{m})$$
, the fitting-step problem (4.4) is equivalent to

178 (4.8)
$$\min_{\boldsymbol{\beta}\in\mathbb{R}^k} \langle \boldsymbol{\beta}, [\widehat{W}_{\circ}^{(k)}]_{[1:k,1:k]} \boldsymbol{\beta} \rangle - 2\langle [\widehat{W}_{\circ}^{(k)}]_{[1:k,k+1]}, \boldsymbol{\beta} \rangle$$

• Let
$$\boldsymbol{v} := [(\boldsymbol{\beta}^k)^\top, -1]^\top$$
, the splitting-step problem (4.5) is equivalent to

180 (4.9)
$$\max_{\boldsymbol{\epsilon}\in E_{ad}} \langle \boldsymbol{v}, [W_{\circ}(\boldsymbol{\epsilon})]_{[1:k+1,1:k+1]} \boldsymbol{v} \rangle.$$

181Moreover, problems (4.3)-(4.7), (4.4)-(4.8), and (4.5)-(4.9) are well posed. 182 *Proof.* The proof is similar to the ones of [11, Lemma 5.12]. For an arbitrary $k \in$ $\{0,\ldots,K-1\}$ let $\boldsymbol{v} \in \mathbb{R}^{k+1}$ and $A(\boldsymbol{v}) = \sum_{j=1}^{k+1} \boldsymbol{v}_j A_j$. We have $\|C\delta \boldsymbol{y}_{\circ}(A(\boldsymbol{v}),\boldsymbol{\epsilon};T)\|_2^2 = \|C\delta \boldsymbol{y}_{\circ}(A(\boldsymbol{v}),\boldsymbol{\epsilon};T)\|_2^2$ 183 $\langle \boldsymbol{v}, [W_{\circ}(\boldsymbol{\epsilon})]_{[1:k+1,1:k+1]} \boldsymbol{v} \rangle$. Recalling that $\delta \boldsymbol{y}_{\circ}(A(\boldsymbol{v}), \boldsymbol{\epsilon}; T) = \sum_{j=1}^{k+1} \boldsymbol{v}_{j} \delta \boldsymbol{y}_{\circ}(A_{j}, \boldsymbol{\epsilon}; T)$, we obtain the equivalence between (4.7), (4.9), and (4.3), (4.5) for suitable k and \boldsymbol{v} . 184185For the equivalence between (4.8) and (4.4), notice that for $\boldsymbol{v} = [\boldsymbol{\beta}^{\top}, -1]^{\top} \in \mathbb{R}^{k+1}$ 186 and any $W \in \mathbb{R}^{(k+1) \times (k+1)}$ we have $\langle \boldsymbol{v}, W \boldsymbol{v} \rangle = \langle \boldsymbol{\beta}, [W]_{[1:k,1:k]} \boldsymbol{\beta} \rangle - 2 \langle [W]_{[1:k,k+1]}, \boldsymbol{\beta} \rangle + 2 \langle [W]_{[1:k,k+1]}, \boldsymbol{\beta} \rangle$ 187 $[W]_{k+1,k+1}$. The well-posedness of the three problems follows by standard arguments; 188 see, e.g., [11, Lemma 5.2]. Π 189

The matrix representation given in Lemma 4.1 allows us to nicely describe the mathematical mechanism behind Algorithm 4.1 (see also [11, section 5.1]). Assume that at the k-th iteration the set $(\boldsymbol{\epsilon}_m)_{m=1}^k$ has been computed, the submatrix $[\widehat{W}_{\circ}^{(k)}]_{[1:k,1:k]}$ is PD and $[\widehat{W}_{\circ}^{(k)}]_{[1:k+1,1:k+1]}$ has a nontrivial (one-dimensional) kernel. Then the fitting step of Algorithm 4.1 identifies this nontrivial kernel. This can be proved by the following technical lemma (for a proof see [11, Lemma 5.3]).

196 LEMMA 4.2 (kernel of some symmetric PSD matrices). Consider a symmetric
197 PSD matrix
$$\widetilde{G} = \begin{bmatrix} G & \mathbf{b} \\ \mathbf{b}^{\top} & c \end{bmatrix} \in \mathbb{R}^{n \times n}$$
, where $G \in \mathbb{R}^{(n-1) \times (n-1)}$ is symmetric PD, and $\mathbf{b} \in \mathbb{R}^{n \times n}$

198 \mathbb{R}^{n-1} and $c \in \mathbb{R}$ are such that $\ker(\widetilde{G})$ is nontrivial. Then $\ker(\widetilde{G}) = \operatorname{span}\left\{ \begin{bmatrix} G^{-1}\boldsymbol{b} \\ -1 \end{bmatrix} \right\}$.

In our case, we have $\widetilde{G} = [\widehat{W}_{\circ}^{(k)}]_{[1:k+1,1:k+1]}$, $G = [\widehat{W}_{\circ}^{(k)}]_{[1:k,1:k]}$ and $\boldsymbol{b} = [\widehat{W}_{\circ}^{(k)}]_{[1:k,k+1]}$. In this notation, the solution to (4.8) is given by $\boldsymbol{\beta}^k = G^{-1}\boldsymbol{b}$. Thus, Lemma 4.2 implies 199 200 that the kernel of $[\widehat{W}_{\circ}^{(k)}]_{[1:k+1,1:k+1]}$ is spanned by $\boldsymbol{v} := [(\boldsymbol{\beta}^k)^{\top}, -1]^{\top}$. Now, the 201 splitting step attempts to compute a new control $\boldsymbol{\epsilon}^{k+1}$ such that $[\widehat{W}_{\circ}(\boldsymbol{\epsilon}^{k+1})]_{[1:k+1,1:k+1]}$ 202 is PD on the span of \boldsymbol{v} . If this is successful, then $[\widehat{W}_{\circ}^{(k+1)}]_{[1:k+1,1:k+1]}$ is PD. The 203 equivalence of (4.5) and (4.9) implies that $[\widehat{W}_{\circ}(\boldsymbol{\epsilon}^{k+1})]_{[1:k+1,1:k+1]}$ is PD on the span of \boldsymbol{v} 204 if and only if $\boldsymbol{\epsilon}^{k+1}$ satisfies $\|C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{k+1}; T) - C\delta \boldsymbol{y}_{\circ}(A_{k+1}, \boldsymbol{\epsilon}^{k+1}; T)\|_{2}^{2} > 0$. The 205existence of such a control depends on the controllability and observability properties 206of system (3.9), as shown in sections 5 and 6. We conclude this section with a remark 207that is useful hereafter. 208

209 Remark 4.3. The GN matrix $\widehat{W}_{\star} := \sum_{m=1}^{K} R'_m(\boldsymbol{\alpha}_{\star})^{\top} R'_m(\boldsymbol{\alpha}_{\star}) \in \mathbb{R}^{K \times K}$ can be 210 written as $[\widehat{W}_{\star}]_{i,j} = \sum_{m=1}^{K} \langle C \delta \boldsymbol{y}_{\star}(A_i, \boldsymbol{\epsilon}^m; T), C \delta \boldsymbol{y}_{\star}(A_j, \boldsymbol{\epsilon}^m; T) \rangle$ for $i, j \in \{1, \dots, K\}$, 211 where $\delta \boldsymbol{y}_{\star}(A_i, \boldsymbol{\epsilon}; T)$ denotes the solution at time T of

212
$$\begin{cases} \dot{\delta} \boldsymbol{y}_{\star} = \partial_{\boldsymbol{y}} f(A(\boldsymbol{\alpha}_{\star}), \boldsymbol{y}_{\star}, \boldsymbol{\epsilon}) \delta \boldsymbol{y}_{\star} + \left(\partial_{A} f(A(\boldsymbol{\alpha}_{\star}), \boldsymbol{y}_{\star}, \boldsymbol{\epsilon})(A_{i}) \right), & \delta \boldsymbol{y}_{\star}(0) = 0, \\ \dot{\boldsymbol{y}}_{\star} = f(A(\boldsymbol{\alpha}_{\star}), \boldsymbol{y}_{\star}, \boldsymbol{\epsilon}), & \boldsymbol{y}(0) = \boldsymbol{y}^{0}. \end{cases}$$

5. Reconstruction of drift matrix in linear systems. Consider (3.1) with $f(A, y, \epsilon) := Ay + B\epsilon$, where A and B are real matrices:

215 (5.1)
$$\dot{\boldsymbol{y}}(t) = A_{\star} \boldsymbol{y}(t) + B\boldsymbol{\epsilon}(t), \ t \in (0,T], \ \boldsymbol{y}(0) = 0$$

This is a linear system, where $B \in \mathbb{R}^{N \times M}$ is a given matrix for $N, M \in \mathbb{N}^+$, and

217 $\boldsymbol{\epsilon} \in E_{ad}$ denotes a control function belonging to E_{ad} , a nonempty and weakly compact 218 subset of $L^2(0,T;\mathbb{R}^M)$ that contains $\boldsymbol{\epsilon} \equiv 0$ as an interior point.¹

 $^{^{1}}$ This hypothesis is used in our analysis and is a reasonable assumption, since it is, for example, satisfied for standard box constraints, which are quite often used in the applications.

The drift matrix $A_{\star} \in \mathbb{R}^{N \times N}$ is unknown and assumed to lie in the space spanned by a set of linearly independent matrices $\mathcal{A} = \{A_1, \ldots, A_K\} \subset \mathbb{R}^{N \times N}, 1 \leq K \leq N^2$. We write $A_{\star} = \sum_{j=1}^{K} \boldsymbol{\alpha}_{\star,j} A_j =: A(\boldsymbol{\alpha}_{\star})$. As stated in section 3, we want to identify the unknown drift matrix A_{\star} by using a set of control functions $(\boldsymbol{\epsilon}^m)_{m=1}^K \subset E_{ad}$ in order to perform K laboratory experiments and obtain the experimental data $(\boldsymbol{\varphi}_{data}^{\star}(\boldsymbol{\epsilon}^m))_{m=1}^K \subset \mathbb{R}^P$, as defined in (3.2).

225 Remark 5.1. The hypothesis $\mathbf{y}(0) = 0$ in (5.1) can be made without loss of gen-226 erality. Indeed, if $\mathbf{y}(0) = \mathbf{y}^0 \neq 0$, one can use $\boldsymbol{\epsilon} = 0$ (case of uncontrolled system), 227 generate the data $\boldsymbol{\varphi}_{data}^{\star}(0)$, and then subtract this from all other data $(\boldsymbol{\varphi}_{data}^{\star}(\boldsymbol{\epsilon}^m))_{m=1}^K$ 228 to get back (by linearity) to the case of system (5.1) with $\mathbf{y}(0) = 0$.

Using $(\boldsymbol{\epsilon}^m)_{m=1}^K$ and $(\boldsymbol{\varphi}_{data}^{\star}(\boldsymbol{\epsilon}^m))_{m=1}^K$, the unknown vector $\boldsymbol{\alpha}_{\star}$ is obtained by solving (3.3), in which $\boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^m; T)$ now solves (5.1), with A_{\star} replaced by $A(\boldsymbol{\alpha})$. Thus, we use the LGR Algorithm 4.1 to generate $(\boldsymbol{\epsilon}^m)_{m=1}^K$ with the goal of making (4.2) uniquely solvable, that means making PD the GN matrix \widehat{W}_{\circ} , defined in (4.6). In (4.2), $\delta \boldsymbol{y}_{\circ}(A(\delta \boldsymbol{\alpha}), \boldsymbol{\epsilon}; t)$ is now the solution to

234 (5.2)
$$\begin{cases} \delta \dot{\boldsymbol{y}}_{\circ}(t) = A(\boldsymbol{\alpha}_{\circ})\delta \boldsymbol{y}_{\circ}(t) + \sum_{j=1}^{K} \delta \boldsymbol{\alpha}_{j} A_{j} \boldsymbol{y}_{\circ}(t), \quad t \in (0,T], \quad \delta \boldsymbol{y}_{\circ}(0) = 0, \\ \dot{\boldsymbol{y}}_{\circ}(t) = A(\boldsymbol{\alpha}_{\circ}) \boldsymbol{y}_{\circ}(t) + B\boldsymbol{\epsilon}(t), \quad t \in (0,T], \quad \boldsymbol{y}_{\circ}(0) = 0. \end{cases}$$

In what follows, we show that the LGR Algorithm 4.1 does produce $(\boldsymbol{\epsilon}^{m})_{m=1}^{K}$ that make \widehat{W}_{\circ} PD under appropriate assumptions on observability and controllability of the considered linear system. Let us recall these properties for an input/output system (A, B, C) of the form (2.1) with $A \in \mathbb{R}^{N \times N}$, $B \in \mathbb{R}^{N \times M}$, $C \in \mathbb{R}^{P \times N}$; see, e.g., [32, Theorem 3, Theorem 23].

DEFINITION & LEMMA 5.2 (observable input-output linear systems). The linear system (2.1) is said to be observable if the initial state $\mathbf{y}(0) = \mathbf{y}^0$ can be uniquely determined from input/output measurements. Equivalently, (2.1) is observable if and only if the observability matrix $\mathcal{O}_N(C, A) := \begin{bmatrix} C & CA & \cdots & CA^{N-1} \end{bmatrix}^\top$ has full rank. DEFINITION & LEMMA 5.3 (controllable input-output linear systems). The linear system (2.1) is said to be controllable if for any final state \mathbf{y}^f there exists an input sequence that transfers \mathbf{y}^0 to \mathbf{y}^f . Equivalently, (2.1) is controllable if and only if the controllability matrix $\mathcal{C}_N(A, B) := \begin{bmatrix} B & AB & \cdots & A^{N-1}B \end{bmatrix}$ has full rank.

In Section 5.1, we analyze Algorithm 4.1 in the case of fully observable and controllable systems (namely, rank($\mathcal{O}_N(C, A(\boldsymbol{\alpha}_\circ))$) = rank($\mathcal{C}_N(A(\boldsymbol{\alpha}_\circ), B)$) = N). However, similar to [11, Section 5.3], one can also formulate the following results for non-fully observable and controllable systems, if appropriate matrices A_1, \ldots, A_K are chosen. For further details, we refer the reader to the supplementary material [12].

Notice that the analysis that we are going to presented is also valid in the case of the reconstruction of a linear control matrix considered in [11, Section 5], i.e. $f(A, y, \epsilon) = My + A\epsilon$, and is therefore an extension of the results obtained in [11].

5.1. Analysis for linear systems. We define $\mathcal{O}_N^{\circ} := \mathcal{O}_N(C, A(\boldsymbol{\alpha}_{\circ}))$ and $\mathcal{C}_N^{\circ} := \mathcal{C}_N(A(\boldsymbol{\alpha}_{\circ}), B)$ and assume that the system $(A(\boldsymbol{\alpha}_{\circ}), B, C)$ is observable and controllable, namely $\mathcal{R} := \operatorname{rank}(\mathcal{O}_N^{\circ}) \cdot \operatorname{rank}(\mathcal{C}_N^{\circ}) = N^2$. In what follows, we show that this is a sufficient condition for \widehat{W}_{\circ} to be PD with the controls generated by Algorithm 4.1. First, we need the following result [3, Ch. 3, Theorem 2.11].

LEMMA 5.4 (controllability of time-invariant systems). Consider the system $\dot{\boldsymbol{x}} =$ 262 $A\boldsymbol{x} + B\boldsymbol{\epsilon}$ with $\boldsymbol{x}(0) = 0$ and its solution $\boldsymbol{x}(\boldsymbol{\epsilon}, t) := \int_0^t e^{(t-s)A(\boldsymbol{\alpha}_\circ)} B\boldsymbol{\epsilon}(s) ds$. For any finite time $t_0 > 0$, there exists a control $\boldsymbol{\epsilon}$ that transfers the state to \boldsymbol{w} in time t_0 , i.e.

264 $\boldsymbol{x}(\boldsymbol{\epsilon},t_0) = \boldsymbol{w}$, if and only if $\boldsymbol{w} \in \operatorname{im}(\mathcal{C}_N(A,B))$. Furthermore, an appropriate $\boldsymbol{\epsilon}$ that

265 will accomplish this transfer in time t_0 is given by $\boldsymbol{\epsilon}(t) = B^{\top} e^{(t_0 - t)A^{\top}} \boldsymbol{\nu}$, for $t \in [0, t_0]$ 266 and $\boldsymbol{\nu}$ such that $\mathcal{W}_c(0, t_0) \boldsymbol{\nu} = \boldsymbol{w}$, where $\mathcal{W}_c(0, T) := \int_0^T e^{\tau A} B B^{\top} e^{\tau A^{\top}} d\tau$.

Now, we prove the following lemma regarding the initialization problem (4.3) and the

splitting step problem (4.5). Notice that the proof of this result is inspired by classical

269 Kalman controllability theory; see, e.g., [15].

LEMMA 5.5 (LGR initialization and splitting steps (linear systems)). Assume that the matrices $A(\boldsymbol{\alpha}_{\circ}) \in \mathbb{R}^{N \times N}$, $B \in \mathbb{R}^{N \times M}$ and $C \in \mathbb{R}^{P \times N}$ are such that $\operatorname{rank}(\mathcal{O}_{N}^{\circ}) = \operatorname{rank}(\mathcal{C}_{N}^{\circ}) = N$, and let $\widetilde{A} \in \mathbb{R}^{N \times N} \setminus \{0\}$ be arbitrary. Then any solution $\widetilde{\boldsymbol{\epsilon}}$ of the problem $\max_{\boldsymbol{\epsilon} \in E_{ad}} \|C\delta \boldsymbol{y}_{\circ}(\widetilde{A}, \boldsymbol{\epsilon}; T)\|_{2}^{2}$ satisfies

$$\|C\delta \boldsymbol{y}_{\circ}(\widetilde{A}, \widetilde{\boldsymbol{\epsilon}}; T)\|_{2}^{2} > 0,$$

270 where $\dot{\delta} \boldsymbol{y}_{\circ} = A(\boldsymbol{\alpha}_{\circ})\delta \boldsymbol{y}_{\circ} + \widetilde{A}\boldsymbol{y}^{\circ}$, with $\delta \boldsymbol{y}_{\circ}(0) = 0$, and $\dot{\boldsymbol{y}}_{\circ} = A(\boldsymbol{\alpha}_{\circ})\boldsymbol{y}_{\circ} + B\boldsymbol{\epsilon}$ with $\boldsymbol{y}_{\circ}(0) = 0$

271 Proof. To prove the result, it is sufficient to construct an $\tilde{\boldsymbol{\epsilon}} \in E_{ad}$ such that 272 $C\delta \boldsymbol{y}_{\circ}(\tilde{A}, \tilde{\boldsymbol{\epsilon}}; T) \neq 0$. Since $\tilde{A} \neq 0$, there exists $\boldsymbol{w} \in \mathbb{R}^{N} \setminus \{0\}$ such that $\tilde{A}\boldsymbol{w} \neq 0$. Since 273 $(A(\boldsymbol{\alpha}_{\circ}), B, C)$ is observable, there exists $\tilde{t} > 0$ such that $Ce^{\tilde{t}A(\boldsymbol{\alpha}_{\circ})}\tilde{A}\boldsymbol{w} \neq 0$. The map f: 274 $\mathbb{R} \to \mathbb{R}^{P}, t \mapsto Ce^{tA(\boldsymbol{\alpha}_{\circ})}\tilde{A}\boldsymbol{w}$ is analytic with derivatives $f^{(i)}(t) = CA(\boldsymbol{\alpha}_{\circ})^{i}e^{tA(\boldsymbol{\alpha}_{\circ})}\tilde{A}\boldsymbol{w}$. 275 Since \mathcal{O}_{N}° has full rank and $e^{\tilde{t}A(\boldsymbol{\alpha}_{\circ})}\tilde{A}\boldsymbol{w} \neq 0$, there exists $i \in \{0, \ldots, N\}$ such that 276 $f^{(i)}(\tilde{t}) = CA(\boldsymbol{\alpha}_{\circ})^{i}e^{\tilde{t}A(\boldsymbol{\alpha}_{\circ})}\tilde{A}\boldsymbol{w} \neq 0$. Hence, f is nonconstant, and there exists $t_{0} \in (0, T)$ 277 with $Ce^{t_{0}A(\boldsymbol{\alpha}_{\circ})}\tilde{A}\boldsymbol{w} \neq 0$.

Now, we use that $\boldsymbol{y}_{\circ}(\boldsymbol{\epsilon}, s) := \int_{0}^{s} e^{(s-\tau)A(\boldsymbol{\alpha}_{\circ})} B\boldsymbol{\epsilon}(\tau) d\tau$ is the solution at time s of $\boldsymbol{y}_{\circ} = A(\boldsymbol{\alpha}_{\circ})\boldsymbol{y}_{\circ} + B\boldsymbol{\epsilon}$, with $\boldsymbol{y}_{\circ}(0) = 0$. Since C_{N}° has full rank, we have $\boldsymbol{w} \in \operatorname{im}(C_{N}^{\circ})$. Thus, Lemma 5.4 guarantees that $\boldsymbol{\hat{\epsilon}}(t) = B^{\top}e^{(t_{0}-t)A(\boldsymbol{\alpha}_{\circ})^{\top}}\boldsymbol{\nu}$, for $t \in [0, t_{0}]$ and some $\boldsymbol{\nu} \in \mathbb{R}^{N}$, satisfies $\boldsymbol{y}_{\circ}(\boldsymbol{\hat{\epsilon}}, t_{0}) = \boldsymbol{w}$. Clearly, $\boldsymbol{\hat{\epsilon}}$ is analytic in $[0, t_{0}]$ and thereby the same holds for $\boldsymbol{y}_{\circ}(\boldsymbol{\hat{\epsilon}}, s)$. Note that, since $\boldsymbol{\epsilon} \equiv 0$ is an interior point of E_{ad} , there exists $\lambda > 0$ such that $\lambda \boldsymbol{\hat{\epsilon}} \in E_{ad}$ with $Ce^{t_{0}A(\boldsymbol{\alpha}_{\circ})} \tilde{A} \boldsymbol{y}_{\circ}(\lambda \boldsymbol{\hat{\epsilon}}, t_{0}) = \lambda Ce^{t_{0}A(\boldsymbol{\alpha}_{\circ})} \tilde{A} \boldsymbol{y}_{\circ}(\boldsymbol{\hat{\epsilon}}, t_{0}) \neq 0$. Hence, we can assume without loss of generality that $\boldsymbol{\hat{\epsilon}} \in E_{ad}$.

In conclusion, we obtain that the map

286
$$\boldsymbol{g}: \mathbb{R} \to \mathbb{R}^p, s \mapsto C e^{(T-s)A(\boldsymbol{\alpha}_\circ)} \widetilde{A} \int_0^s e^{(s-\tau)A(\boldsymbol{\alpha}_\circ)} B \widehat{\boldsymbol{\epsilon}}(\tau) d\tau$$

is analytic in $(0, t_0)$ with $\boldsymbol{g}(t_0) \neq 0$. Thus, \boldsymbol{g} is nonzero in an open subinterval of $(0, t_0)$. Hence, there exists $t_1 \in (0, t_0)$ such that $\int_0^{t_1} \boldsymbol{g}(s) ds \neq 0$. By choosing

289
$$\widetilde{\boldsymbol{\epsilon}}(s) := \begin{cases} 0, & 0 \le s < T - t_1, \\ \widehat{\boldsymbol{\epsilon}}(s - t_1), & T - t_1 \le s \le T \end{cases}$$

and using that $C\delta \boldsymbol{y}_{\circ}(\widetilde{A}, \widetilde{\boldsymbol{\epsilon}}; T) = \int_{0}^{T} C e^{(T-s)A(\boldsymbol{\alpha}_{\circ})} \widetilde{A} \int_{0}^{s} e^{(s-\tau)A(\boldsymbol{\alpha}_{\circ})} B\widetilde{\boldsymbol{\epsilon}}(\tau) d\tau ds$, we obtain

291
$$C\delta \boldsymbol{y}_{\circ}(\widetilde{A}, \widetilde{\boldsymbol{\epsilon}}; T) = \int_{T-t_{1}}^{T} Ce^{(T-s)A(\boldsymbol{\alpha}_{\circ})} \widetilde{A} \int_{T-t_{1}}^{s} e^{(s-\tau)A(\boldsymbol{\alpha}_{\circ})} B\widetilde{\boldsymbol{\epsilon}}(\tau-t_{1}) d\tau ds$$

$$= \int_0^{\iota_1} C e^{(\iota_1 - s)A(\boldsymbol{\alpha}_\circ)} \widetilde{A} \int_0^s e^{(s - \tau)A(\boldsymbol{\alpha}_\circ)} B\widehat{\boldsymbol{\epsilon}}(\tau) d\tau ds = \int_0^{\iota_1} \boldsymbol{g}(s) ds \neq 0.$$

Lemma 5.5 can be applied to both (4.3) and (4.5), choosing $\widetilde{A} = A_1$ and $\widetilde{A} = (A^{(k)}(\boldsymbol{\beta}^k) - A_{k+1})$, respectively. Now, we can prove our first main convergence result.

THEOREM 5.6 (positive definiteness of the GN matrix \widehat{W}_{\circ} (linear systems)). Assume that $A(\boldsymbol{\alpha}_{\circ}) \in \mathbb{R}^{N \times N}$, $B \in \mathbb{R}^{N \times M}$ and $C \in \mathbb{R}^{P \times N}$ are such that $\operatorname{rank}(\mathcal{O}_{N}^{\circ}) =$ rank $(\mathcal{C}_{N}^{\circ}) = N$. For $K \leq N^{2}$, let $\mathcal{A} = \{A_{1}, \ldots, A_{K}\} \subset \mathbb{R}^{N \times N}$ be a set of linearly independent matrices such that $A(\boldsymbol{\alpha}_{\circ}) \in \operatorname{span}(\mathcal{A})$, and let $\{\boldsymbol{\epsilon}^{1}, \ldots, \boldsymbol{\epsilon}^{K}\} \subset E_{ad}$ be generated by Algorithm 4.1. Then the GN matrix \widehat{W}_{\circ} , defined in (4.6), is PD.

301 Proof. We proceed by induction. Lemma 5.5 guarantees that there exists an $\boldsymbol{\epsilon}^1$ 302 such that $[W_{\circ}(\boldsymbol{\epsilon}^1)]_{1,1} = \|C\delta \boldsymbol{y}_{\circ}(A_1, \boldsymbol{\epsilon}; T)\|_2^2 > 0$. Now, we assume that $[\widehat{W}_{\circ}^{(k)}]_{[1:k,1:k]} =$ 303 $\sum_{m=1}^k [W_{\circ}(\boldsymbol{\epsilon}^m)]_{[1:k,1:k]}$ is PD. By construction, $[\widehat{W}_{\circ}^{(k+1)}]_{[1:k+1,1:k+1]}$ is PSD. Thus, if 304 $[\widehat{W}_{\circ}^{(k)}]_{[1:k+1,1:k+1]}$ is PD, then

305
$$[\widehat{W}_{\circ}^{(k+1)}]_{[1:k+1,1:k+1]} = [\widehat{W}_{\circ}^{(k)}]_{[1:k+1,1:k+1]} + [W_{\circ}(\boldsymbol{\epsilon}^{k+1})]_{[1:k+1,1:k+1]}$$

is PD as well, since $[W_{\circ}(\boldsymbol{\epsilon}^{k})]_{[1:k+1,1:k+1]}$ is PSD. Assume now that the submatrix $[\widehat{W}_{\circ}^{(k)}]_{[1:k+1,1:k+1]}$ has a nontrivial kernel. Since $[\widehat{W}_{\circ}^{(k)}]_{[1:k,1:k]}$ is PD (induction hypothesis), problem (4.4) is uniquely solvable with solution $\boldsymbol{\beta}^{k}$. Then, by Lemma 4.2 the (one-dimensional) kernel of $[\widehat{W}_{\circ}^{(k)}]_{[1:k+1,1:k+1]}$ is the span of the vector $\boldsymbol{v} =$ $[(\boldsymbol{\beta}^{k})^{\top}, -1]^{\top}$. Using Lemma 5.5 we obtain that the solution $\boldsymbol{\epsilon}^{k+1}$ to the splitting step problem satisfies

312
$$\langle \boldsymbol{v}, [W_{\circ}(\boldsymbol{\epsilon}^{k+1})]_{[1:k+1,1:k+1]}\boldsymbol{v} \rangle = \left\| C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}) - A_{k+1}, \boldsymbol{\epsilon}; T) \right\|_{2}^{2} > 0.$$

Thus, $[W(\boldsymbol{\epsilon}^{k+1})]_{[1:k+1,1:k+1]}$ is PD on the span of \boldsymbol{v} , and $[\widehat{W}_{\circ}^{(k+1)}]_{[1:k+1,1:k+1]}$ is PD. Notice that Theorem 5.6 does not require any assumption on the matrices A_1, \ldots, A_K . These can be arbitrarily chosen with the only constraint to be linearly independent. Also the ordering of these matrices does not affect the result of Theorem 5.6. This is, however, different for non-fully observable and controllable systems, i.e. for $\mathcal{R} < N^2$ (see the supplementary material [12]).

Now that we proved that Algorithm 4.1 makes \widehat{W}_{\circ} PD, the obvious question is whether this is sufficient for the convergence of GN, as described in Lemma 3.1. We answer this question in Section 5.2.

5.2. Positive definiteness of the GN matrix. To guarantee convergence of GN, we need to show that $\widehat{W}(\boldsymbol{\alpha}) := \sum_{m=1}^{K} R'_m(\boldsymbol{\alpha})^\top R'_m(\boldsymbol{\alpha})$ (defined in section 3) remains PD in a neighborhood of $\boldsymbol{\alpha}_{\star}$. Indeed, in Section 5.1, we proved that the control functions generated by Algorithm 4.1 make the GN matrix $\widehat{W}_{\circ} = \widehat{W}(\boldsymbol{\alpha}_{\circ})$ PD. Thus, it is sufficient to prove that $\widehat{W}(\boldsymbol{\alpha})$ remains PD in a neighborhood of $\boldsymbol{\alpha}_{\circ}$ containing $\boldsymbol{\alpha}_{\star}$. To do so, let us rewrite $\widehat{W}(\boldsymbol{\alpha})$ as

328 (5.3)
$$[\widehat{W}(\boldsymbol{\alpha})]_{i,j} := \sum_{m=1}^{K} \langle \boldsymbol{\gamma}_i(\boldsymbol{\alpha}, \boldsymbol{\epsilon}^m), \boldsymbol{\gamma}_j(\boldsymbol{\alpha}, \boldsymbol{\epsilon}^m) \rangle, \quad i, j \in \{1, \dots, K\},$$

$$\begin{array}{l} {}_{329} \\ {}_{330} \end{array} (5.4) \qquad \boldsymbol{\gamma}_j(\boldsymbol{\alpha}, \boldsymbol{\epsilon}^m) := \int_0^T C e^{(T-s)A(\boldsymbol{\alpha})} A_j \boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^m; s) ds, \quad j \in \{1, \ldots, K\}, \end{array}$$

and recall the next lemma, which follows from the Bauer-Fike theorem [6].

LEMMA 5.7 (rank stability). Consider two natural numbers N_D and M_D with N_D $\geq M_D$, and an arbitrary matrix $D \in \mathbb{R}^{N_D \times M_D}$ with rank \mathcal{R}_D and (positive) singular values $\sigma_1, \ldots, \sigma_{\mathcal{R}_D}$ in descending order. Then it holds that

335
$$\min_{\widehat{D}\in\mathbb{R}^{N_D\times M_D}} \{\|\widehat{D}\|_2 \mid \operatorname{rank}(D+\widehat{D}) < \mathcal{R}_{\mathcal{D}}\} = \sigma_{\mathcal{R}_{\mathcal{D}}}.$$

Using this lemma, we can prove the following approximation result.

LEMMA 5.8 (positive definiteness of $\widehat{W}(\boldsymbol{\alpha})$ (linear systems)). Let \widehat{W}_{\circ} defined in (4.6) be PD and let $\sigma_{K}^{\circ} > 0$ be its smallest singular value. Then, there exists $\delta := \delta(\sigma_{K}^{\circ}) > 0$ such that $\widehat{W}(\boldsymbol{\alpha})$ (in (5.3)) is PD for any $\boldsymbol{\alpha} \in \mathbb{R}^{K}$ with $\|\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\circ}\|_{2} < \delta$.

Proof. Our first goal is to show that $\widehat{W}(\boldsymbol{\alpha})$ is continuous in $\boldsymbol{\alpha}$. From (5.3) and (5.4) we know that $\widehat{W}(\boldsymbol{\alpha})$ is the sum over products of $\int_{0}^{T} Ce^{(T-s)A(\boldsymbol{\alpha})}A_{j}\boldsymbol{y}(A(\boldsymbol{\alpha}),\boldsymbol{\epsilon}^{m};s)ds$, where $\boldsymbol{y}(A(\boldsymbol{\alpha}),\boldsymbol{\epsilon}^{m};s) = \int_{0}^{s} e^{(s-\tau)A(\boldsymbol{\alpha})}B\boldsymbol{\epsilon}^{m}(\tau)d\tau$. Now, recall that $A(\boldsymbol{\alpha}) = \sum_{j=1}^{K} \boldsymbol{\alpha}_{j}A_{j}$, meaning that $A(\boldsymbol{\alpha})$ is continuous in $\boldsymbol{\alpha}$. Since the exponential map $\mathbb{R}^{N} \to \mathbb{R}^{N \times N}, \boldsymbol{\alpha} \mapsto e^{sA(\boldsymbol{\alpha})}$ and the integral map $\mathbb{R}^{N \times N} \to \mathbb{R}^{N}, X \mapsto \int_{0}^{s} XB\boldsymbol{\epsilon}(\tau)d\tau$ are continuous, we obtain that $\boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^{m};s)$ is continuous in $\boldsymbol{\alpha}$. Since products of continuous functions are continuous, we obtain that $\widehat{W}(\boldsymbol{\alpha})$ is continuous in $\boldsymbol{\alpha}$.

By assumption, \widehat{W}_{\circ} is PD, and therefore $\sigma_{K}^{\circ} > 0$. Since $\widehat{W}(\boldsymbol{\alpha})$ is continuous in $\boldsymbol{\alpha}$, we obtain that there exists a $\delta := \delta(\sigma_{K}^{\circ}) > 0$ such that for any $\boldsymbol{\alpha}$ with $\|\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\circ}\|_{2} < \delta(\sigma_{K}^{\circ})$ it holds that $\|\widehat{W}(\boldsymbol{\alpha}) - \widehat{W}(\boldsymbol{\alpha}_{\circ})\|_{2} < \sigma_{K}^{\circ}$. Now, let $\widehat{\boldsymbol{\alpha}}$ be such that $\|\widehat{\boldsymbol{\alpha}} - \boldsymbol{\alpha}_{\circ}\|_{2} < \delta(\sigma_{K}^{\circ})$ and hence $\|\widehat{W}(\widehat{\boldsymbol{\alpha}}) - \widehat{W}(\boldsymbol{\alpha}_{\circ})\|_{2} < \sigma_{K}^{\circ}$. Setting $D = \widehat{W}(\boldsymbol{\alpha}_{\circ})$ and $\widehat{D} = \widehat{W}(\widehat{\boldsymbol{\alpha}}) - \widehat{W}(\widehat{\boldsymbol{\alpha}})$, Lemma 5.7 implies that $K = \operatorname{rank}(\widehat{W}(\boldsymbol{\alpha}_{\circ})) \leq \operatorname{rank}(\widehat{W}(\widehat{\boldsymbol{\alpha}}))$. Because of (5.3), $\widehat{W}(\widehat{\boldsymbol{\alpha}}) \in \mathbb{R}^{K \times K}$ meaning that $\operatorname{rank}(\widehat{W}(\widehat{\boldsymbol{\alpha}})) = K$. Since $\widehat{W}(\boldsymbol{\alpha})$ is PSD by construction, rank $(\widehat{W}(\widehat{\boldsymbol{\alpha}})) = K$ implies that $\widehat{W}(\widehat{\boldsymbol{\alpha}})$ is PD.

Lemma 5.8 implies that the positive definiteness of $\widehat{W}(\boldsymbol{\alpha})$ is locally preserved near $\boldsymbol{\alpha}_{\circ}$. Now, we can prove our main convergence result.

THEOREM 5.9 (convergence of GN (linear systems)). Let $\boldsymbol{\alpha}_{\circ} \in \mathbb{R}^{K}$ be such that the matrices $A(\boldsymbol{\alpha}_{\circ}) \in \mathbb{R}^{N \times N}$, $B \in \mathbb{R}^{N \times M}$ and $C \in \mathbb{R}^{P \times N}$ satisfy rank $(\mathcal{O}_{N}^{\circ}) \cdot$ rank $(\mathcal{C}_{N}^{\circ}) = N^{2}$. Let $(\boldsymbol{\epsilon}^{m})_{m=1}^{K} \subset E_{ad}$ be a set of controls generated by Algorithm 4.1. Finally, let $\widehat{\sigma}_{K}$ be the K-th (smallest) singular value of \widehat{W}_{\circ} defined in (4.6). Then there exists $\delta = \delta(\widehat{\sigma}_{K}) > 0$ such that if $\boldsymbol{\alpha}_{\star} \in \mathbb{R}^{K}$ satisfies $\|\boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}_{\circ}\| < \delta$, then GN method for the problem

362 (5.5)
$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{K}} \frac{1}{2} \sum_{m=1}^{K} \|C\boldsymbol{y}(A(\boldsymbol{\alpha}_{\star}), \boldsymbol{\epsilon}^{m}; T) - C\boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^{m}; T)\|_{2}^{2},$$

initialized with $\boldsymbol{\alpha}_{\circ}$, converges to $\boldsymbol{\alpha}_{j} = \boldsymbol{\alpha}_{\star,j}, j = 1, \ldots, K$.

Proof. Theorem 5.6 guarantees that \widehat{W}_{\circ} is PD and hence $\widehat{\sigma}_{K} > 0$. Thus, by Lemma 5.8 there exists $\delta = \delta(\widehat{\sigma}_{K}) > 0$ such that, for $\boldsymbol{\alpha} \in \mathbb{R}^{K}$ with $\|\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\circ}\|_{2} < \delta$, the matrix $\widehat{W}(\boldsymbol{\alpha})$ is also PD. Moreover, we know from section 3 that $\widehat{W}(\boldsymbol{\alpha}_{c})$ is the GN matrix for the iterate $\boldsymbol{\alpha}_{c} \in \mathbb{R}^{K}$ of GN for (3.3). Analogously to the proof of Lemma 5.8, one can also show that the functions $R_{m}(\boldsymbol{\alpha})$, defined in (3.4), are Lipschitz continuously differentiable in $\boldsymbol{\alpha}$ for all $m \in \{1, \ldots, K\}$. Hence, if $\|\boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}_{\circ}\| < \delta$, then the result follows by Lemma 3.1. 5.3. Local uniqueness of solutions. Theorem 5.9 says that GN converges to $\boldsymbol{\alpha}_{\star}$ if an appropriate initialization vector $\boldsymbol{\alpha}_{\circ}$ is used. However, in the linear case corresponding to (5.1) we can specify the local properties of problem (3.3) around the solution $\boldsymbol{\alpha}_{\star}$. To this end, we start by rewriting the cost function in a matrix form.

LEMMA 5.10 (online identification problem in matrix form (linear systems)). *Problem* (3.3) *is equivalent to*

377 (5.6)
$$\min_{\boldsymbol{\alpha}\in\mathbb{R}^{K}}\frac{1}{2}\langle\boldsymbol{\alpha}_{\star}-\boldsymbol{\alpha},\widetilde{W}(\boldsymbol{\alpha}_{\star},\boldsymbol{\alpha})(\boldsymbol{\alpha}_{\star}-\boldsymbol{\alpha})\rangle,$$

378 where $\widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}) \in \mathbb{R}^{K \times K}$ is defined as²

379 (5.7)
$$\widetilde{W}(\boldsymbol{\alpha}_{\star},\boldsymbol{\alpha}) := \sum_{m=1}^{K} W(\boldsymbol{\alpha}_{\star},\boldsymbol{\alpha},\boldsymbol{\epsilon}^{m}),$$

380 with $W(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}, \boldsymbol{\epsilon}^{m}) \in \mathbb{R}^{K \times K}$ given by

381 (5.8)
$$[W(\boldsymbol{\alpha}_{\star},\boldsymbol{\alpha},\boldsymbol{\epsilon}^{m})]_{i,j} := \langle \boldsymbol{\gamma}_{i}(\boldsymbol{\alpha}_{\star},\boldsymbol{\alpha},\boldsymbol{\epsilon}^{m}), \boldsymbol{\gamma}_{j}(\boldsymbol{\alpha}_{\star},\boldsymbol{\alpha},\boldsymbol{\epsilon}^{m}) \rangle, \quad i,j \in \{1,\ldots,K\},$$

$$\begin{array}{l} {}_{382} \quad (5.9) \qquad \boldsymbol{\gamma}_j(\boldsymbol{\alpha}_\star, \boldsymbol{\alpha}, \boldsymbol{\epsilon}^m) := \int_0^T C e^{(T-s)A(\boldsymbol{\alpha}_\star)} A_j \boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^m; s) ds, \quad j \in \{1, \ldots, K\}. \end{array}$$

³⁸⁴ Proof. Let $J(\boldsymbol{\alpha}) := \frac{1}{2} \sum_{m=1}^{K} \|C\boldsymbol{y}(A_{\star}, \boldsymbol{\epsilon}^{m}; T) - C\boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^{m}; T)\|_{2}^{2}$. For $t \in [0, T]$ ³⁸⁵ and $m \in \{1, \ldots, K\}$ define $\Delta \boldsymbol{y}_{m}(t) := \boldsymbol{y}(A_{\star}, \boldsymbol{\epsilon}^{m}; t) - \boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^{m}; t)$. Then we have

$$\dot{\Delta y}_m(t) = A(\boldsymbol{\alpha}_{\star})\boldsymbol{y}(A_{\star},\boldsymbol{\epsilon}^m;t) + B\boldsymbol{\epsilon}^m(t) - A(\boldsymbol{\alpha})\boldsymbol{y}(A(\boldsymbol{\alpha}),\boldsymbol{\epsilon}^m;t) - B\boldsymbol{\epsilon}^m(t)$$

$$= A(\boldsymbol{\alpha}_{\star})\Delta \boldsymbol{y}_m(t) + A(\boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha})\boldsymbol{y}(A(\boldsymbol{\alpha}),\boldsymbol{\epsilon}^m;t),$$

389 whose solution at time T is given by

390
$$\Delta \boldsymbol{y}_m(T) = \int_0^T e^{(T-s)A(\boldsymbol{\alpha}_\star)} \Big[A(\boldsymbol{\alpha}_\star - \boldsymbol{\alpha}) \boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^m; s) \Big] ds.$$

391 Thus, recalling $A(\boldsymbol{\alpha}) = \sum_{j=1}^{K} \boldsymbol{\alpha}_j A_j$, the function $J(\boldsymbol{\alpha})$ can be written as

392
$$J(\boldsymbol{\alpha}) = \frac{1}{2} \sum_{m=1}^{K} \left\| \int_{0}^{T} C e^{(T-s)A(\boldsymbol{\alpha}_{\star})} \Big(\sum_{j=1}^{K} (\boldsymbol{\alpha}_{\star,j} - \boldsymbol{\alpha}_{j})A_{k} \Big) \boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^{m}; s) ds \right\|_{2}^{2}$$

393

$$\stackrel{(5.9)}{=} \frac{1}{2} \sum_{m=1} \sum_{i=1} \sum_{j=1} (\boldsymbol{\alpha}_{\star,i} - \boldsymbol{\alpha}_i) (\boldsymbol{\alpha}_{\star,j} - \boldsymbol{\alpha}_j) \langle \boldsymbol{\gamma}_i (\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}, \boldsymbol{\epsilon}^m), \boldsymbol{\gamma}_j (\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}, \boldsymbol{\epsilon}^m) \rangle$$

$$\stackrel{(5.8)}{=} \frac{1}{2} \langle \boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}, \sum_{m=1}^{K} W(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}, \boldsymbol{\epsilon}^{m})(\boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}) \rangle = \frac{1}{2} \langle \boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}, \widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha})(\boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}) \rangle. \ \Box$$

Now, the set of global solutions to problem (5.6) is given by $S_{global} := \left\{ \boldsymbol{\alpha} \in \mathbb{R}^{K} : (\boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}) \in \ker \widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}) \right\}$. Since $\widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha})$ is symmetric PSD, (5.6) is locally uniquely solvable if and only if $\widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha})$ is PD for $\boldsymbol{\alpha}$ close to $\boldsymbol{\alpha}_{\star}$. Now, assume that the system

²Notice that the notations (5.3) and (5.7) are related in the sense that $\widetilde{W}(\boldsymbol{\alpha}, \boldsymbol{\alpha}) = \widehat{W}(\boldsymbol{\alpha})$.

is fully observable and controllable, meaning that $\mathcal{R} = N^2$. Theorem 5.9 guarantees that Algorithm 4.1 computes $(\boldsymbol{\epsilon}_m)_{m=1}^{N^2}$ such that $\widehat{W}(\boldsymbol{\alpha}_{\star}) = \widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}_{\star})$ is PD, if $\boldsymbol{\alpha}_{\star}$ is close enough to the estimate $\boldsymbol{\alpha}_{\circ}$. Similar to the proof of Lemma 5.8, one can prove that $\widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha})$ is continuous in $\boldsymbol{\alpha}$. Hence, we obtain that if the matrix $\widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}_{\star})$ is PD, then the same is true for $\widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha})$, when $\boldsymbol{\alpha}$ is close to $\boldsymbol{\alpha}_{\star}$, which implies that (5.6) is locally uniquely solvable with $\boldsymbol{\alpha} = \boldsymbol{\alpha}_{\star}$.

6. Bilinear reconstruction problem. In this section, we extend the results of section 5 to the case of skew-symmetric bilinear systems. We consider (3.1) with a right-hand side $f(A, \mathbf{y}, \epsilon) = (A + \epsilon B)\mathbf{y}$, that is

408 (6.1)
$$\dot{\boldsymbol{y}}(t) = (A_{\star} + \epsilon(t)B)\boldsymbol{y}(t), \ t \in (0,T], \ \boldsymbol{y}(0) = \boldsymbol{y}^{0},$$

409 where $B \in \mathfrak{so}(N)$ is a given skew-symmetric matrix for $N \in \mathbb{N}^+$, the initial state is 410 $\mathbf{y}^0 \in \mathbb{R}^N$, and $\epsilon \in E_{ad} \subset L^2(0,T;\mathbb{R})$ denotes a control function belonging to E_{ad} , a 411 nonempty, closed, convex and bounded subset of $L^2(0,T;\mathbb{R})$ that contains $\epsilon \equiv 0$ as 412 an interior point. The matrix $A_{\star} \in \mathfrak{so}(N)$ is unknown and assumed to lie in the space 413 spanned by a set of linearly independent matrices $\mathcal{A} = \{A_1, \ldots, A_K\} \subset \mathbb{R}^{N \times N}, 1 \leq$ 414 $K \leq N^2$, and we write $A_{\star} = \sum_{j=1}^{K} \boldsymbol{\alpha}_{\star,j} A_j =: A(\boldsymbol{\alpha}_{\star})$. Notice that, since the matrices 415 A_{\star} and B are skew-symmetric, system (6.1) is norm preserving, i.e. $\|\mathbf{y}(t)\|_2 = \|\mathbf{y}^0\|_2$ 416 for all $t \in [0, T]$.³

To identify the true matrix A_{\star} , one can consider a set of control functions (ϵ^m) $_{m=1}^K \subset E_{ad}$ and use it experimentally to obtain the data ($\varphi_{data}^{\star}(\epsilon^m)$) $_{m=1}^K \subset \mathbb{R}^P$, as defined in (3.2). The unknown vector $\boldsymbol{\alpha}_{\star}$ is then obtained by solving the problem

420 (6.2)
$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{K}} \frac{1}{2} \sum_{m=1}^{K} \|\boldsymbol{\varphi}_{data}^{\star}(\boldsymbol{\epsilon}^{m}) - C\boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^{m}; T)\|_{2}^{2}.$$

421 We assume to be provided with a known estimate $\boldsymbol{\alpha}_{\circ}$ of $\boldsymbol{\alpha}_{\star}$. For this estimate, we can 422 derive the linearized state equation

423 (6.3)
$$\begin{cases} \delta \dot{\boldsymbol{y}}_{\circ}(t) = (A_{\circ} + \epsilon(t)B)\delta \boldsymbol{y}_{\circ}(t) + \sum_{j=1}^{K} \delta \boldsymbol{\alpha}_{j} A_{j} \boldsymbol{y}_{\circ}(t), & t \in (0,T], \\ \dot{\boldsymbol{y}}_{\circ}(t) = (A_{\circ} + \epsilon(t)B) \boldsymbol{y}_{\circ}(t), & t \in (0,T], & \boldsymbol{y}_{\circ}(0) = \boldsymbol{y}^{0}, \end{cases}$$

424 where $A_{\circ} := A(\boldsymbol{\alpha}_{\circ})$. Denoting by $\delta \boldsymbol{y}_{\circ}(A(\delta \boldsymbol{\alpha}), \epsilon; t)$ the solution of (6.3) at time $t \in$ 425 [0, T], the GN matrix \widehat{W}_{\circ} is defined as in (4.6), and LGR is detailed in Algorithm 4.1. 426 Let us recall the following definition and result from [10, Corollary 4.11].

DEFINITION & LEMMA 6.1 (Controllability of skew-symmetric bilinear systems).
 Consider a system of the form

429 (6.4)
$$\dot{\boldsymbol{y}}(t) = (A_{\circ} + \epsilon(t)B)\boldsymbol{y}(t), \quad \boldsymbol{y}(0) = \boldsymbol{y}^{0},$$

430 where $A_{\circ}, B \in \mathfrak{so}(N)$. System (6.4) is said to be controllable if for any final state 431 \mathbf{y}^{f} that lies on the sphere of radius $\|\mathbf{y}^{0}\|_{2}$ there exists a control $\epsilon(t)$ that transfers \mathbf{y}^{0} 432 to \mathbf{y}^{f} . Furthermore, if the Lie algebra $L = Lie\{A_{\circ}, B\} \subset \mathfrak{so}(N)$, generated by the 433 matrices A_{\circ} and B, has dimension $\frac{N(N-1)}{2}$, then there exists a constant $\tilde{t} \geq 0$ such 434 that for any $T \geq \tilde{t}$ controllability of (6.4) holds.

³To see this, we observe that $\frac{1}{2} \frac{d}{dt} \| \boldsymbol{y}(t) \|_2^2 = \langle \boldsymbol{y}(t), \dot{\boldsymbol{y}}(t) \rangle = \langle \boldsymbol{y}(t), (A_\star + \epsilon(t)B) \boldsymbol{y}(t) \rangle = 0.$

As in section 5, we also need to make some assumptions on the observability of 435 436the linearized equation in (6.3). However, recalling the proof of Lemma 5.5, these assumptions are only required to prove the existence of a control function that guar-437 antees a positive cost function value in the splitting step. If we assume this function 438to be constant, at least on a subinterval of [0, T], then we get a system of the form 439

440 (6.5)
$$\dot{\delta y}_{\circ}(t) = (A_{\circ} + cB)\delta y_{\circ}(t) + A(\delta \alpha)y_{\circ}(t),$$

for a scalar $c \in \mathbb{R}$. In this case, system (6.5) is again a linear system, for which observ-441

ability is defined in Definition 5.2. Hence, the observability matrix is $\mathcal{O}_N(C, A_\circ + cB)$. 442 Let us state our assumptions on controllability and observability of (6.4) and (6.5). 443

Assumption 6.2. Let the matrices A_{\circ} , B and C be such that the following con-444 ditions are satisfied. 445

1. The Lie algebra $L = Lie\{A_{\circ}, B\} \subset \mathfrak{so}(N)$, generated by the matrices A_{\circ} and 446 The Lie algebra L = Lie (A₀, D_f ⊂ B(A), generative of the matrice of the B, has dimension N(N-1)/2.
 The final time T > 0 is sufficiently large, such that the controllability result 447

448 from Lemma 6.1 holds. 449

3. There exists $c \in \mathbb{R}$ such that system (6.5) is observable, i.e. the observability 450matrix $\mathcal{O}_N(C, A_\circ + cB)$ has full rank. 451

In addition, let the set of admissible controls $E_{ad} \subset L^2(0,T;\mathbb{R})$ be chosen such that 452the controllability result from Lemma 6.1 holds, and such that $\epsilon \equiv c$ is an interior 453point of E_{ad} for the constant $c \in \mathbb{R}$ mentioned above. 454

Remark 6.3. The analysis presented in the following sections can be applied to the 455case where the matrix $A = A_{\star}$ is assumed to be known and $B = B(\boldsymbol{\alpha}) := \sum_{j=1}^{K} \boldsymbol{\alpha}_j B_j$ 456is unknown and to be identified. The main differences in the case of the identification 457of B is that the state equation is linearized around an initial guess B_{0} , leading to 458

459
$$\begin{cases} \delta \dot{\boldsymbol{y}}_{\circ}(t) = (A + \epsilon(t)B_{\circ})\delta \boldsymbol{y}_{\circ}(t) + \sum_{j=1}^{K} \delta \boldsymbol{\alpha}_{j}\epsilon(t)B_{j}\boldsymbol{y}_{\circ}(t), \quad t \in (0,T], \quad \delta \boldsymbol{y}_{\circ}(0) = 0, \\ \dot{\boldsymbol{y}}_{\circ}(t) = (A + \epsilon(t)B_{\circ})\boldsymbol{y}_{\circ}(t), \quad t \in (0,T], \quad \boldsymbol{y}_{\circ}(0) = \boldsymbol{y}^{0}. \end{cases}$$

Assumption 6.2 would be the same, only with A instead of A_{\circ} and B_{\circ} instead of B. 460Notice that, in this case, we also cover Schrödinger-type systems of the form 461

462
$$i\hat{\boldsymbol{\psi}}(t) = (H + \epsilon(t)\mu_{\star})\boldsymbol{\psi}(t), \ t \in (0,T], \quad \boldsymbol{\psi}(0) = \boldsymbol{\psi}^0$$

as considered in [30], for Hermitian matrices $H, \mu_{\star} \in \mathbb{C}^{N \times N}$. This can be seen by 463 writing $\boldsymbol{\psi} = \boldsymbol{\psi}_R + i\boldsymbol{\psi}_I, \ \boldsymbol{\psi}^0 = \boldsymbol{\psi}_R^0 + i\boldsymbol{\psi}_I^0, \ H = H_R + iH_I \text{ and } \mu_\star = \mu_{\star,R} + i\mu_{\star,I}, \text{ to get}$ 464

465 (6.6)
$$\dot{\boldsymbol{y}}(t) = \left(\underbrace{\begin{bmatrix} H_I & H_R \\ -H_R & H_I \end{bmatrix}}_{=:A} + \epsilon(t) \underbrace{\begin{bmatrix} \mu_{\star,I} & \mu_{\star,R} \\ -\mu_{\star,R} & \mu_{\star,I} \end{bmatrix}}_{:=B_{\star}} \right) \boldsymbol{y}(t),$$

for $\boldsymbol{y}(t) := \begin{bmatrix} \boldsymbol{\psi}_R(t) & \boldsymbol{\psi}_I(t) \end{bmatrix}^\top$ and skew-symmetric matrices $A, B_\star \in \mathbb{R}^{N \times N}$ (compare 466 also [10, Section 2.12.2]). 467

468 6.1. Analysis for skew-symmetric bilinear systems. We show in this section that Assumption 6.2 is a sufficient condition for the GN matrix W_{\circ} , defined as in 469(4.6), to be PD if the controls generated by Algorithm 4.1 are used. The idea of the 470analysis is similar to the one considered in section 5, meaning that we first have to 471show the existence of a control that makes the cost function of (4.5) strictly positive. 472

13

473 LEMMA 6.4 (GR initialization and splitting steps (bilinear systems)). Let the 474 matrices A_{\circ} , B and C satisfy Assumption 6.2. Let $\widetilde{A} \in \text{span}(\mathcal{A})$ be an arbitrary 475 matrix. If T > 0 is sufficiently large, then any solution $\widetilde{\epsilon}$ to the problem

476 $\max_{\boldsymbol{\epsilon}\in E_{ad}} \left\| C\delta \boldsymbol{y}_{\circ}(\widetilde{A},\boldsymbol{\epsilon};T) \right\|_{2}^{2},$

477
$$s.t. \ \dot{\delta y}_{\circ}(t) = (A_{\circ} + \epsilon(t)B)\delta y_{\circ}(t) + \widetilde{A}y_{\circ}(t), \quad \delta y_{\circ}(0) = 0,$$

$$\dot{\boldsymbol{y}}_{\circ}(t) = (A_{\circ} + \epsilon(t)B)\boldsymbol{y}_{\circ}(t), \quad \boldsymbol{y}_{\circ}(0) = \boldsymbol{y}^{0}$$

480 satisfies $\left\|C\delta \boldsymbol{y}_{\circ}(\widetilde{A},\widetilde{\epsilon};T)\right\|_{2}^{2} > 0.$

481 Proof. It is sufficient to show that there exists a control $\hat{\epsilon}_c \in E_{ad}$ such that 482 $C\delta \boldsymbol{y}_{\circ}(\widetilde{A}, \hat{\epsilon}_c; T) \neq 0$ for T sufficiently large. Let us define $\hat{\epsilon}_c$ as

483
$$\widehat{\epsilon}_c(s) := \begin{cases} \widehat{\epsilon}(s), & \text{for } 0 \le s \le \widehat{t}, \\ c, & \text{for } \widehat{t} < s \le T, \end{cases}$$

where $c \in \mathbb{R}$, $\hat{\epsilon} \in E_{ad}$, T > 0 and $\hat{t} \in (0, T)$ are to be chosen. Since $\tilde{A} \neq 0$, there exists 484 $\boldsymbol{v} \in \mathbb{R}^N, \|\boldsymbol{v}\|_2 = \|\boldsymbol{y}^0\|_2$ such that $\widetilde{A}\boldsymbol{v} \neq 0$. By the first and second part of Assumption 4856.2, we know that (6.4) is controllable on the sphere of radius $\|\boldsymbol{y}^0\|_2$, meaning that 486 there exist $\hat{t} > 0$ and $\hat{\epsilon} \in E_{ad}$ such that $\boldsymbol{y}_{\circ}(\tilde{A}, \hat{\epsilon}; \hat{t}) = \boldsymbol{v}$. Defining $A_c := A_{\circ} + cB$, we 487 notice that $f_{\boldsymbol{v}}(t) := \widetilde{A}e^{tA_c}\boldsymbol{v}$ is analytic in t, and since $f_{\boldsymbol{v}}(0) = \widetilde{A}\boldsymbol{v} \neq 0$, it is not equal to 488 zero everywhere and therefore has only isolated roots, see, e.g., [31, Theorem 10.18]. 489Recalling that exponential matrices are always invertible (see, e.g., [24, Theorem 4902.6.38]), we obtain that there exists $t_1 > 0$ such that $e^{-t_1(A_c)} \tilde{A} e^{(t_1-\hat{t})A_c} \boldsymbol{v} \neq 0$. By defining $\boldsymbol{w} := \delta \boldsymbol{y}_{\circ}(\tilde{A}, \hat{\epsilon}; \hat{t})$ and $\boldsymbol{g}(t) := \int_{\hat{t}}^{t} e^{-s(A_c)} \tilde{A} e^{(s-\hat{t})A_c} \boldsymbol{v} ds + e^{-\hat{t}A_c} \boldsymbol{w}$, we observe that $\frac{d\boldsymbol{g}(t_1)}{dt} = e^{-t_1(A_c)} \tilde{A} e^{(t_1-\hat{t})A_c} \boldsymbol{v} \neq 0$. Since $\frac{d\boldsymbol{g}(t)}{dt}$ is analytic in t, the same holds for 491 492493 g(t),⁴ and since $\frac{dg(t_1)}{dt} \neq 0$ we obtain that g(t) has only isolated roots. Notice that 494

495
$$e^{-tA_c}\delta\boldsymbol{y}(\widetilde{A},\widehat{\epsilon}_c;t) = e^{-tA_c} \int_{\widehat{t}}^t e^{(t-s)(A_c)} \widetilde{A} e^{(s-\widehat{t})A_c} \boldsymbol{v} ds + e^{(t-\widehat{t})A_c} \boldsymbol{w} = \boldsymbol{g}(t),$$

for $t > \hat{t}$. Thus, it remains to show that there exists $T > \hat{t}$ such that $Ce^{TA_c} \boldsymbol{q}(T) \neq 0$. 496 Assumption 6.2 guarantees that there exists $c \in \mathbb{R}$ such that the observability matrix 497 $\mathcal{O}_N(C, A_\circ + cB)$ has full rank. Hence, for any $\boldsymbol{u} \in \mathbb{R}^N \setminus \{0\}$ there exists a $t_{\boldsymbol{u}} > \hat{t}$ such 498that $Ce^{t_{\boldsymbol{u}}A_c}\boldsymbol{u}\neq 0$. Since $t\mapsto Ce^{tA_c}\boldsymbol{u}$ is analytic in $t, Ce^{t_{\boldsymbol{u}}A_c}\boldsymbol{u}\neq 0$ implies that it has 499only isolated roots. Thus, for $t > \hat{t}, t \mapsto Ce^{tA_c} g(t)$ is the composition of two analytic 500functions which both have only isolated roots, and is therefore also analytic with 501isolated roots. Hence, there exists $T > \hat{t}$ such that $C\delta \boldsymbol{y}(\tilde{A}, \hat{\epsilon}_c; T) = Ce^{TA_c}\boldsymbol{g}(T) \neq 0.\square$ 502Now, we can prove our main result, whose proof is the same as the one of Theorem 503

503 Now, we can prove our main result, whose proof is the same as the one of Theorem 504 5.6, in which Lemma 6.4 has to be used instead of Lemma 5.5.

THEOREM 6.5 (positive definiteness of the GN matrix \widehat{W}_{\circ} (bilinear systems)). Let $\boldsymbol{\alpha}_{\circ} \in \mathbb{R}^{K}$ be such that the matrices $A(\boldsymbol{\alpha}_{\circ}), B \in \mathfrak{so}(N)$ and $C \in \mathbb{R}^{P \times N}$ satisfy Assumption 6.2. For $K \leq N^{2}$, let $\mathcal{A} = \{A_{1}, \ldots, A_{K}\} \subset \mathfrak{so}(N)$ be a set of linearly independent matrices such that $A_{\star} \in \operatorname{span} \mathcal{A}$, and let $\{\epsilon^{1}, \ldots, \epsilon^{K}\} \subset E_{ad}$ be controls generated by Algorithm 4.1. Then the GN matrix \widehat{W}_{\circ} , defined in (4.6), is PD.

479

⁴This follows directly from the fundamental theorem of calculus.

510 **6.2.** Positive definiteness of the GN matrix. As in section 5.2, we show 511 that if the GN matrix in α_{\circ} is PD, then the same is true locally, for all iterates α_c of 512 GN. We start by writing the matrix $\widehat{W}(\alpha)$ as a function of α :

513 (6.7)
$$[\widehat{W}(\boldsymbol{\alpha})]_{i,j} := \sum_{m=1}^{K} \langle C \delta \boldsymbol{y}(\boldsymbol{\alpha}, A_i, \boldsymbol{\epsilon}^m; T), C \delta \boldsymbol{y}(\boldsymbol{\alpha}, A_j, \boldsymbol{\epsilon}^m; T) \rangle, \quad i, j \in \{1, \dots, K\},$$

514 where $\delta \boldsymbol{y}(\boldsymbol{\alpha}, \widehat{A}, \epsilon; T)$ denotes the solution at time T of

515 (6.8)
$$\begin{cases} \delta \boldsymbol{y}(t) = (A(\boldsymbol{\alpha}) + \epsilon(t)B)\delta \boldsymbol{y}(t) + A\boldsymbol{y}(t), \quad \delta \boldsymbol{y}(0) = 0, \\ \dot{\boldsymbol{y}}(t) = (A(\boldsymbol{\alpha}) + \epsilon(t)B)\boldsymbol{y}(t), \quad \boldsymbol{y}(0) = \boldsymbol{y}^{0}. \end{cases}$$

516 Now, we want to prove the same positive definiteness result of in Lemma 5.8.

517 LEMMA 6.6 (positive definiteness of \widehat{W}_{\circ} (bilinear systems)). Let \widehat{W}_{\circ} , defined in 518 (4.6), be PD and denote by $\sigma_{K}^{\circ} > 0$ the smallest singular value of \widehat{W}_{\circ} . Then, there 519 exists $\delta := \delta(\sigma_{K}^{\circ}) > 0$ such that for any $\boldsymbol{\alpha} \in \mathbb{R}^{K}$ with $\|\boldsymbol{\alpha} - \boldsymbol{\alpha}_{\circ}\|_{2} < \delta$, the matrix 520 $\widehat{W}(\boldsymbol{\alpha})$, defined as in (6.7), is also PD.

521 Proof. Recalling the proof of Lemma 5.8, it is sufficient to show that the solution 522 $\delta \boldsymbol{y}(\boldsymbol{\alpha}, \hat{A}, \epsilon; T)$ of (6.8) is continuous in $\boldsymbol{\alpha}$. By [10, Proposition 3.26],⁵ we obtain continu-523 ity of the map $\boldsymbol{\alpha} \mapsto \boldsymbol{y}(A(\boldsymbol{\alpha}), \epsilon; T)$ and analogously the continuity of $\boldsymbol{\alpha} \mapsto \delta \boldsymbol{y}(\boldsymbol{\alpha}, \hat{A}, \epsilon; T)$.

524 Using the result from Lemma 6.6, we can directly prove our main result.

THEOREM 6.7 (convergence of GN (bilinear systems)). Let $\boldsymbol{\alpha}_{\circ} \in \mathbb{R}^{K}$ be such that the matrices $A(\boldsymbol{\alpha}_{\circ})$, B and C satisfy Assumption 6.2, and let $(\epsilon^{m})_{m=1}^{K} \subset E_{ad}$ be generated by Algorithm 4.1. Denote by $\hat{\sigma}_{K}$ the smallest singular value of \widehat{W}_{\circ} , defined in (4.6). Then there exists $\delta = \delta(\widehat{\sigma}_{K}) > 0$ such that, if $\boldsymbol{\alpha}_{\star} \in \mathbb{R}^{K}$ satisfies $\|\boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}_{\circ}\| \leq \delta$, then GN for the solution (6.2), initialized with $\boldsymbol{\alpha}_{\circ}$, converges to $\boldsymbol{\alpha}_{\star}$.

530 Proof. Theorem 6.5 guarantees that \widehat{W}_{\circ} is PD, meaning that $\widehat{\sigma}_{K} > 0$. Anal-531 ogously to the proof of Lemma 6.6, one can also show that the functions $R_{m}(\boldsymbol{\alpha})$, 532 defined in (3.4), are Lipschitz continuously differentiable in $\boldsymbol{\alpha}$ for all $m \in \{1, \ldots, K\}$. 533 Thus, the result follows by Lemma 6.6.

6.3. Local uniqueness of solutions. Let us study the local properties of problem (6.2) around α_{\star} . We use the same approach as in the linear case, and start by rewriting problem (6.2) in a matrix-vector form.

LEMMA 6.8 (online identification problem in matrix form (bilinear systems)).
 Problem (3.3) is equivalent to

539
$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{K}} \frac{1}{2} \langle \boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}, \widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha})(\boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}) \rangle$$

543

540 where $\widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}) \in \mathbb{R}^{K \times K}$ is defined as $\widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}) = \sum_{m=1}^{K} W(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}, \epsilon^{m})$ with

541
$$[W(\boldsymbol{\alpha}_{\star},\boldsymbol{\alpha},\epsilon^{m})]_{i,j} := \langle C\delta \boldsymbol{y}_{m}(\boldsymbol{\alpha}_{\star},\boldsymbol{\alpha},A_{j};T), C\delta \boldsymbol{y}_{m}(\boldsymbol{\alpha}_{\star},\boldsymbol{\alpha},A_{j};T) \rangle,$$

542 for $i, j \in \{1, ..., K\}$ and where $C\delta \boldsymbol{y}_m(\boldsymbol{\alpha}_\star, \boldsymbol{\alpha}, A; T)$ is the solution at time T of

$$\begin{cases} \dot{\delta} \boldsymbol{y}(t) &= (A(\boldsymbol{\alpha}_{\star}) + \epsilon^{m}(t)B)\delta \boldsymbol{y}(t) + A\boldsymbol{y}(t), \quad \delta \boldsymbol{y}(0) = 0, \\ \dot{\boldsymbol{y}}(t) &= (A(\boldsymbol{\alpha}) + \epsilon^{m}(t)B)\boldsymbol{y}(t), \quad \boldsymbol{y}(0) = \boldsymbol{y}^{0}. \end{cases}$$

⁵This result is a special case of the implicit function theorem; see, e.g., [10, Theorem 3.4].

Algorithm	7.1	Nonlinear	Greedy	Reconstruction	Algorithm
-----------	-----	-----------	--------	----------------	-----------

Require: A set of linearly independent operators $\mathcal{A} = \{A_1, \ldots, A_K\}$, an (initial) operator $A(\boldsymbol{\alpha}_{\circ}) \in \text{span } \mathcal{A}$ and a family of compact sets $\mathcal{K}_j \subset \mathbb{R}^j, j = 1, \ldots, K-1$.

1: Compute the control $\boldsymbol{\epsilon}^1$ by solving

(7.1)
$$\max_{\boldsymbol{\epsilon}\in E_{+}} \|C\boldsymbol{y}(A(\boldsymbol{\alpha}_{\circ}),\boldsymbol{\epsilon};T) - C\boldsymbol{y}(A(\boldsymbol{\alpha}_{\circ}) + A_{1},\boldsymbol{\epsilon};T)\|_{2}^{2}.$$

(I unified the notation here regarding the OGR Algorithm 7.2 and Assumption 7.6. Before, the A_1 -state was split against the uncontrolled state)

2: for k = 1, ..., K - 1 do

3: Fitting step: $A^{(k)}(\boldsymbol{\beta}) := \sum_{j=1}^{k} \boldsymbol{\beta}_{j} A_{j}$, find $\boldsymbol{\beta} = (\boldsymbol{\beta}_{j}^{k})_{j=1,\dots,k}$ that solves

(7.2)
$$\min_{\boldsymbol{\beta}\in\mathcal{K}_k}\sum_{m=1}^k \left\| C\boldsymbol{y}(A(\boldsymbol{\alpha}_\circ) + A^{(k)}(\boldsymbol{\beta}), \boldsymbol{\epsilon}^m; T) - C\boldsymbol{y}(A(\boldsymbol{\alpha}_\circ) + A_{k+1}, \boldsymbol{\epsilon}^m; T) \right\|_2^2$$

4: Splitting step: Find ϵ^{k+1} that solves

(7.3)
$$\max_{\boldsymbol{\epsilon}\in E_{ad}} \left\| C\boldsymbol{y}(A(\boldsymbol{\alpha}_{\circ}) + A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}; T) - C\boldsymbol{y}(A(\boldsymbol{\alpha}_{\circ}) + A_{k+1}, \boldsymbol{\epsilon}; T) \right\|_{2}^{2}$$

5: **end for**

The proof of Lemma 6.8 is analogous to the one of Lemma 5.10 (for details see the supplementary material [12]). Notice that the notations in (6.7) and Lemma 6.8 are related in the sense that $\widehat{W}(\boldsymbol{\alpha}) = \widetilde{W}(\boldsymbol{\alpha}, \boldsymbol{\alpha})$. Now, proceeding as in Section 5.3 and defining the set of all global solutions $S_{global} := \left\{ \boldsymbol{\alpha} \in \mathbb{R}^{K} : (\boldsymbol{\alpha}_{\star} - \boldsymbol{\alpha}) \in \ker \widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}) \right\}$, we obtain the same local uniqueness of the solution $\boldsymbol{\alpha}_{\star}$ to (6.2), meaning that if $\widehat{W}(\boldsymbol{\alpha}_{\star}) = \widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha}_{\star})$ is PD, the same holds for $\widetilde{W}(\boldsymbol{\alpha}_{\star}, \boldsymbol{\alpha})$ when $\boldsymbol{\alpha}$ is close to $\boldsymbol{\alpha}_{\star}$.

7. Towards general nonlinear GR algorithms. The LGR algorithm introduced in the previous sections only considers the linearized system. Thus it does not have access to the full (nonlinear) dynamics and can only capture the local characteristics of the considered system. Moreover, as we will show in section 8, the standard 553GR algorithm can outperform LGR when α_{\circ} is far from the solution. However, the 554analysis of LGR allows us to better understand the local behavior of GR and prove 555that locally it is capable to construct control functions that guarantee convergence 556 of GN. This analysis is carried out in section 7.1. This is the first analysis of GR algorithms for nonlinear problems. While section 7.1 focuses on GR, we also briefly 558 discuss its optimized version called optimized GR (OGR), introduced in [11], and propose a slight improvement of the original version. 560

7.1. A local analysis for nonlinear GR algorithms. This section is con-561cerned with general nonlinear systems of the form $\dot{\boldsymbol{y}}(t) = f(A(\boldsymbol{\alpha}^0) + A(\delta\alpha_{\star}), \boldsymbol{y}(t), \boldsymbol{\epsilon}(t))$ 562 with the goal of reconstructing $A(\delta \alpha_{\star}) = A_{\star} - A(\boldsymbol{\alpha}^0)$. Here, the shift of A_{\star} is con-563 sidered to perform a local analysis near $A(\boldsymbol{\alpha}^0)$. The goal is to prove convergence of 564565 GN for the controls generated by the GR Algorithm 7.1 using a local analogy to Algorithm 4.1. Notice that there are a few differences between Algorithms 7.1 and 4.1. 566 To derive a local analogy between them, all operators from the set \mathcal{A} are shifted by 567 $A(\boldsymbol{\alpha}_{\circ})$. Additionally, the fitting step problem (7.2) only minimizes over a compact set 568 $\mathcal{K}_k \subset \mathbb{R}^k$. However, this is not restrictive since the set \mathcal{K}_k can be chosen arbitrarily 569

large. Finally, the initialization problem (7.1) is different from the initialization (4.3). 570

571This is due to results obtained in [11] which suggest that one should not simply max-

imize the state corresponding to the first element A_1 in the set, but rather maximize 572

the difference to the state that is observed when no elements from \mathcal{A} are considered. We recall that, in order to obtain our main results for Algorithm 4.1, it is sufficient 574

to prove two points. First, that the fitting step identifies the kernel of the submatrix 575 $[\widehat{W}^{(k)}_{\circ}]_{[1:k+1,1:k+1]}$. Second, that for the initialization and each splitting step there 576 exists at least one control for which the corresponding cost function is strictly positive (making the submatrix $[\widehat{W}_{\circ}^{(k+1)}]_{[1:k+1,1:k+1]}$ PD). 578

To prove the fitting step result, we need some continuity properties of the argmin 579 operator. For this purpose, we introduce the following definition of hemi-continuous 580set-valued correspondences (see, e.g., [8, Chapter VI, §1]). 581

DEFINITION 7.1 (hemi-continuity). Let $X \subset \mathbb{R}$ be an open interval. A set-valued 582 correspondence $c: X \rightrightarrows \mathbb{R}^k$ is called upper hemi-continuous (u.h.c.) if for each $x_0 \in X$ 583and each open set $G \subset \mathbb{R}^k$ with $c(x_0) \subset G$ there exists a neighborhood $U(x_0)$ such that 584 $x \in U(x_0) \Rightarrow c(x) \subset G$, and called lower hemi-continuous (l.h.c.) if for each $x_0 \in X$ 585 and each open set $G \subset \mathbb{R}^k$ meeting $c(x_0)$ there exists a neighborhood $U(x_0)$ such that 586 $x \in U(x_0) \Rightarrow c(x) \cap G \neq \emptyset$. Furthermore, $c: X \rightrightarrows \mathbb{R}^k$ is called hemi-continuous if it 587 is u.h.c. and l.h.c. 588

Using Definition 7.1, we can recall the Berge maximum theorem [2, Theorem 17.31]. 589

LEMMA 7.2 (Berge maximum theorem). Let $X \subset \mathbb{R}$ be an open interval. Let 590 $J: \mathbb{R}^k \times X \to \mathbb{R}$ be a continuous function and $\phi: X \rightrightarrows \mathbb{R}^k$ be a hemi-continuous, 591 set-valued correspondence such that $\phi(x)$ is nonempty and compact for any $x \in X$. 592Then the correspondence $c: X \rightrightarrows \mathbb{R}^k$ defined by $c(x) := \arg \min J(z; x)$ is u.h.c.

 $z \in \phi(x)$

We will also need the following technical lemma. 594

LEMMA 7.3 (limit of set-valued correspondence). Let $X \subset \mathbb{R}$ be an open interval 595 with $0 \in X$, and $c : X \rightrightarrows \mathbb{R}^k$ be a u.h.c. correspondence. If $c(0) = \{0\}$, then 596 $\lim_{k\to\infty} c(x_k) = \{0\} \text{ for any sequence } \{x_k\}_{k=1}^{\infty} \text{ such that } \lim_{k\to\infty} x_k = 0.$ 597

Proof. Consider an arbitrary sequence $\{x_k\}_{k=1}^{\infty}$ with $\lim_{k\to\infty} x_k = 0$, and let 598 $c(0) = \{0\}$. It is sufficient to show that for any $\epsilon > 0$ there exists $n_{\epsilon} \in \mathbb{N}$ such that for 599 all $k \ge n_{\epsilon}$ we have $c(x_k) \subset \mathcal{B}^k_{\epsilon}(0)$. Let $\epsilon > 0$ and define $G_{\epsilon} := \mathcal{B}^k_{\epsilon}(0)$. Since $c(0) = \{0\}$ 600 and c is u.h.c., there exists a neighborhood $U_{\epsilon}(0) \subset \mathbb{R}$ such that $c(x) \subset G_{\epsilon}$ for any 601 $x \in U_{\epsilon}(0)$. Since $U_{\epsilon}(0)$ is an open neighborhood of 0, there exists $\xi_{\epsilon} > 0$ such that 602 $(-\xi_{\epsilon},\xi_{\epsilon}) \subset U_{\epsilon}(0)$. Since $\lim_{k\to\infty} x_k = 0$, there exists n_{ϵ} such that for all $k \geq n_{\epsilon}$ we 603 have $x_k \in (-\xi_{\epsilon}, \xi_{\epsilon})$ and hence $c(x_k) \subset \mathcal{B}^k_{\epsilon}(0)$. 604

To use Lemmas 7.2 and 7.3, we make the following assumptions. 605

ASSUMPTION 7.4. Let $k \in \{1, \ldots, K-1\}$ and define, 606

607
$$J_k(\boldsymbol{\beta}; A_{k+1}) := \sum_{m=1}^k \|C\boldsymbol{y}(A(\boldsymbol{\alpha}_\circ) + A^{(k)}(\boldsymbol{\beta}), \boldsymbol{\epsilon}^m; T) - C\boldsymbol{y}(A(\boldsymbol{\alpha}_\circ) + A_{k+1}, \boldsymbol{\epsilon}^m; T)\|_2^2.$$

• If $||A_{k+1}||$ is small enough, then there exists a $\boldsymbol{\beta}^k = \boldsymbol{\beta}^k(A_{k+1})$ that solves 608 (7.2) with $J_k(\boldsymbol{\beta}^k; A_{k+1}) = 0$. • There exists $\nu > 0$ such that $\mathcal{B}^k_{\nu}(0) \subset \mathcal{K}_k$ and $\arg\min_{\boldsymbol{\beta} \in \overline{\mathcal{B}^k_{\nu}(0)}} J_k(\boldsymbol{\beta}; 0) = \{0\}.$ 609

610

The first point in Assumption 7.4 guarantees that locally near $A(\boldsymbol{\alpha}_{\circ})$, for $||A_{k+1}||$ 611 612 small enough, one can solve (7.2) making the cost function zero, meaning that one 613 can find a linear combination of the first k elements for which the final state cannot 614 be distinguished from the k + 1-th element by any of the k computed controls. On

615 the other hand, if the minimum function value is strictly positive, then there already

exists a control in the set $(\boldsymbol{\epsilon}_m)_{m=1}^k$ that discriminates (splits) these two states.

The second point in Assumption 7.4 ensures that $\{0\} = \arg \min_{\boldsymbol{\beta} \in \overline{\mathcal{B}_{\nu}^{k}(0)}} J_{k}(\boldsymbol{\beta}, 0)$. If this was not true, it would mean that, for any radius $\nu > 0$, the ball $\mathcal{B}_{\nu}^{k}(0)$ would contain infinitely many $\boldsymbol{\beta} \in \mathbb{R}^{k} \setminus \{0\}$ satisfying $J_{k}(\boldsymbol{\beta}, 0) = 0$. Hence, for an infinite number of linear combinations in the set $\{A_{1}, \ldots, A_{k}\}$, the corresponding states could not be distinguished by any of the previously selected controls. However, this implies that at least one of the previous splitting steps was not successful, which contradicts what we assume to reach iteration k.

Now, we can show that the local nonlinear fitting step problem (7.2) is able to identify the kernel of the submatrix $[\widehat{W}_{\circ}^{(k)}]_{[1:k+1,1:k+1]}$, if it exists.

THEOREM 7.5 (nonlinear GR fitting step problems). Let $k \in \{1, \ldots, K\}$ and let $\boldsymbol{\beta}^k$ be a solution to (7.2). If $||A_{k+1}||$ is sufficiently small and Assumption 7.4 holds, then $\boldsymbol{\beta}^k$ also solves (4.4) with

$$\sum_{m=1}^{k} \|C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{m}; T) - C\delta \boldsymbol{y}_{\circ}(A_{k+1}, \boldsymbol{\epsilon}^{m}; T)\|_{2}^{2} = 0.$$

Proof. Define $\widehat{J}_k(\boldsymbol{\beta}, \delta_k) := J_k(\boldsymbol{\beta}, \delta_k A_{k+1})$ for $\delta_k > 0$. The first point of Assumption 7.4 implies that there exists a $\widehat{\delta}_k > 0$ such that for all $|\delta_k| < \widehat{\delta}_k$ we have $\widehat{J}_k(\boldsymbol{\beta}, \delta_k) = 0$. Thus, Lemma 7.2 guarantees that the correspondence $c_k : (-\widehat{\delta}_k, \widehat{\delta}_k) \Rightarrow$ $\mathbb{R}^k, c_k(\delta_k) = \arg\min_{\boldsymbol{\beta}\in\mathcal{K}_k} \widehat{J}_k(\boldsymbol{\beta}; \delta_k)$ is u.h.c.⁶

According to the second point of Assumption 7.4, $c_k(0) = 0$ is an isolated solution of (7.2). Hence, the upper hemi-continuity of c_k guarantees that for $\delta_k \to 0$ we have $\beta^k \to 0$ for any corresponding solution $\beta^k = \beta^k(\delta_k)$ of (7.2).

Now, let $m \in \{1, \ldots, k\}$. If $\widehat{J}_k(\boldsymbol{\beta}^k; \delta_k) = 0$, then

634 (7.4)
$$C\boldsymbol{y}(A(\boldsymbol{\alpha}_{\circ}) + A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{m}; T) - C\boldsymbol{y}(A(\boldsymbol{\alpha}_{\circ}) + \delta_{k}A_{k+1}, \boldsymbol{\epsilon}^{m}; T) = 0$$

We define $g(\boldsymbol{\alpha}) := C\boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}^m; T)$. Since $f(A, \boldsymbol{y}, \boldsymbol{\epsilon})$ in (3.1) is assumed to be differentiable with respect to A and \boldsymbol{y} , we obtain that the map $A \mapsto \boldsymbol{y}(A, \boldsymbol{\epsilon}; T)$ is differentiable with respect to A by the implicit function theorem (see, e.g., [14, Theorem 17.13-1]). Hence, $C\boldsymbol{y}(A(\boldsymbol{\alpha}), \boldsymbol{\epsilon}; T)$ is also differentiable with respect to $\boldsymbol{\alpha}$. By Taylor's theorem, we get $g(\boldsymbol{\alpha}_{\circ} + \boldsymbol{v}) = g(\boldsymbol{\alpha}_{\circ}) + g'(\boldsymbol{\alpha}_{\circ})(\boldsymbol{v}) + O(\|\boldsymbol{v}\|_2^2)$ for $\boldsymbol{v} \in \mathbb{R}^k$. Defining $\widehat{\boldsymbol{\beta}^k}$ and $\widehat{\boldsymbol{\delta}_k}$ as $\widehat{\boldsymbol{\beta}^k} := [\boldsymbol{\beta}^k, 0, \cdots, 0]^\top \in \mathbb{R}^k$ and $\widehat{\boldsymbol{\delta}_k} := [0, \cdots, 0, \delta_k]^\top \in \mathbb{R}^k$, we can rewrite (7.4) as

$$\underset{\mathbb{R}^{41}}{\overset{641}{\oplus}} \quad 0 = g(\boldsymbol{\alpha}_{\circ} + \widehat{\boldsymbol{\beta}^{k}}) - g(\boldsymbol{\alpha}_{\circ} + \widehat{\boldsymbol{\delta}}_{k+1}) = g'(\boldsymbol{\alpha}_{\circ})(\widehat{\boldsymbol{\beta}^{k}}) - g'(\boldsymbol{\alpha}_{\circ})(\widehat{\boldsymbol{\delta}}_{k+1}) + O(\|\widehat{\boldsymbol{\beta}^{k}}\|_{2}^{2}) + O(|\boldsymbol{\delta}_{k}|^{2}).$$

643 Since $g'(\boldsymbol{\alpha}_{\circ})(\widehat{\boldsymbol{\beta}^{k}}) = C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{m}; T)$ and $g'(\boldsymbol{\alpha}_{\circ})(\widehat{\boldsymbol{\delta}}_{k+1}) = C\delta \boldsymbol{y}_{\circ}(\delta_{k}A_{k+1}, \boldsymbol{\epsilon}^{m}; T),$ 644 we obtain

645 (7.5) $0 = C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{m}; T) - C\delta \boldsymbol{y}_{\circ}(\delta \alpha_{k} A_{k+1}, \boldsymbol{\epsilon}^{m}; T) + O(\|\boldsymbol{\widehat{\beta}^{k}}\|_{2}^{2}) + O(|\delta_{k}|^{2}).$

646 Since $\beta^k = \beta^k(\delta_k) \to 0$ for $\delta_k \to 0$, we know that all four terms vanish for $\delta_k \to 0$.

However,
$$O(|\delta_k|^2)$$
 converges faster than $C\delta \boldsymbol{y}_{\circ}(\delta_k A_{k+1}, \boldsymbol{\epsilon}^m; T)$ and $O(||\boldsymbol{\beta}^k||_2^2)$ faster

⁶Note that, in this setting, the correspondence $\phi : (-\widehat{\delta}_k, \widehat{\delta}_k) \rightrightarrows \mathbb{R}^k$ mentioned in Lemma 7.2 is defined as $\phi(x) = \mathcal{K}_k$ for any $x \in (-\widehat{\delta}_k, \widehat{\delta}_k)$ with \mathcal{K}_k compact, and is therefore hemi-continuous.

648 than $C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{m}; T)$. Hence, (7.5) can only be true for $\delta_{k} \to 0$ if 649 $C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{m}; T) - C\delta \boldsymbol{y}_{\circ}(\delta_{k}A_{k+1}, \boldsymbol{\epsilon}^{m}; T) = 0$ for δ_{k} small enough, which is equiv-650 alent to $C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{m}; T) - C\delta \boldsymbol{y}_{\circ}(A_{k+1}, \boldsymbol{\epsilon}^{m}; T) = 0$ for $||A_{k+1}||$ sufficiently small.

Regarding the initialization and splitting step result, we make now the assumption that there always exists a control that makes the corresponding cost function value strictly positive, and discuss specific cases where this assumption holds.

ASSUMPTION 7.6. Let $k \in \{1, ..., K-1\}$ and $\boldsymbol{\beta}^k \in \mathbb{R}^k$ be the solution of (7.2). Then there exists a solution $\boldsymbol{\epsilon}^{k+1} \in E_{ad}$ to (7.3) that simultaneously satisfies

656 (7.6)
$$\|C\boldsymbol{y}(A(\boldsymbol{\alpha}_{\circ}) + A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{k+1}; T) - C\boldsymbol{y}(A(\boldsymbol{\alpha}_{\circ}) + A_{k+1}, \boldsymbol{\epsilon}^{k+1}; T)\|_{2}^{2} > 0,$$

657 and

658 (7.7)
$$\|C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}^{k+1}; T) - C\delta \boldsymbol{y}_{\circ}(A_{k+1}, \boldsymbol{\epsilon}^{k+1}; T)\|_{2}^{2} > 0.$$

659 Let (7.6)-(7.7) also hold for a solution $\boldsymbol{\epsilon}^1 \in E_{ad}$ to (7.1) with k = 0 and $\boldsymbol{\beta}^0 = 0$.

In Theorem 7.10, we will investigate Assumption 7.6 for the two settings considered
in sections 5 and 6. Now, we state the following theorem, relating the two Algorithms
4.1 and 7.1.

THEOREM 7.7. Consider the general setting of system (3.1) with a set of linearly independent matrices $\{A_1, \ldots, A_K\}$ such that $||A_k||$ be sufficiently small for all $k \in$ $\{1, \ldots, K\}$. Let $(\boldsymbol{\epsilon}^m)_{m=1}^K \subset E_{ad}$ be generated by Algorithm 7.1 such that Assumption 7.4 holds for all $k \in \{1, \ldots, K-1\}$ and $\boldsymbol{\epsilon}^m$ satisfies Assumption 7.6 for all $m \in$ $\{1, \ldots, K\}$. Then the GN matrix \widehat{W}_{\circ} , defined in (4.6), is PD.

668 The proof of Theorem 7.7 is exactly the one of Theorem 5.6.

It remains to show that Assumption 7.6 holds in the settings considered in sections 5 and 6. First, we require the following results (see, e.g., [35, p. 1079]).

671 LEMMA 7.8 (on analytic functions in Banach spaces). Let X, Y denote real Ba-672 nach spaces and $\mathcal{B}_r(x) \subset X$ the open ball with center $x \in X$ and radius r > 0. For an 673 open set $D \subset X$, let the functions $f, g: D \to Y$ be analytic. If there exist $x_f, x_g \in D$ 674 such that $f(x_f) \neq 0$ and $g(x_g) \neq 0$, then for any $x \in D$ and any r > 0 there exists a 675 $\widetilde{x} \in \mathcal{B}_r(x) \subset D$ such that $f(\widetilde{x}) \neq 0$ and $g(\widetilde{x}) \neq 0$.

We also require the following result about the analycity of control-to-state maps, which follows directly from the implicit function theorem (see, e.g., [35, p. 1081]).

LEMMA 7.9 (analycity of control-to-state maps). Consider system (3.1) and 678 define the map $c: U \times Y \to Z$ as $c(\boldsymbol{\epsilon}, \boldsymbol{y}) := [\boldsymbol{\dot{y}} - f(A, \boldsymbol{y}, \boldsymbol{\epsilon}), \boldsymbol{y}(0) - \boldsymbol{y}^0]$, where U is the 679 680 Hilbert space of control functions, Y is the (Banach) space where solutions to (3.1)lie and Z is a Banach space. If c is analytic in $\boldsymbol{\epsilon}$ and \boldsymbol{y} , (3.1) has a unique solution 681 $\boldsymbol{y} = \boldsymbol{y}(\boldsymbol{\epsilon}) \in Y$ such that $c(\boldsymbol{y}(\boldsymbol{\epsilon}), \boldsymbol{\epsilon}) = 0$ for each $\boldsymbol{\epsilon} \in E_{ad} \subset U$ and the linearized state 682 equation $\delta \mathbf{y} = \delta_{\mathbf{y}} f(A, \mathbf{y}(\boldsymbol{\epsilon}), \boldsymbol{\epsilon})(\delta \mathbf{y}) - \varphi$ with $\delta \mathbf{y}(0) = \varphi^0$ is uniquely solvable for any 683 $[\varphi, \varphi^0] \in Z$, then the control-to-state map $L : E_{ad} \to Y, \boldsymbol{\epsilon} \mapsto \boldsymbol{y}(\boldsymbol{\epsilon})$ is analytic. If the solution space Y is such that the evaluation map $S_T : Y \to \mathbb{R}^N, \boldsymbol{y} \mapsto \boldsymbol{y}(T)$ is linear and continuous, then also the map $S : E_{ad} \to \mathbb{R}^N, \boldsymbol{\epsilon} \mapsto (\boldsymbol{y}(\boldsymbol{\epsilon}))(T)$ is analytic. 684 685 686

687 Proof. First, we prove that the control-to-state map $L : E_{ad} \to Y, \boldsymbol{\epsilon} \mapsto \boldsymbol{y}(\boldsymbol{\epsilon})$ is 688 analytic. This follows directly from the implicit function theorem [35, p. 1081] if we 689 can show that the map $D_{\boldsymbol{y}}c(\boldsymbol{\epsilon}, \boldsymbol{y})$ is an isomorphism of Y on Z for any pair $(\boldsymbol{\tilde{\epsilon}}, \boldsymbol{\tilde{y}}) \subset U \times$ 690 Y such that $\boldsymbol{\tilde{y}}$ is the unique solution to (3.1) for $\boldsymbol{\tilde{\epsilon}}$, i.e. $c(\boldsymbol{\tilde{\epsilon}}, \boldsymbol{\tilde{y}}) = 0$. Since the equation for the derivative $D_{\boldsymbol{y}}c(\tilde{\boldsymbol{\epsilon}}, \tilde{\boldsymbol{y}})(\delta \boldsymbol{y}) = \varphi$, which is equivalent to $\delta \boldsymbol{y} = \delta_{\boldsymbol{y}} f(A, \tilde{\boldsymbol{y}}, \tilde{\boldsymbol{\epsilon}})(\delta \boldsymbol{y}) - \varphi$ with $\delta \boldsymbol{y}(0) = \varphi^0$, admits a unique solution $\delta \boldsymbol{y} \in Y$ for any $[\varphi, \varphi^0] \in Z$, $D_{\boldsymbol{y}}c(\tilde{\boldsymbol{\epsilon}}, \tilde{\boldsymbol{y}})$ is bijective and therefore an isomorphism of Y on Z.

It remains to show that also the map $S : E_{ad} \to \mathbb{R}^N, \boldsymbol{\epsilon} \mapsto (\boldsymbol{y}(\boldsymbol{\epsilon}))(T)$ is analytic. Consider an arbitrary $\boldsymbol{\epsilon}_0 \in E_{ad}$. Since the control-to-state map L is analytic, there exist (by definition, see, e.g., [35, p. 1078]) ℓ -linear, symmetric and continuous maps $a_\ell : (E_{ad})^\ell \to \mathbb{R}^N, (\boldsymbol{\epsilon}_1, \dots, \boldsymbol{\epsilon}_\ell) \mapsto a_\ell(\boldsymbol{\epsilon}_1, \dots, \boldsymbol{\epsilon}_\ell)$ such that $\boldsymbol{y}(\boldsymbol{\epsilon}) = \sum_{\ell=0}^{\infty} a_\ell(\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_0)^\ell$. Now, define the maps $b_\ell : (E_{ad})^\ell \to \mathbb{R}^N$ as $b_\ell(\boldsymbol{\epsilon})^\ell := (a_\ell(\boldsymbol{\epsilon})^\ell)(T)$, meaning that $\sum_{\ell=0}^{\infty} b_\ell(\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_0)^\ell = (\boldsymbol{y}(\boldsymbol{\epsilon}))(T)$. Since the evaluation map $S_T : Y \to \mathbb{R}^N, \boldsymbol{y} \mapsto \boldsymbol{y}(T)$ is linear and continuous, the maps b_ℓ are ℓ -linear, symmetric and continuous. Thus, the map $S : E_{ad} \to \mathbb{R}^N, \boldsymbol{\epsilon} \mapsto (\boldsymbol{y}(\boldsymbol{\epsilon}))(T) = \sum_{\ell=0}^{\infty} b_\ell(\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_0)^\ell$ is analytic by definition. \Box

In our case, we consider $U = L^2(0,T;\mathbb{R}^M)$ in the linear and $U = L^2(0,T;\mathbb{R})$ in the bilinear setting, $Y = H^1(0,T;\mathbb{R}^N)$ and $Z = L^2(0,T;\mathbb{R}^N) \times \mathbb{R}^N$. Then, the assumptions in Lemma 7.9 on the ODE system and its linearization are satisfied for (5.1) and (5.2) in the linear setting, and for (6.1) and (6.3) in the bilinear setting.⁷ Notice that all solutions lie in $H^1(0,T;\mathbb{R}^N) \in C(0,T;\mathbb{R}^N)$ (see, e.g., [14]), which implies that the evolution map $S_T : H^1(0,T;\mathbb{R}^N) \to \mathbb{R}^N, \mathbf{y} \mapsto \mathbf{y}(T)$ is also linear and continuous.

709 Now, we can prove our main result.

THEOREM 7.10. Consider the linear setting (5.1) or the bilinear setting (6.1). For brevity, we assume that the systems are sufficiently observable and controllable, i.e. fully observable and controllable in the linear case, and satisfying Assumption 6.2 in the bilinear case. If $||A_{k+1}||$ is sufficiently small, then there exists a control $\epsilon \in E_{ad}$ which satisfies (7.6)-(7.7) in Assumption 7.6.

715 Proof. For brevity, we denote $A_{\boldsymbol{\beta}} := A(\boldsymbol{\alpha}_{\circ}) + A^{(k)}(\boldsymbol{\beta}^{k}), A_{+} := A(\boldsymbol{\alpha}_{\circ}) + A_{k+1},$ 716 $\boldsymbol{y}_{\boldsymbol{\beta}}(\boldsymbol{\epsilon};t) := \boldsymbol{y}(A_{\boldsymbol{\beta}},\boldsymbol{\epsilon};t) \text{ and } \boldsymbol{y}_{+}(\boldsymbol{\epsilon};t) := \boldsymbol{y}(A_{+},\boldsymbol{\epsilon};t).$

We start with the linear setting (5.1) from section 5. First, we derive observability 717 and controllability properties for the systems (A_+, B, C) and (A_{β}, B, C) . Denote by 718 $\sigma_k > 0$ the smallest singular value of $\mathcal{O}_N(C, A(\boldsymbol{\alpha}_\circ))$. Let $k \in \{1, \ldots, K\}$ and $\boldsymbol{\beta}^k \in \mathbb{R}^k$ 719 be the solution of (7.2) for $||A_{k+1}|| > 0$ sufficiently small such that $||\mathcal{O}_N(C, A(\boldsymbol{\alpha}_\circ)) - C(C, A(\boldsymbol{\alpha}_\circ))||$ 720 $\mathcal{O}_N(C, A_+) \|_2 < \sigma_k$. From the proof of Theorem 7.5, we obtain that also $\boldsymbol{\beta}^k$ can be 721 assumed to be sufficiently small such that $\|\mathcal{O}_N(C, A(\boldsymbol{\alpha}_o)) - \mathcal{O}_N(C, A_{\boldsymbol{\beta}})\|_2 < \sigma_k$. Now, 722 Lemma 5.7 guarantees that $\operatorname{rank}(\mathcal{O}_N(C, A_+)) = \operatorname{rank}(\mathcal{O}_N(C, A_\beta)) = N$. Using the 723 same argument for the rank of the controllability matrices, we obtain that the systems 724 (A_+, B, C) and (A_{β}, B, C) are fully observable and controllable. 725

Next, we consider the state of the difference $\mathbf{z}(t) = \mathbf{y}(A_+, \boldsymbol{\epsilon}; t) - \mathbf{y}(A_{\boldsymbol{\beta}}, \boldsymbol{\epsilon}; t)$ with $\dot{\mathbf{z}} = A_+ \mathbf{z} + (A_+ - A_{\boldsymbol{\beta}})\mathbf{y}(A_{\boldsymbol{\beta}}, \boldsymbol{\epsilon}; t)$. Since $A_+ \neq A_{\boldsymbol{\beta}}$, there exists $\mathbf{v} \in \mathbb{R}^N$ such that $(A_+ - A_{\boldsymbol{\beta}})\mathbf{v} \neq 0$. Recalling that $(A_{\boldsymbol{\beta}}, B)$ is controllable, we can find $\boldsymbol{\epsilon}_{t_1}$ for any $t_1 \in (0, T]$ such that $\mathbf{y}_{\boldsymbol{\beta}}(\boldsymbol{\epsilon}_{t_1}; t) = \mathbf{v}$ and therefore $(A_+ - A_{\boldsymbol{\beta}})\mathbf{y}_{\boldsymbol{\beta}}(\boldsymbol{\epsilon}_{t_1}; t_1) \neq 0$. We define

730
$$\widetilde{\boldsymbol{\epsilon}}(s) := \begin{cases} \boldsymbol{\epsilon}_{t_1}(s), & \text{for } 0 \leq s < t_1, \\ \boldsymbol{c}, & \text{for } t_1 \leq s \leq T, \end{cases}$$

⁷Existence and uniqueness of all solutions $\boldsymbol{y}, \delta \boldsymbol{y}$ follow by Carathéodory's existence theorem (see, e.g., [32, Theorem 54] and related propositions). For $\boldsymbol{\epsilon} \in L^2(0,T;\mathbb{R}^M)$ in the linear and $\boldsymbol{\epsilon} \in L^2(0,T;\mathbb{R})$ in the bilinear setting, we obtain $\boldsymbol{y}, \delta \boldsymbol{y} \in L^2(0,T;\mathbb{R}^N)$ and thus $\boldsymbol{y}, \delta \boldsymbol{y} \in H^1(0,T;\mathbb{R}^N)$.

731 where $\boldsymbol{c} \in \mathbb{R}^N$ is to be chosen later. For $t > t_1$, we have

732 (7.8)
$$\boldsymbol{z}(t) = e^{(t-t_1)A_+} \boldsymbol{z}(t_1) + \int_{t_1}^t e^{(t-s)A_+} (A_+ - A_{\boldsymbol{\beta}}) \boldsymbol{y}_{\boldsymbol{\beta}}(\boldsymbol{\tilde{\epsilon}}; s) ds.$$

733 Multiplying (7.8) with $e^{-(t-t_1)A_+}$ from the left, we get

734
$$\widetilde{\boldsymbol{z}}(t) := e^{-(t-t_1)A_+} \boldsymbol{z}(t) = \boldsymbol{z}(t_1) + \int_{t_1}^t e^{(t_1-s)A_+} (A_+ - A_{\boldsymbol{\beta}}) \boldsymbol{y}_{\boldsymbol{\beta}}(\widetilde{\boldsymbol{\epsilon}}; s) ds.$$

Notice that for $s > t_1$, the terms $e^{(t_1-s)A_+}$ and $\boldsymbol{y}_{\boldsymbol{\beta}}(\boldsymbol{\tilde{\epsilon}};s) = e^{(s-t_1)A_{\boldsymbol{\beta}}}\boldsymbol{v} + \int_0^s e^{(s-\tau)A_{\boldsymbol{\beta}}} B\boldsymbol{c} ds$ are continuous in s. Since exponential matrices are invertible (see, e.g., [24, pag. 369, 5.6.P43]) and $\boldsymbol{z}(t_1)$ is independent of t, there exists a $t > t_1$ such that $\boldsymbol{z}(t_1) + \int_{t_1}^t e^{(t_1-s)A_+} (A_+ - A_{\boldsymbol{\beta}}) \boldsymbol{y}_{\boldsymbol{\beta}}(\boldsymbol{\tilde{\epsilon}};s) ds \neq 0$ and thus $\boldsymbol{\tilde{z}}(t) \neq 0$. Using (7.8), we obtain

739 (7.9)
$$C\mathbf{z}(t) = Ce^{(t-t_1)A_+} \widetilde{\mathbf{z}}(t) = \sum_{j=0}^{\infty} \frac{(t-t_1)^j}{j!} CA_+^j \widetilde{\mathbf{z}}(t).$$

Now, the observability of (A_+, C) guarantees the existence of some $i \in \{0, \ldots, N-1\}$ such that $CA_+^i \tilde{\boldsymbol{z}}(t) \neq 0$. We have $\frac{(t-t_1)^i}{i!} > 0$ for $t > t_1$ and all terms of the sum in (7.9) converge to zero at different rates for different j. Hence, there exists $t > t_1$ such that $C\boldsymbol{z}(t) \neq 0$. Since $t_1 \in (0,T]$ was chosen arbitrarily, we obtain $C\boldsymbol{z}(T) \neq 0$ and thus $C\boldsymbol{y}_{\boldsymbol{\beta}}(\tilde{\boldsymbol{\epsilon}};T) - C\boldsymbol{y}_+(\tilde{\boldsymbol{\epsilon}};T) \neq 0$.

Regarding the linearized system (5.2), we have already shown in Lemma 5.5 that there exists an $\boldsymbol{\epsilon} \in E_{ad}$ such that $C\delta \boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^{k}), \boldsymbol{\epsilon}; T) - C\delta \boldsymbol{y}_{\circ}(A_{k+1}, \boldsymbol{\epsilon}; T) \neq 0.$

Finally, the maps $S, S_{\delta} : L^2(0, T; \mathbb{R}^M) \to \mathbb{R}^N$, $S(\boldsymbol{\epsilon}) := C\boldsymbol{y}_{\boldsymbol{\beta}}(\boldsymbol{\epsilon}; T) - C\boldsymbol{y}_+(\boldsymbol{\epsilon}; T)$, $S_{\delta}(\boldsymbol{\epsilon}) := C\delta\boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^k), \boldsymbol{\epsilon}; T) - C\delta\boldsymbol{y}_{\circ}(A_{k+1}, \boldsymbol{\epsilon}; T)$ are analytic by Lemma 7.9. Using Lemma 7.8, we obtain the existence of an $\boldsymbol{\epsilon} \in E_{ad}$ such that $C\boldsymbol{y}(A_{\boldsymbol{\beta}}, \boldsymbol{\epsilon}; T) - C\delta\boldsymbol{y}_{\circ}(A_{k+1}, \boldsymbol{\epsilon}; T) \neq 0$ and $C\delta\boldsymbol{y}_{\circ}(A^{(k)}(\boldsymbol{\beta}^k), \boldsymbol{\epsilon}; T) - C\delta\boldsymbol{y}_{\circ}(A_{k+1}, \boldsymbol{\epsilon}; T) \neq 0$.

The proof for the <u>bilinear setting</u> (6.1) from Section 6 is analogous to the one above. For a detailed proof, we refer to the supplementary material [12].

Remark 7.11. Notice that we did not prove exactly Assumption 7.6 in Theorem 7537.10, but only the existence of a general control $\boldsymbol{\epsilon} \in E_{ad}$ that satisfies (7.6)-(7.7). How-754 ever, this implies that any solution $\boldsymbol{\epsilon}^{k+1}$ to (7.3) always satisfies (7.6). Additionally, 755we recall from the proof of Theorem 7.10 that the maps $S, S_{\delta} : L^2(0,T;\mathbb{R}^M) \to \mathbb{R}^N$, 756 defined by $S(\boldsymbol{\epsilon}) := \boldsymbol{y}(A, \boldsymbol{\epsilon}; T), \ S_{\delta}(\boldsymbol{\epsilon}) := \delta \boldsymbol{y}_{\circ}(A, \boldsymbol{\epsilon}; T)$ are analytic and not the zero 757 functional. Thus, we obtain by Lemma 7.8 that any neighborhood of ϵ^{k+1} contains 758 infinitely many ϵ that do satisfy (7.7). This implies that it is rather unlucky to choose 759 an $\boldsymbol{\epsilon}^{k+1}$ that does not satisfy (7.7). On the other hand, one can also add inequality 760 (7.7) as a constraint to (7.3) to ensure that both inequalities are met by ϵ^{k+1} . 761

As a consequence of Theorems 7.7, 7.10 and Remark 7.11, the controls generated by Algorithm 7.1 for the linear (5.1) and bilinear (6.1) setting make the GN matrix \widehat{W}_{\circ} , defined in (4.6), PD under certain assumptions. Thus, the results from Sections 5.2 and 6.2 imply that GN for the reconstruction problems (5.5) and (6.2), initialized with $\boldsymbol{\alpha}_{\circ}$, converges to $\boldsymbol{\alpha}_{\star}$.

767 **7.2. Optimized GR Algorithm.** The analysis discussed in the previous sec-768 tions are based on certain hypotheses of observability and controllability of the dynam-769 ical system. However, as shown already in [11] and also discussed in the supplementary

material [12], if these hypotheses are not satisfied, the choice of the elements in the 770 771 set \mathcal{A} becomes very relevant and can strongly affect the online reconstruction process.

For this reason, a modified GR algorithm called Optimized GR (OGR) has been in-772 troduced in [11] to identify important basis elements by solving in each iteration the 773 fitting and splitting step problems (in parallel) for all remaining basis elements, and 774 not just the next one. This also allows us to initialize the algorithm with a number of 775 elements $(A_j)_{j=1}^K$ with $K > N^2$. Even though some of the matrices A_j will inevitably be linearly dependent if $K > N^2$, the OGR algorithm manipulates them to construct 776 777 a new subset of linearly independent ones. In the spirit of the previous analysis, we 778 add a new feature to the original OGR algorithm. At iteration k, after all fitting 779 780 step problems have been solved, we check whether there exists $\ell \in \{k+1,\ldots,K\}$ for which the optimal cost function value is different from zero (i.e. larger than a 781 tolerance tol₂) If this is the case, then there exists a control $\boldsymbol{\epsilon}^m$, $m \in \{1, \ldots, k\}$, that 782 already satisfies $\|C\boldsymbol{y}(A^{(k)}(\boldsymbol{\beta}^{\ell}), \boldsymbol{\epsilon}^{m}; T) - C\boldsymbol{y}(A_{\ell}, \boldsymbol{\epsilon}^{m}; T)\|_{2}^{2} > \text{tol}_{2}$ for at least one index $\ell_{k+1} \in \{k+1, \ldots, K\}$ (see Step 8 in Algorithm 7.2). Hence, we can add the basis 783 784element $A_{\ell_{k+1}}$ to the already selected ones without computing a new control. This 785 new improvement can also be motivated with the matrix formulation we used for our 786 analysis. If $\operatorname{rank}(\widehat{W}_{\circ}^{(k)}) = r > k$, one can appropriately permute rows and columns of $\widehat{W}_{\circ}^{(k)}$ such that $[\widehat{W}_{\circ}^{(k)}]_{[1:r,1:r]}$ has rank r and is thus PD. The rank of $\widehat{W}_{\circ}^{(k)} = \sum_{m=1}^{k} W_{\circ}(\boldsymbol{\epsilon}^{m})$ is bounded by kP, where P is the number of rows of the observer matrix C. This can be seen by writing $W_{\circ}(\boldsymbol{\epsilon}^{m})$, as defined in 787 788

789 790 (4.6), as $W_{\circ}(\boldsymbol{\epsilon}^m) = \delta Y_{\circ}^{\top} C^{\top} C \delta Y_{\circ}$, where $\delta Y_{\circ} := [\delta \boldsymbol{y}_{\circ}(A_1, \boldsymbol{\epsilon}^m; T), \cdots, \delta \boldsymbol{y}_{\circ}(A_K, \boldsymbol{\epsilon}^m; T)].$ 791 Hence, $\operatorname{rank}(W_{\circ}(\epsilon^{m})) \leq \operatorname{rank}(C) \leq P$, and therefore $\operatorname{rank}(\widehat{W}_{\circ}^{(k)}) \leq kP$. 792

The full OGR algorithm is stated in Algorithm 7.2, where the new feature that 793 we described correspond to the steps 7-8. Algorithm 7.2 can be formulated for the 794 795 linearized setting considered the previous sections by simply replacing the state \boldsymbol{y} with 796 its linearization y_{\circ} . We call OLGR the OGR algorithm for the linearized system.

797 8. Numerical experiments. In this section, efficiency and robustness of the GR and OGR algorithms are studied by direct numerical experiments. In particular, 798 first we consider the reconstruction of a drift matrix in Section 8.1. Second, we focus 799 on the reconstruction of a bilinear dipole momentum operator as Section 8.2. All 800 optimization problems inside of the GR algorithms are solved by a BFGS descent-801 802 direction method, while the online identification problem is solved by GN.

8.1. Reconstruction of drift matrices. We consider system (5.1) with (full 803 rank) randomly generated matrices $A_{\star}, B, C \in \mathbb{R}^{3 \times 3}$. The final time is T = 1 and 804 the initial value is $\boldsymbol{y}^0 = [0, 0, 0]^{\top}$. First, we study the algorithms for system (5.2). 805 This is obtained by linearizing (5.1) around two different A_{\circ} , which are randomly 806 chosen approximations to A_{\star} , one with 1% and the other with 10% relative error, 807 meaning that, e.g., $\frac{\|A_* - A_0\|_F}{\|A_*\|_F} = 0.01$ for the one with 1% error, where $\|\cdot\|_F$ is the Frobenius norm. The LGR Algorithm 4.1 is run for two different choices for the basis 808 809 \mathcal{A} : the canonical basis of $\mathbb{R}^{3\times 3}$ and a basis consisting of 9 randomly generated (linearly 810 independent) 3×3 matrices. LGR is also compared with the OLGR Algorithm 7.2, 811 812 which is run with a set of 18 matrices, namely, the 9 canonical basis elements and the 9 random matrices. The controls generated by the respective algorithms are then used to 813 reconstruct the matrix A_{\star} by solving the online least-squares problem (3.3) with GN. 814 To test the robustness of the control functions, we consider a nine-dimensional sphere 815 centered in the global minimum A_{\star} and with given relative radius r, and repeat the 816

Algorithm 7.2 Optimized Greedy Reconstruction (OGR) Algorithm

Require: A set of K matrices $\mathcal{A} = \{A_1, \ldots, A_K\}$ and two tolerances $tol_1 > 0$ and $tol_2 > 0$.

1: Set $\boldsymbol{\epsilon}^0 = 0$ and compute $\boldsymbol{\epsilon}^1$ and the index ℓ_1 by solving the initialization problem

$$\max_{\ell \in \{1,...,K\}} \max_{\boldsymbol{\epsilon} \in E_{ad}} \|C\boldsymbol{y}(0,\boldsymbol{\epsilon};T) - C\boldsymbol{y}(A_{\ell},\boldsymbol{\epsilon};T)\|_{2}^{2}$$

- 2: Swap A_1 and A_{ℓ_1} in \mathcal{A} , and set k = 1 and $A^{(0)}(\boldsymbol{\beta}^{\ell_1}) = 0$. 3: while $k \leq K 1$ and $\left\| C \boldsymbol{y}(A^{(k-1)}(\boldsymbol{\beta}^{\ell_k}), \boldsymbol{\epsilon}^k; T) C \boldsymbol{y}(A_k, \boldsymbol{\epsilon}^k; T) \right\|_2^2 > \text{tol}_1$ do
- for $\ell = k + 1, \dots, K$ do 4:
- Orthogonalize all basis elements (A_{k+1}, \ldots, A_K) with respect to (A_1, \ldots, A_k) , re-5:move any that are linearly dependent and update K accordingly.
- Fitting step: Find $(\boldsymbol{\beta}_{i}^{\ell})_{j=1,\ldots,k}$ that solve the problem 6:

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^k} \sum_{m=1}^k \left\| C \boldsymbol{y}(A^{(k)}(\boldsymbol{\beta}), \boldsymbol{\epsilon}^m; T) - C \boldsymbol{y}(A_\ell, \boldsymbol{\epsilon}^m; T) \right\|_2^2$$

and set $f_{\ell} = \sum_{m=1}^{k} \left\| C \boldsymbol{y}(A^{(k)}(\boldsymbol{\beta}^{\ell}), \boldsymbol{\epsilon}^{m}; T) - C \boldsymbol{y}(A_{\ell}, \boldsymbol{\epsilon}^{m}; T) \right\|_{2}^{2}$

- 7: end for
- 8: if $\max_{\ell=k+1,\ldots,K} f_{\ell} > \operatorname{tol}_2$ then
- Set $\ell_{k+1} = \arg \max_{\ell=k+1,\dots,K} f_{\ell}$. 9:
- 10: else
- Extended splitting step: Find $\boldsymbol{\epsilon}^{k+1}$ and ℓ_{k+1} that solve the problem 11:

$$\max_{\ell \in \{k+1,\ldots,K\}} \max_{\boldsymbol{\epsilon} \in E_{ad}} \left\| C \boldsymbol{y}(A^{(k)}(\boldsymbol{\beta}^{\ell}), \boldsymbol{\epsilon}; T) - C \boldsymbol{y}(A_{\ell}, \boldsymbol{\epsilon}; T) \right\|_{2}^{2}$$

12:end if Swap A_{k+1} and $A_{\ell_{k+1}}$ in \mathcal{A} , and set k = k+1. 13:14: end while

minimization for 1000 initialization vectors randomly chosen on this sphere. We then 817 count the percentage of times that GN converges to the global solution $A_{\star} = A(\boldsymbol{\alpha}_{\star})$ 818 up to a tolerance of Tol = 0.005 (half of the smallest considered radius), meaning 819 that $\frac{\|A_{\star} - A(\boldsymbol{\alpha}_{comp})\|_{F}}{\|A_{\star}\|_{F}} \leq Tol$, where $\boldsymbol{\alpha}_{comp}$ denotes the solution computed by GN. 820 Repeating this experiment for different radii of the sphere, we obtain the results 821 reported in the two panels on the left in Figure 8.1. All control sets make GN capable 822 of reliably reconstructing the global minimum A_{\star} up to a relative radius r = 2, which 823 824 corresponds to a relative error of 200%. This demonstrates that the choice of the basis is not crucial for fully observable and controllable systems. However, OLGR 825 is able to reduce the number of controls down to 3 and still outperforms any set of 826 9 controls generated by LGR, while staying reliable up to a relative error of 250%. 827 828 Thus, OLGR is able to compute better basis, thereby optimizing the performance, and to omit unnecessary controls. 829

830 Next, we repeat the same experiments for the GR Algorithm 7.1. However, we replace the case for the approximation A_{\circ} with a relative error of 1% by $A_{\circ} = 0$. This 831 effectively removes the shift and makes the algorithm independent of the choice of A_{\circ} , 832 which is the version of the algorithm that was also considered in [11, 30] We obtain 833 the results shown in the two panels on the right in Figure 8.1. The performance of 834



Fig. 8.1: Percentage of runs that converged (up to a tolerance) to the global minimum A_{\star} starting from randomly chosen vectors on a nine-dimensional sphere with radius r, for controls generated by LGR and OLGR for 1% (top left) and 10% (bottom left) relative error between A_{\star} and A_{\circ} , and GR and OGR in the version of Algorithm 7.1 (bottom right) and without the shift by A_{\circ} (top right).

the control sets is similar to the ones for the linearized system, with an increase in performance for the GR algorithm with the canonical basis, without the shift by A_{\circ} , and a decrease in performance for the GR algorithm with the random basis and an A_{\circ} that has a 10% relative error with respect to A_{\star} . As in the linearized setting, OGR is able to reduce the number of controls down to 3 and still outperforms any set of 9 controls generated by LGR.

841 **8.2. Bilinear reconstruction problem.** Similar to [30] and [11], we consider a Schrödinger-type equation, written as a real system as in (6.6). We also use similar matrices H and μ^* as in [11], namely

844
$$H = H_R = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 8 & 0 \\ 0 & 0 & 16 \end{bmatrix}, \ \mu^* = \begin{bmatrix} -0.3243 & -3.4790 + 0.7359i & -0.5338 + 1.9254i \\ -3.4790 - 0.7359i & -3.8342 & -1.1697 + 2.0256i \\ -0.5338 - 1.9254i & -1.1697 - 2.0256i & 1.0551 \end{bmatrix}$$

The final time is $T = 10\pi$ and the initial state is $\boldsymbol{\psi}_0 = [1, 0, 0]^{\top}$. The observer matrix 845 is $C = [\psi_1, i\psi_1]$, which means that the final state is measured against the fixed state 846 $\boldsymbol{\psi}_1 = \frac{1}{\sqrt{3}} [1, 1, 1]^{\top}$. Again, we consider two bases, each consisting of 9 elements: the 847 canonical and a random one for the space of Hermitian matrices in $\mathbb{C}^{3\times 3}$. We then 848 perform the same experiments as in Section 8.1. The results are reported in Figure 8.2. 849 We observe that the radii, up to which the control sets make GN capable of reliably 850 reconstructing the global minimum, are much smaller than for the linear setting in 851 Section 8.1. When the initial relative error between $\mu_{\circ} = \mu(\boldsymbol{\alpha}_{\circ})$ and $\mu_{\star} = \mu(\boldsymbol{\alpha}_{\star})$ is 852 very small (1%) then LGR and OLGR have the most stable performance regarding the 853 854 choice of the basis, making GN capable of reliably reconstructing the global minimum μ_{\star} up to a relative error of 4-5%. However, when the initial relative error is larger 855 856 (10%) then only the LGR algorithm for the random basis can keep its performance, while even OLGR fails at errors of over 1%. The results for OGR, on the other hand, 857 show the best performance, with and without a shift by μ_{\circ} . The controls generated 858 by the GR algorithms can not match OGR or LGR and OLGR for small initial errors, 859 but are still more stable with respect to larger initial errors. 860



Fig. 8.2: Percentage of runs that converged (up to a tolerance) to the global minimum μ_{\star} starting from randomly chosen vectors on a nine-dimensional sphere with radius r, for controls generated by LGR and OLGR for 1% (top left) and 10% (bottom left) relative error between μ_{\star} and μ_{\circ} , and GR and OGR in the version of Algorithm 7.1 (bottom right) and without the shift by μ_{\circ} (top right).

9. Conclusion. In this paper, we developed and analyzed greedy reconstruction 861 algorithms based on the strategy presented in [30]. In particular, we tackled the case 862 of nonlinear problems consisting in the reconstruction of drift operators in linear and 863 bilinear dynamical systems. In these cases, we proved that the controls obtained 864 with the greedy algorithm on the corresponding linearized systems lead to the local 865 convergence of the classical Gauss-Newton method applied to the online nonlinear 866 identification problem. These results were extended to the controls obtained on the 867 868 fully nonlinear system (without linearization) where a local convergence result was also obtained. 869

Acknowledgements. G. Ciaramella is member of GNCS Indam. Simon Buchwald is funded by the DFG via the collaborative research center SFB1432, Project-ID
425217212. Julien Salomon acknowledges support from the ANR/RGC ALLOWAPP
project (ANR-19-CE46-0013/A-HKBU203/19).

874

REFERENCES

- [1] A. ALEXANDERIAN, N. PETRA, G. STADLER, AND O. GHATTAS, A fast and scalable method
 for A-optimal design of experiments for infinite-dimensional Bayesian nonlinear inverse
 problems, SIAM J. Sci. Comput., 38 (2016), pp. A243–A272.
- [2] C. D. ALIPRANTIS AND K. C. BORDER, Infinite Dimensional Analysis: a Hitchhiker's Guide, Springer, 2006.
- [3] P. J. ANTSAKLIS AND A. N. MICHEL, *Linear Systems*, Birkhäuser Basel, 2006.
- [4] A. C. ATKINSON, Optimum Experimental Design, Springer Berlin Heidelberg, 2011.
- [5] L. BAUDOUIN AND A. MERCADO, An inverse problem for Schrödinger equations with discontinuous main coefficient, Appl. Anal., 87 (2008), pp. 1145–1165.
- [6] F. BAUER AND C. FIKE, Norms and exclusion theorems, Numer. Math., 2 (1960), pp. 137–141.
- [7] I. BAUER, H. G. BOCK, S. KÖRKEL, AND J. P. SCHLÖDER, Numerical methods for optimum
 experimental design in dae systems, J. Comput. Appl. Math., 120 (2000), pp. 1 25.
- [8] C. BERGE, Topological spaces: including a treatment of multi-valued functions, vector spaces and convexity; Translated by E.M. Patterson, Oliver & Boyd Edinburgh, 1963.
- [9] S. BONNABEL, M. MIRRAHIMI, AND P. ROUCHON, Observer-based Hamiltonian identification for quantum systems, Automatica, 45 (2009), pp. 1144 – 1155.
- 891 [10] A. BORZÌ, G. CIARAMELLA, AND M. SPRENGEL, Formulation and Numerical Solution of Quan-

- 892 tum Control Problems, SIAM, Philadelphia, PA, 2017. 893 [11] S. BUCHWALD, G. CIARAMELLA, AND J. SALOMON, Analysis of a greedy reconstruction algo-894 rithm, SIAM J. Control Optim., 59 (2021), pp. 4511-4537. 895 [12] S. BUCHWALD, G. CIARAMELLA, AND J. SALOMON, Gauss-newton oriented greedy-type algo-896 rithms for the reconstruction of nonlinear operators: Supplementary material, (2023). 897 [13] S. BUCHWALD, G. CIARAMELLA, J. SALOMON, AND D. SUGNY, Greedy reconstruction algorithm 898 for the identification of spin distribution, Phys. Rev. A, 104 (2021), p. 063112. [14] P. G. CIARLET, Linear and Nonlinear Functional Analysis with Applications, Applied mathe-899 900 matics, SIAM, Philadelphia, PA, 2013. J. CORON, Control and Nonlinearity, Math. Surveys Monogr., AMS, 2007. 901 15 902 [16] B. DE SCHUTTER, Minimal state-space realization in linear system theory: An overview, J. 903 Comput. Appl. Math., 121 (2000), pp. 331-354. 904 [17] A. DONOVAN AND H. RABITZ, Exploring the Hamiltonian inversion landscape, Phys. Chem., 16 905 (2014), pp. 15615-15622. 906 [18] Y. FU AND G. TURINICI, Quantum Hamiltonian and dipole moment identification in presence 907 of large control perturbations, ESAIM: Contr. Optim. Ca., 23 (2017), pp. 1129–1143. [19] J. M. GEREMIA AND H. RABITZ, Global, nonlinear algorithm for inverting quantum-mechanical 908 909 observations, Phys. Rev. A, 64 (2001), p. 022710. 910 [20] J. M. GEREMIA AND H. RABITZ, Optimal Hamiltonian identification: The synthesis of quantum 911 optimal control and quantum inversion, J. Chem. Phys., 118 (2003), pp. 5369–5382. [21] J. M. GEREMIA, W. ZHU, AND H. RABITZ, Incorporating physical implementation concerns into 912 913 closed loop quantum control experiments, J. Chem. Phys., 113 (2000), pp. 10841–10848. 914 [22] E. GILBERT, Controllability and observability in multivariable control systems, J. SIAM Control 915 Ser. A, 1 (1963), pp. 128–151. 916 [23] S. GLASER AND ET AL, Training schrödinger's cat: quantum optimal control, Eur. Phys. J. D, 917 69 (2015), p. 279. 918 [24] R. A. HORN AND C. R. JOHNSON, Topics in Matrix Analysis, Cambridge Univ. Press, 1991. 919[25]J. N. JUANG AND R. S. PAPPA, An eigensystem realization algorithm for modal parameter 920identification and model reduction, J. Guid. Control Dynam., 8 (1985), pp. 620-627. 921 [26] B. KALTENBACHER, A. NEUBAUER, AND O. SCHERZER, Iterative Regularization Methods for 922 Nonlinear Ill-Posed Problems, De Gruyter, Berlin, New York, 2008. 923 C. T. KELLEY, Iterative Methods for Optimization, SIAM, Philadelphia, 1999. [27]924 [28] K. KOBZAR, T. E. SKINNER, N. KHANEJA, S. J. GLASER, AND B. LUY, Exploring the limits of 925 broadband excitation and inversion: Ii. rf-power optimized pulses, J. Magn. Reson., 194 926 (2008), pp. 58-66. 927 [29] C. LE BRIS, M. MIRRAHIMI, H. RABITZ, AND G. TURINICI, Hamiltonian identification for quantum systems: Well posedness and numerical approaches, ESAIM: Contr. Optim. Ca., 928 929 13 (2007), pp. 378–395.
- [30] Y. MADAY AND J. SALOMON, A greedy algorithm for the identification of quantum systems, in
 Proceedings of the 48th IEEE Conference on Decision and Control, , 2009, pp. 375–379.
- 932 [31] W. RUDIN, Real and Complex Analysis, 3rd Ed., McGraw-Hill, Inc., USA, 1987.
- [32] E. D. SONTAG, Mathematical Control Theory: Deterministic Finite Dimensional Systems (2Nd B34
 Ed.), Springer-Verlag, Berlin, Heidelberg, 1998.
- [33] M. TADI AND H. RABITZ, Explicit method for parameter identification, J. Guid. Control Dyn.,
 20 (1997), pp. 486–491.
- [34] Y. WANG, D. DONG, B. QI, J. ZHANG, I. R. PETERSEN, AND H. YONEZAWA, A quantum
 Hamiltonian identification algorithm: Computational complexity and error analysis, IEEE
 Trans. Autom. Control, 63 (2018), pp. 1388–1403.
- 940
 [35] E. F. WHITTLESEY, Analytic functions in Banach spaces, Proceedings of the American Math-941

 941
 ematical Society, 16 (1965), pp. 1077–1083.
- [36] S. XUE, R. WU, D. LI, AND M. JIANG, A gradient algorithm for Hamiltonian identification of open quantum systems, Phys. Rev. A, 103 (2021), p. 022604.
- [37] J. ZHANG AND M. SAROVAR, Quantum Hamiltonian identification from measurement time
 traces, Phys. Rev. Lett., 113 (2014), p. 080401.
- [38] W. ZHOU, S. SCHIRMER, E. GONG, H. XIE, AND M. ZHANG, Identification of Markovian open system dynamics for qubit systems, Chinese Sci. Bull., 57 (2012), pp. 2242–2246.
- [39] W. ZHU AND H. RABITZ, Potential surfaces from the inversion of time dependent probability density data, J. Chem. Phys., 111 (1999), pp. 472–480.

MOX Technical Reports, last issues

Dipartimento di Matematica Politecnico di Milano, Via Bonardi 9 - 20133 Milano (Italy)

- **08/2023** Bonizzoni, F.; Hu, K.; Kanschat, G.; Sap, D. Discrete tensor product BGG sequences: splines and finite elements
- 07/2023 Garcia-Contreras, G.; Còrcoles, J.; Ruiz-Cruz, J.A.; Oldoni, M; Gentili, G.G.; Micheletti, S.;
 Perotto, S.
 Advanced Modeling of Rectangular Waveguide Devices with Smooth Profi les by Hierarchical Model Reduction
- **06/2023** Artoni, A.; Antonietti, P. F.; Mazzieri, I.; Parolini, N.; Rocchi, D. A segregated finite volume - spectral element method for aeroacoustic problems
- **05/2023** Fumagalli, I.; Vergara, C. Novel approaches for the numerical solution of fluid-structure interaction in the aorta
- **04/2023** Quarteroni, A.; Dede', L.; Regazzoni, F.; Vergara, C. A mathematical model of the human heart suitable to address clinical problems
- **03/2023** Africa, P.C.; Perotto, S.; de Falco, C. Scalable Recovery-based Adaptation on Quadtree Meshes for Advection-Diffusion-Reaction Problems
- **01/2023** Zingaro, A.; Bucelli, M.; Piersanti, R.; Regazzoni, F.; Dede', L.; Quarteroni, A. *An electromechanics-driven fluid dynamics model for the simulation of the whole human heart*
- **02/2023** Boon, W. M.; Fumagalli, A.; Scotti, A. *Mixed and multipoint finite element methods for rotation-based poroelasticity*
- **83/2022** Ciaramella, G.; Gander, M.; Mazzieri, I. Unmapped tent pitching schemes by waveform relaxation
- **82/2022** Ciaramella, G.; Gander, M.; Van Criekingen, S.; Vanzan, T. A PETSc Parallel Implementation of Substructured One- and Two-level Schwarz Methods