#### PBDW METHOD FOR STATE ESTIMATION: ERROR ANALYSIS 2 FOR NOISY DATA AND NONLINEAR FORMULATION\*

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Abstract. We present an error analysis and further numerical investigations of the Parameter-4 ized-Background Data-Weak (PBDW) formulation to variational Data Assimilation (state estima-5 6 tion), proposed in [Y Maday, AT Patera, JD Penn, M Yano, Int J Numer Meth Eng, 102(5), 933-965]. 7 The PBDW algorithm is a state estimation method involving reduced models. It aims at approximating an unknown function  $u^{\text{true}}$  living in a high-dimensional Hilbert space from M measurement 8 9 observations given in the form  $y_m = \ell_m(u^{\text{true}}), m = 1, \ldots, M$ , where  $\ell_m$  are linear functionals. The method approximates  $u^{\text{true}}$  with  $\hat{u} = \hat{z} + \hat{\eta}$ . The background  $\hat{z}$  belongs to an N-dimensional linear 10 space  $\mathcal{Z}_N$  built from reduced modelling of a parameterized mathematical model, and the update  $\hat{\eta}$ 11 belongs to the space  $\mathcal{U}_M$  spanned by the Riesz representers of  $(\ell_1, \ldots, \ell_M)$ . When the measurements 12 are noisy, — i.e.,  $y_m = \ell_m(u^{\text{true}}) + \epsilon_m$  with  $\epsilon_m$  being a noise term — the classical PBDW formu-13 14 lation is not robust in the sense that, if N increases, the reconstruction accuracy degrades. In this paper, we propose to address this issue with an extension of the classical formulation, which consists 15 in searching for the background  $\hat{z}$  either on the whole  $\mathcal{Z}_N$  in the noise-free case, or on a well-chosen 1617 subset  $\mathcal{K}_N \subset \mathcal{Z}_N$  in presence of noise. The restriction to  $\mathcal{K}_N$  makes the reconstruction be nonlinear 18 and is the key to make the algorithm significantly more robust against noise. We further present 19an a priori error and stability analysis, and we illustrate the efficiency of the approach on several 20 numerical examples.

21Key words. variational data assimilation; parameterized partial differential equations; model 22order reduction.

#### 23 AMS subject classifications. 62-07, 93E24

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1. Introduction. Let  $\mathcal{U}$  be a Hilbert space defined over a domain  $\Omega \subset \mathbb{R}^d$  and equipped with inner product  $(\cdot, \cdot)$  and induced norm  $\|\cdot\| = \sqrt{(\cdot, \cdot)}$ . In this paper, we consider the following state estimation problem: we want to recover an unknown function  $u^{\text{true}} \in \mathcal{U}$  that represents the state of a physical system of interest from M measurements given in the form

$$y_m = \ell_m(u^{\text{true}}) + \epsilon_m \quad m = 1, \dots, M,$$

where  $\ell_1 \ldots, \ell_M$  are M independent linear functionals over  $\mathcal{U}$  and  $\epsilon_1, \ldots, \epsilon_M$  reflect the experimental noise. In the following, we gather in the vector

$$\mathbf{y} = [y_1, \dots, y_M]^T \in \mathbb{R}^M$$

the set of measurement data. 24

Several authors have proposed to exploit Bayesian approaches [14, 23, 9] that 25consist in adding certain prior assumptions and then searching through the most 26plausible solution through sampling strategies of the posterior density. Since this 2728 is very costly in a high-dimensional framework, approaches involving dimensionality

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29 reduction techniques have become a very active research field in recent years. Our

focus lies on strategies involving reduced modelling of parameterized PDEs for which a number of different approaches have been proposed in recent years, see [15, 16, 17, 13,

32 3]. Note, however, that other compression approaches are possible and, in particular,

33 we cite the works of [1, 5] in the field of signal processing and compressive sensing, 34 which share similarities with the main ideas propagated in the reduced modelling 35 approach as well.

Our starting point is the so-called Parameterized-Background Data-Weak method (PBDW) that was originally introduced in [17]. The method has been further developed and analyzed in several works. We cite [6, 8] for relevant works on the theoretical front, [7] for works on sensor placement. The methodology has been applied to nontrivial applications in [17, 12, 11] and an analysis on how the method can be used as a vehicle to find optimal sensor locations can be found in [7]. Our paper is devoted to the topic of the noise in measurements for which previous works are [18, 25, 24]. We outline our contribution on this topic in what follows.

The PBDW method exploits the knowledge of a parameterized best-knowledge (bk) model that describes the physical system, to improve performance. We denote by  $u^{bk}(\mu) \in \mathcal{U}$ , the solution to the parameterized model for the parameter value  $\mu \in \mathcal{P}^{bk}$ ,

$$G^{\mathrm{bk},\mu}(u^{\mathrm{bk}}(\mu)) = 0.$$

Here,  $G^{\mathrm{bk},\mu}(\cdot)$  denotes the parameterized bk model associated with the system, and  $\mathcal{P}^{\mathrm{bk}} \subset \mathbb{R}^P$  is a compact set that reflects the lack of knowledge in the value of the parameters of the model. We further define the bk manifold

$$\mathcal{M}^{\mathrm{bk}} = \{ u^{\mathrm{bk}}(\mu) : \, \mu \in \mathcal{P}^{\mathrm{bk}} \},\,$$

which collects the solution to the bk model for all values of the parameter. Note that 44 45 here, for simplicity of exposition, the model is defined over  $\Omega$ : in [26], the authors considered the case in which the model is defined over a domain  $\Omega^{bk}$  that strictly 46contains the domain of interest  $\Omega$ . We here intend, but we do not assume, that  $u^{\text{true}}$ 47 is close to the bk manifold: there exists  $\mu^{\text{true}} \in \mathcal{P}^{\text{bk}}$  such that  $\|u^{\text{true}} - u^{\text{bk}}(\mu^{\text{true}})\|$ 48is small. In our state estimation problem, we are given the vector  $\mathbf{y} \in \mathbb{R}^M$  of mea-49surement data but the value of  $\mu^{\text{true}}$  is unknown so we cannot simply run a forward 50computation to approximate  $u^{\text{true}}$  with  $u^{\text{bk}}(\mu^{\text{true}})$ . That is why we refer to the lack of knowledge of the value of  $\mu^{\text{true}}$  as to anticipated or parametric ignorance. On the 52other hand, we refer to  $\inf_{\mu \in \mathcal{P}^{bk}} \|u^{true} - u^{bk}(\mu)\|$  as to unanticipated or nonparametric 53 model error. 54

The PBDW method seeks an approximation

$$\hat{u} = \hat{z} + \hat{\eta}$$

employing projection by data. For perfect measurements, that is  $\epsilon_m = 0$ ,  $m = 1, \ldots, M$ , the estimate  $\hat{u}$  is built by searching  $\hat{\eta}$  of minimum norm subject to the observation constraints  $\ell_m(\hat{u}) = y_m$  for  $m = 1, \ldots, M$ . In presence of noise, PBDW can be formulated as a Tikhonov regularization of the perfect-measurement statement that depends on an hyper-parameter  $\xi > 0$  which should be tuned using out-ofsample data. We refer to the above mentioned literature (see in particular [17, 25]) for a detailed discussion of the connections between PBDW and other existing state estimation techniques. 63 The first contribution to  $\hat{u}$ , is the *deduced background estimate*, (1,1)

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$$\hat{z} = \sum_{n=1}^{N} \hat{z}_n \zeta_n \in \mathcal{K}_N = \left\{ \sum_{n=1}^{N} z_n \zeta_n : \mathbf{z} = [z_1, \dots, z_N]^T \in \Phi_N \right\} \subset \mathcal{Z}_N := \operatorname{span}\{\zeta_n\}_{n=1}^N,$$

where  $\mathcal{Z}_N$  is an *N*-dimensional linear space spanned by the basis  $\{\zeta_n\}_{n=1}^N$ , and  $\mathcal{K}_N \subseteq \mathcal{Z}_N$  is a subset of  $\mathcal{Z}_N$ . The space  $\mathcal{Z}_N$  is built based on the bk manifold  $\mathcal{M}^{\mathrm{bk}}$  and summarizes two approximations:

- (i) the approximation coming from the model, which suffers from a bias (*unan-ticipated model error*),
- (ii) the approximation of the elements of  $\mathcal{M}^{bk}$  due to the finite dimension N of  $\mathcal{Z}_N$ .

Note that, while the second approximation can be systematically improved by increas-72 ing N, the first one is incompressible and inherent to the choice of the model. One of 73 the novelties with respect to previous works on noise is that we restrict the search of 74  $\hat{z}$  to a well-chosen subset  $\mathcal{K}_N$  of  $\mathcal{Z}_N$ . The information that is encoded in  $\mathcal{K}_N$  reflects 75some "learning" acquisition on the behavior of the coefficients  $\hat{\mathbf{z}} = [\hat{z}_1, \dots, \hat{z}_N]^T$  of the 76 solutions to the best-knowledge model when the parameter varies. The relevance of 77 this set is a more complete formalization of the decrease of the Kolmogorov thickness 78 and of course depends on the proper choice of the reduced basis  $\{\zeta_n\}_{n=1}^N$ . We will see 79 further how this can be taken into account. As shown later in the paper, the state 80 estimate  $\hat{u}$  is a linear function of the measurements **y** if and only if  $\Phi_N = \mathbb{R}^N$  (i.e., 81  $\mathcal{K}_N = \mathcal{Z}_N$ : for this reason, we refer to the case  $\Phi_N = \mathbb{R}^N$  as linear PBDW, and to 82 the case  $\Phi_N \subsetneq \mathbb{R}^N$  (i.e.,  $\mathcal{K}_N \subsetneq \mathcal{Z}_N$ ) as nonlinear PBDW. 83

The second term in  $\hat{u}, \hat{\eta} \in \mathcal{U}_M$  is the *update estimate*: the linear *M*-dimensional space  $\mathcal{U}_M$  is the span of Riesz representers  $q_1, \ldots, q_M \in \mathcal{U}$  of the *M* observation functionals  $\{\ell_m\}_{m=1}^M$ ,

$$\mathcal{U}_M \coloneqq \operatorname{span}\{q_m\}_{m=1}^M, \qquad (q_m, v) = \ell_m(v) \quad \forall v \in \mathcal{U}.$$

The background  $\hat{z}$  addresses the lack of knowledge in the value of the model parameters, while the update  $\hat{\eta}$  accomodates the non-parametric model error.

86 The contributions of the present work are twofold.

(i) We present a complete *a priori* error analysis of linear PBDW, and we present 87 a stability analysis for the nonlinear case. More in detail, we present an error 88 analysis for general linear recovery algorithms, which relies on the definition of 89 three computable constants; we specialize our analysis to linear PBDW; and 90 we present, once again for linear PBDW, two optimality results that motivate 91 our approach. Furthermore, for the nonlinear case, we prove that, if  $\Phi_N$  is 92 convex, small perturbations in the measurements lead to small perturbations in the state estimate. As explained in section 3, in the linear case, our analysis 94 is based on an extension of the framework presented in [5] to a broader class 95 of linear recovery algorithms. The extension is necessary since linear PBDW 96 does not belong to the recovery class of [5]. For the analysis of the nonlinear 97 case, we use tools originally developed in the inverse problem literature (see, 98 e.g., [10]). 99

(ii) We present several numerical results that empirically motivate the introduction of the constraints for the background coefficients  $\hat{\mathbf{z}}$  (i.e.,  $\Phi_N \subsetneq \mathbb{R}^N$ ). We consider the specific case where  $\Phi_N = \bigotimes_{n=1}^N [a_n, b_n]$  and  $\{a_n, b_n\}_n$  are estimated based on the bk manifold. We present numerical investigations of

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104 the stability of the formulation as a function of (i) the hyper-parameter  $\xi$ 105 associated with the regularizer, (ii) the background dimension N, and (iii) 106 the measurement locations. Note that the idea of introducing box constraints 107 has originally been introduced in [4] to stabilize the Generalized Empirical 108 Interpolation Method in presence of noise (GEIM, [15]). In this respect, the 109 present paper can be understood as an extension of the latter methodology 110 to PBDW.

The paper is organized as follows. In section 2, we present the PBDW method: 111 we discuss the well-posedness of the mathematical formulation, and we present the 112actionable algebraic form which is used in the numerical implementation. In section 113 3, we present the analysis of the method: we here discuss the error analysis for linear 114 115 PBDW and the stability bound for the nonlinear case. To simplify the exposition, in sections 2 and 3 we consider real-valued problems; the extension to the complex-116 valued case is straightforward and is briefly outlined at the end of section 2. In section 117 4 we present several numerical results for a two-dimensional and a three-dimensional 118model problem, and in section 5 we draw some conclusions. 119

## 120 **2.** Formulation.

**2.1. PBDW statement.** In view of the presentation of the PBDW formulation,
 we recall the definition of the experimental measurements

123 (2.1) 
$$y_m = \ell_m(u^{\text{true}}) + \epsilon_m, \quad m = 1, ..., M,$$

where  $\{\ell_m\}_{m=1}^M \subset \mathcal{U}'$  and  $\{\epsilon_m\}_{m=1}^M$  are unknown disturbances, and of the parameterized bk mathematical model

126 (2.2) 
$$G^{bk,\mu}(u^{bk}(\mu)) = 0,$$

127 where  $\mu$  corresponds to the set of uncertain parameters in the model and belongs to 128 the compact set  $\mathcal{P}^{bk} \subset \mathbb{R}^{P}$ . We here assume that  $G^{bk,\mu}$  is well-posed for all  $\mu \in \mathcal{P}^{bk}$ 129 over a domain  $\Omega^{bk}$  that contains  $\Omega$ ; we further assume that the restriction of  $u^{bk}(\mu)$ 130 to  $\Omega$ ,  $u^{bk}(\mu)|_{\Omega}$ , belongs to  $\mathcal{U}$ . Then, we introduce the rank-N approximation of  $u^{bk}|_{\Omega}$ , 131  $u_{N}^{bk}(\mu)|_{\Omega} = \sum_{n=1}^{N} z_{n}^{bk}(\mu)\zeta_{n}$ , and we denote by  $\Phi_{N} \subset \mathbb{R}^{N}$  a suitable bounding box of 132 the set  $\{\mathbf{z}^{bk}(\mu) : \mu \in \mathcal{P}^{bk}\}$ .

We can now introduce the PBDW statement: find  $\hat{u}_{\xi} = \sum_{n=1}^{N} (\hat{\mathbf{z}}_{\xi})_n \zeta_n + \hat{\eta}_{\xi}$  such that  $(\hat{\mathbf{z}}_{\xi}, \hat{\eta}_{\xi}) \in \Phi_N \times \mathcal{U}$  minimizes

135 (2.3) 
$$\min_{(\mathbf{z},\eta)\in\Phi_N\times\mathcal{U}}\mathcal{J}_{\xi}(\mathbf{z},\eta) := \xi \|\eta\|^2 + \left\|\boldsymbol{\ell}\left(\sum_{n=1}^N z_n\zeta_n + \eta\right) - \mathbf{y}\right\|_2^2,$$

with  $\boldsymbol{\ell} = [\ell_1, \dots, \ell_M]^T : \boldsymbol{\mathcal{U}} \to \mathbb{R}^M$ , and where  $\|\cdot\|_2$  is the Euclidean  $\ell^2$ -norm in  $\mathbb{R}^N$ . For reasons that will become clear soon, we further introduce the limit formulations:

138 (2.4) 
$$(\hat{\mathbf{z}}_0, \hat{\eta}_0) \in \arg\min_{(\mathbf{z}, \eta) \in \Phi_N \times \mathcal{U}} \|\eta\|, \text{ subject to } \boldsymbol{\ell}\left(\sum_{n=1}^N z_n \zeta_n + \eta\right) = \mathbf{y};$$

139 and

140 (2.5) 
$$\hat{\mathbf{z}}_{\infty} \in \arg\min_{\mathbf{z}\in\Phi_{N}} \left\| \boldsymbol{\ell}\left(\sum_{n=1}^{N} z_{n}\zeta_{n}\right) - \mathbf{y} \right\|_{2}^{2}.$$

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We anticipate that (2.4) and (2.5) can be rigorously linked to (2.3): we address this issue in the next section.

We shall now interpret the PBDW statement introduced above. The first term 143 in (2.3) penalizes the distance of the state estimate from the set  $\mathcal{K}_N$  defined in (1.1), 144which is an approximation of the bk solution manifold  $\mathcal{M}^{bk}$ ; the second term penalizes 145 the data misfit; finally, the hyper-parameter  $\xi > 0$  regulates the relative importance 146 of the background compared to the data. We remark that PBDW can be interpreted 147as a relaxation of the Partial Spline Model presented in [28]: we refer to [24, section 1482 and [19, section 2] for a detailed derivation. We further observe that in (2.3) we 149consider the  $\ell^2$  loss,  $V_M(\cdot) = \|\cdot\|_2^2$ , to penalize the data misfit: in presence of a priori 150information concerning the properties of the measurement noise, other loss functions 151152could also be considered.

Model order reduction techniques for data compression are here employed to 153generate the background space  $\mathcal{Z}_N = \operatorname{span}\{\zeta_n\}_{n=1}^N$  from the bk manifold. We refer to 154[17] and to the references therein for a detailed discussion; we further refer to [26] for 155the construction of local approximation spaces when  $\Omega$  is strictly contained in  $\Omega^{bk}$ . 156On the other hand,  $\Phi_N \subset \mathbb{R}^N$  is built by exploiting (estimates of) snapshots of the 157bk solution manifold for selected values of the parameters  $\mu^1, \ldots, \mu^{n_{\text{train}}} \in \mathcal{P}^{\text{bk}}$ . In particular, we here consider two choices for  $\Phi_N$ :  $\Phi_N = \mathbb{R}^N$  and  $\Phi_N = \bigotimes_{n=1}^N [a_n, b_n]$ . 158 159In the former case, it is easy to verify that PBDW reduces to the original linear 160 algorithm of [17], while for the second case we anticipate that computation of the 161 state estimate requires the solution to a quadratic programming problem with box 162 163constraints. We defer the detailed description of the definition of  $\{a_n, b_n\}_n$  to the numerical examples presented in section 4. 164

**2.2. Finite-dimensional formulation and limit cases.** We introduce the matrices

$$\mathbf{L} = (\mathbf{L}_{m,n})_{\substack{1 \le m \le M \\ 1 \le n \le N}} \in \mathbb{R}^{M,N}, \quad \mathbf{L}_{m,n} = \ell_m(\zeta_n)$$

and

$$\mathbf{K} = (\mathbf{K}_{m,m'})_{1 \le m, m' \le M} \in \mathbb{R}^{M,M}, \quad \mathbf{K}_{m,m'} = (q_m, q_{m'})$$

In the remainder of this work, we assume that

 $M \ge N.$ 

Given a symmetric positive definite matrix  $\mathbf{W} \in \mathbb{R}^{M,M}$ , we define the weighted norm  $\|\cdot\|_{\mathbf{W}}$ , such that for all  $\mathbf{y} \in \mathbb{R}^M$  we have  $\|\mathbf{y}\|_{\mathbf{W}} := \sqrt{\mathbf{y}^T \mathbf{W} \mathbf{y}}$ , and we denote by  $\lambda_{\min}(\mathbf{W})$  and  $\lambda_{\max}(\mathbf{W})$  the minimum and maximum eigenvalues of  $\mathbf{W}$ . Proposition 2.1 summarizes key properties of the PBDW formulation stated in the previous section. The proof is provided in Appendix A.

170 PROPOSITION 2.1. Let  $\ell_1, \ldots, \ell_M \in \mathcal{U}'$  be linear independent. Let  $\hat{u}_{\xi} = \sum_{n=1}^{N} (\hat{\mathbf{z}}_{\xi})_n \zeta_n + \hat{\eta}_{\xi}$  be a solution to (2.3) for  $\xi > 0$ , and let  $\hat{u}_0 = \sum_{n=1}^{N} (\hat{\mathbf{z}}_0)_n \zeta_n + \hat{\eta}_0$  be a solution to (2.4). Then, the following hold.

- 173 1. The updates  $\hat{\eta}_{\xi}$  and  $\hat{\eta}_0$  belong to the space  $\mathcal{U}_M = \operatorname{span}\{q_m\}_{m=1}^M$ .
- 174 2. The vector of coefficients  $\hat{\mathbf{z}}_{\xi}$  associated with the deduced background solves the 175 least-squares problem:

176 (2.6a) 
$$\min_{\mathbf{z}\in\Phi_N} \|\mathbf{L}\mathbf{z}-\mathbf{y}\|_{\mathbf{W}_{\xi}}, \text{ where } \mathbf{W}_{\xi} := (\xi\mathbf{Id}+\mathbf{K})^{-1},$$

177 where **Id** is the identity matrix;  $\hat{\eta}_{\xi}$  is the unique solution to

178 (2.6b) 
$$\min_{\eta \in \mathcal{U}_M} \xi \|\eta\|^2 + \|\boldsymbol{\ell}(\eta) - \mathbf{y}^{\mathrm{err}}(\hat{\mathbf{z}}_{\xi})\|_2^2, \quad \text{where } \mathbf{y}^{\mathrm{err}}(\mathbf{z}) := \mathbf{y} - \mathbf{L}\mathbf{z}.$$

179 In addition, the solution  $(\hat{\mathbf{z}}_0, \hat{\eta}_0)$  to (2.4) solves

180 (2.7) 
$$\begin{cases} \min_{\mathbf{z}\in\Phi_N} \|\mathbf{L}\mathbf{z}-\mathbf{y}\|_{\mathbf{K}^{-1}},\\ \min_{\eta\in\mathcal{U}_M} \|\eta\|, \quad \text{subject to } \boldsymbol{\ell}(\eta) = \mathbf{y}^{\text{err}}(\hat{\mathbf{z}}_0). \end{cases}$$

181 3. Any solution  $\hat{\mathbf{z}}_{\xi}$  to (2.3) satisfies

182 (2.8a) 
$$\|\mathbf{L}\hat{\mathbf{z}}_{\xi} - \mathbf{y}\|_{2}^{2} \leq \frac{\xi + \lambda_{\max}(\mathbf{K})}{\xi + \lambda_{\min}(\mathbf{K})} \min_{\mathbf{z} \in \Phi_{N}} \|\mathbf{L}\mathbf{z} - \mathbf{y}\|_{2}^{2},$$

183 and

184 (2.8b) 
$$\|\mathbf{L}\hat{\mathbf{z}}_{\xi} - \mathbf{y}\|_{\mathbf{K}^{-1}}^2 \leq \frac{\lambda_{\max}(\mathbf{K})}{\lambda_{\min}(\mathbf{K})} \left(\frac{\xi + \lambda_{\min}(\mathbf{K})}{\xi + \lambda_{\max}(\mathbf{K})}\right) \min_{\mathbf{z} \in \Phi_N} \|\mathbf{L}\mathbf{z} - \mathbf{y}\|_{\mathbf{K}^{-1}}^2.$$

185 Furthermore, the optimal update  $\hat{\eta}_{\xi}$  satisfies

186 (2.9) 
$$\|\hat{\eta}_{\xi}\|^2 \leq \frac{1}{\xi} \min_{\mathbf{z} \in \Phi_N} \|\mathbf{L}\mathbf{z} - \mathbf{y}\|_2^2; \quad \|\boldsymbol{\ell}(\hat{\eta}_{\xi}) + \mathbf{L}\hat{\mathbf{z}}_{\xi} - \mathbf{y}\|_2^2 \leq \xi \|\hat{\eta}_0\|^2.$$

- 187 4. If **L** is full rank, any solution to (2.3) is bounded for any choice of  $\Phi_N$  and 188 for any  $\xi > 0$ .
- 189 5. If  $\Phi_N$  is convex and **L** is full rank, then the solution to (2.3) is unique for 190 any  $\xi > 0$ .

191 Estimates (2.8) can be used to prove rigorous links between (2.3) and the limit 192 cases (2.4) and (2.5): we state the formal result in the following corollary, which is an 193 extension of [24, Proposition 2.9]. Motivated by this corollary, with some abuse of no-194 tation, we extend the PBDW formulation (2.3) to  $\xi \in [0, \infty]$ , with the understanding 195 that  $\xi = 0$  corresponds to (2.4) and  $\xi = \infty$  corresponds to (2.5).

196 COROLLARY 2.2. Given the sequence  $\{\xi_i\}_{i=1}^{\infty}$  such that  $\xi_i > 0$ , we define the 197 sequence of solutions  $\{(\hat{\mathbf{z}}_i, \hat{\eta}_i) := (\hat{\mathbf{z}}_{\xi_i}, \hat{\eta}_{\xi_i})\}_{i=1}^{\infty}$  to (2.3). Then, if **L** is full rank with 198  $M \ge N$ , the following hold: (i) if  $\xi_i \to \infty$ , then  $\hat{\eta}_i \to 0$  and any limit point of  $\{\hat{\mathbf{z}}_i\}_{i=1}^{\infty}$ 199 is a solution to (2.5); (ii) if  $\xi_i \to 0$ , then any limit point of  $\{(\hat{\mathbf{z}}_i, \hat{\eta}_i)\}_{i=1}^{\infty}$  is a solution 200 to (2.4); and (iii) if  $\Phi_N$  is convex, then the solution map  $\xi \mapsto (\hat{\mathbf{z}}_{\xi}, \hat{\eta}_{\xi})$  is continuous 201 in  $[0, \infty]$ .

*Proof.* We here prove the first statement. The proofs of the second and of the third statements follow similar ideas. Since **L** is full rank and **K** is invertible, exploiting (2.8a) and (2.9), there exists  $C < \infty$  such that

$$\sup_{i} \|\hat{\mathbf{z}}_{i}\|_{2}, \ \sup_{i} \xi_{i} \|\hat{\eta}_{i}\|_{2} \le C.$$

This implies that  $\hat{\eta}_i \to 0$ , while, applying Bolzano-Weierstrass theorem, we find that  $\{\hat{\mathbf{z}}_i\}_i$  admits convergent subsequences. Let  $\hat{\mathbf{z}}^*$  be a limit of point of  $\{\hat{\mathbf{z}}_i\}_i$ ; then by taking the limit in (2.8a), we obtain

$$\|\mathbf{L}\hat{\mathbf{z}}^{\star} - \mathbf{y}\|_{2}^{2} \leq \limsup_{i \to \infty} \|\mathbf{L}\hat{\mathbf{z}}_{i} - \mathbf{y}\|_{2}^{2} \leq \min_{\mathbf{z} \in \Phi_{N}} \|\mathbf{L}\mathbf{z} - \mathbf{y}\|_{2}^{2},$$

202 which proves the first statement.

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For non-convex domains  $\Phi_N$ , the solution to (2.3) is not in general unique: for this reason, we here restrict our attention to the case in which  $\Phi_N$  is convex. We thus specialize (2.6) to the two choices of  $\Phi_N$  considered in this work. For  $\Phi_N = \mathbb{R}^N$ , the vector  $\hat{\mathbf{z}}_{\xi}$  solves the linear problem:

207 (2.10a) 
$$\mathbf{L}^T \mathbf{W}_{\boldsymbol{\xi}} \mathbf{L} \, \hat{\mathbf{z}}_{\boldsymbol{\xi}} = \mathbf{L}^T \mathbf{W}_{\boldsymbol{\xi}} \mathbf{y}.$$

while the vector  $\hat{\eta}_{\xi}$  associated with the update  $\hat{\eta}_{\xi}$ ,  $\hat{\eta}_{\xi} = \sum_{m=1}^{M} (\hat{\eta}_{\xi})_m q_m$ , satisfies

209 (2.10b) 
$$(\mathbf{K} + \xi \mathbf{Id}) \ \hat{\boldsymbol{\eta}}_{\xi} = \mathbf{y} - \mathbf{L} \, \hat{\mathbf{z}}_{\xi}.$$

Note that in this case there exists a linear map between the data  $\mathbf{y}$  and the solution  $\hat{u}_{\xi}$ . We further observe that the update  $\hat{\eta}_{\xi}$  belongs to  $\mathcal{Z}_N^{\perp} \cap \mathcal{U}_M$  (see [25, Proposition 2.2.2]), where  $\mathcal{Z}_N^{\perp}$  is the orthogonal complement of  $\mathcal{Z}_N$ . On the other hand, for  $\Phi_N = \bigotimes_{n=1}^N [a_n, b_n]$ ,  $\hat{\mathbf{z}}_{\xi}$  solves the quadratic programming problem:

(2.11)  
214 
$$\min_{\mathbf{z}\in\mathbb{R}^{N}} \frac{1}{2} \mathbf{z}^{T} \left( \mathbf{L}^{T} \mathbf{W}_{\xi} \mathbf{L} \right) \mathbf{z} - \mathbf{z}^{T} \mathbf{L}^{T} \mathbf{W}_{\xi} \mathbf{y}, \text{ subject to } a_{n} \leq z_{n} \leq b_{n}, \quad n = 1, \dots, N;$$

which can be easily solved with classical optimization methods. The update  $\hat{\eta}_{\xi}$  can be computed using (2.6b) as for the linear case. Note that in this case the map between data and state estimate is nonlinear, and the update  $\hat{\eta}_{\xi}$  does not in general belong<sup>1</sup> to  $\mathcal{Z}_{N}^{\perp} \cap \mathcal{U}_{M}$ . As anticipated in the introduction, we refer to (2.3) with  $\Phi_{N} = \mathbb{R}^{N}$  as to linear PBDW, and we refer to (2.3) with  $\Phi_{N} = \bigotimes_{n=1}^{N} [a_{n}, b_{n}]$  as to nonlinear PBDW.

220 Remark 2.3. We can easily extend the previous developments to complex-valued 221 problems. If  $\mathcal{U}$  is a space of complex-valued functions, the measurements  $y_1, \ldots, y_M \in$ 222  $\mathbb{C}$  and  $\Phi_N = \mathbb{C}^N$ , we can find the counterpart of (2.10):

223 (2.12) 
$$\mathbf{L}^{H}\mathbf{W}_{\xi}\mathbf{L}\,\hat{\mathbf{z}}_{\xi} = \mathbf{L}^{H}\mathbf{W}_{\xi}\mathbf{y}, \qquad (\mathbf{K} + \xi\mathbf{Id})\,\,\hat{\boldsymbol{\eta}}_{\xi} = \mathbf{y} - \mathbf{L}\,\hat{\mathbf{z}}_{\xi};$$

where  $(\cdot)^{H}$  denotes the Hermitian conjugate. For the nonlinear case, if we set

$$\Phi_N = \left\{ \mathbf{z}^{\mathrm{re}} + \mathrm{i}\mathbf{z}^{\mathrm{im}} : \mathbf{z}^{\mathrm{re}} \in \bigotimes_{n=1}^N [a_n, b_n], \ \mathbf{z}^{\mathrm{im}} \in \bigotimes_{n=1}^N [a_{n+N}, b_{n+N}], \right\}$$

224 for some  $\{a_n, b_n\}_{n=1}^{2N}$ , it is easy to obtain that  $\widehat{\mathbf{z}}_{\xi}^{\star} = [\operatorname{Re}\{\widehat{\mathbf{z}}_{\xi}\}, \operatorname{Im}\{\widehat{\mathbf{z}}_{\xi}\}] \in \mathbb{R}^{2N}$  solves

225 (2.13a) 
$$\min_{\mathbf{z}\in\mathbb{R}^{2N}} \frac{1}{2}\mathbf{z}^T \mathbf{H} \mathbf{z} - \mathbf{f}^T \mathbf{z} \text{ subject to } a_n \leq z_n \leq b_n, \quad n = 1, \dots, 2N;$$

226 where

227 (2.13b) 
$$\mathbf{H} = \begin{bmatrix} \operatorname{Re}\{\mathbf{L}^{H}\mathbf{W}_{\xi}\mathbf{L}\} & -\operatorname{Im}\{\mathbf{L}^{H}\mathbf{W}_{\xi}\mathbf{L}\} \\ \operatorname{Im}\{\mathbf{L}^{H}\mathbf{W}_{\xi}\mathbf{L}\} & \operatorname{Re}\{\mathbf{L}^{H}\mathbf{W}_{\xi}\mathbf{L}\} \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} \operatorname{Re}\{\mathbf{L}^{H}\mathbf{W}_{\xi}\mathbf{y}\} \\ \operatorname{Im}\{\mathbf{L}^{H}\mathbf{W}_{\xi}\mathbf{y}\} \end{bmatrix}$$

**3.** Analysis. We present below a mathematical analysis of the PBDW formulation for noisy measurements. In section 3.1, we extend the analysis presented in [5] to general linear recovery algorithms, and we apply it to PBDW. In section 3.2, we prove that the solution to nonlinear PBDW depends continuously on data. To conclude, in section 3.3, we briefly discuss how the analysis presented in this section could be exploited to choose measurement locations.

<sup>&</sup>lt;sup>1</sup>We found empirically that explicitly adding the constraint  $\eta \in \mathbb{Z}_N^{\perp}$  does not improve reconstruction performance, and can even deteriorate the accuracy of the PBDW estimate in presence of substantial model bias and moderate experimental noise.

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# 3.1. Analysis for linear PBDW: *a priori* error bounds and optimality.

**3.1.1.** A general result for linear recovery algorithms. We first introduce 235some notation. Given the closed linear subspace  $\mathcal{Q} \subset \mathcal{U}$ , we denote by  $\Pi_{\mathcal{Q}} : \mathcal{U} \to \mathcal{Q}$ 236the orthogonal projection operator onto  $\mathcal{Q}$ , and we denote by  $\mathcal{Q}^{\perp}$  its orthogonal 237complement. We also denote by  $\mathcal{L}(\mathcal{X}, \mathcal{Y})$  the space of linear bounded operators from 238 the Hilbert space  $\mathcal{X}$  to the Hilbert space  $\mathcal{Y}$ , equipped with the norm  $||A||_{\mathcal{L}(\mathcal{X},\mathcal{Y})} =$ 239 $\sup_{v \in \mathcal{X}} \frac{\|A(v)\|_{\mathcal{Y}}}{\|v\|_{\mathcal{X}}}.$  Given the algorithm  $A : \mathbb{R}^M \to \mathcal{U}$ , we define the image of A,  $\operatorname{Im}(A) := \{A(\mathbf{y}) : \mathbf{y} \in \mathbb{R}^M\}$ ; we denote by Q the dimension of the space  $\operatorname{Im}(A), Q \leq M$ , and we denote by  $\{\psi_q\}_{q=1}^Q$  an orthonormal basis of  $\operatorname{Im}(A)$ . We further denote by  $A_{\ell} : \mathcal{U} \to \mathcal{U}$ 240241 242the  $\mathcal{L}(\mathcal{U},\mathcal{U})$  operator such that  $A_{\ell}(u) = A(\ell(u))$ . 243

We can now introduce the stability constants associated with A:

245 (3.1) 
$$\Lambda_2(A) := \|A\|_{\mathcal{L}(\mathbb{R}^M, \mathcal{U})} = \sup_{\mathbf{y} \in \mathbb{R}^M} \frac{\|A(\mathbf{y})\|}{\|\mathbf{y}\|_2}$$

246 and

247 (3.2) 
$$\Lambda_{\mathcal{U}}(A) := \|Id - A_{\ell}\|_{\mathcal{L}(\mathcal{U},\mathcal{U})} = \sup_{u \in \mathcal{U}} \frac{\|u - A_{\ell}(u)\|}{\|u\|} .$$

248 We further define the biasing constant

249 (3.3) 
$$\Lambda_{\mathcal{U}}^{\text{bias}}(A) := \|Id - A_{\ell}|_{\text{Im}(A)}\|_{\mathcal{L}(\text{Im}(A),\mathcal{U})} = \sup_{u \in \text{Im}(A)} \frac{\|u - A_{\ell}(u)\|}{\|u\|} .$$

Note that  $\Lambda_{\mathcal{U}}^{\text{bias}}(A) = 0$  if and only if  $A_{\boldsymbol{\ell}}(u) = u$  for all  $u \in \text{Im}(A)$ . Next Lemma summarizes important properties of the constants introduced above. We remark that if  $\Lambda_{\mathcal{U}}^{\text{bias}}(A) \neq 0$ , exact computation of  $\Lambda_{\mathcal{U}}(A)$  is in general not possible. In the numerical experiments, we consider the approximation  $\Lambda_{\mathcal{U}}(A) \approx \sup_{u \in \mathcal{U}_{\mathcal{N}}} \frac{\|u - A_{\boldsymbol{\ell}}(u)\|}{\|u\|}$ , where  $\mathcal{U}_{\mathcal{N}}$ is the  $\mathcal{N}$ -dimensional approximation of the space  $\mathcal{U}$ , based on a high-fidelity (spectral, Finite Element,...) discretization, and then we resort to an Arnoldi iterative method to (approximately) solve the corresponding eigenvalue problem.

LEMMA 3.1. Given the linear algorithm  $A : \mathbb{R}^M \to \mathcal{U}$ , the following hold.

258 1. The constants  $\Lambda_2(A)$  and  $\Lambda_{\mathcal{U}}^{\text{bias}}(A)$  can be computed as follows:

259 (3.4) 
$$\Lambda_2(A) = s_{\max}(\mathbf{A}), \quad \Lambda_{\mathcal{U}}^{\text{bias}}(A) = s_{\max}(\mathbf{Id} - \mathbf{A}_{\ell})$$

260 where  $s_{\max}(\mathbf{W})$  denotes the maximum singular value of  $\mathbf{W}$ . Here,  $\mathbf{A} \in \mathbb{R}^{Q,M}$  and  $\mathbf{A}_{\boldsymbol{\ell}} \in \mathbb{R}^{Q,Q}$  are such that  $\mathbf{A}_{q,m} = (A(\mathbf{e}_m), \psi_q)$  and  $(\mathbf{A}_{\boldsymbol{\ell}})_{q,q'} = (A_{\boldsymbol{\ell}}(\psi_{q'}), \psi_q)$ , where  $\{\mathbf{e}_m\}_m$  is the canonical basis in  $\mathbb{R}^M$ .

263 2. Suppose that 
$$\Lambda_{\mathcal{U}}^{\text{Dias}}(A) = 0$$
. Then,  $A_{\boldsymbol{\ell}}$  is idempotent (i.e.,  $A_{\boldsymbol{\ell}}^{\boldsymbol{\ell}} = A_{\boldsymbol{\ell}}$ ), and  
264  $\Lambda_{\mathcal{U}}(A) = \|A_{\boldsymbol{\ell}}\|_{\mathcal{L}(\mathcal{U},\mathcal{U})}$ . Furthermore, we have  $\Lambda_{\mathcal{U}}(A) = s_{\max}(\mathbf{A}\mathbf{K}^{1/2})$ .

265 *Proof.* Proof of the identities in (3.4) is tedious but straightforward. We omit the 266 details.

To prove the second statement, we recall that  $\Lambda_{\mathcal{U}}^{\text{bias}}(A) = 0$  if and only if  $A_{\ell}(u) = u$ for all  $u \in \text{Im}(A)$ . The latter implies that  $A_{\ell}^2 = A_{\ell}$ . Recalling [21, Corollary 3], we then obtain that  $\Lambda_{\mathcal{U}}(A) = \|Id - A_{\ell}\|_{\mathcal{L}(\mathcal{U},\mathcal{U})} = \|A_{\ell}\|_{\mathcal{L}(\mathcal{U},\mathcal{U})}$ . Finally, we observe

$$\Lambda_{\mathcal{U}}(A) = \sup_{u \in \mathcal{U}} \frac{\|A_{\ell}(u)\|}{\|u\|} = \sup_{u \in \mathcal{U}_M} \frac{\|A_{\ell}(u)\|}{\|u\|} = \sup_{\mathbf{q} \in \mathbb{R}^M} \frac{\|\mathbf{A}\mathbf{K}\mathbf{q}\|_2}{\|\mathbf{K}^{1/2}\mathbf{q}\|_2} = s_{\max}(\mathbf{A}\mathbf{K}^{1/2}),$$

267 which completes the proof.

Proposition 3.2 links the previously-defined quantities to the state estimation error. We observe that  $\Lambda_2(A)$  measures the sensitivity of A to measurement error, while  $\Lambda_{\mathcal{U}}(A)$  measures the sensitivity to the approximation error — given by  $\|\Pi_{\mathrm{Im}(A)^{\perp}} u^{\mathrm{true}}\|$ .

Finally,  $\Lambda_{\mathcal{U}}^{\text{bias}}(A)$  should be interpreted as the maximum possible relative error for per-

fect measurements (i.e.,  $\mathbf{y} = \boldsymbol{\ell}(\boldsymbol{u}^{\text{true}})$ ) and perfect approximation (i.e.,  $\boldsymbol{u}^{\text{true}} \in \text{Im}(A)$ ).

PROPOSITION 3.2. Given the linear algorithm  $A : \mathbb{R}^M \to \mathcal{U}$ , the following estimate holds:

(3.5)  
275 
$$\|A(\mathbf{y}) - u^{\text{true}}\| \leq \Lambda_2(A) \|\mathbf{y} - \boldsymbol{\ell}(u^{\text{true}})\|_2 + \Lambda_{\mathcal{U}}(A) \|\Pi_{\text{Im}(A)^{\perp}} u^{\text{true}}\| + \Lambda_{\mathcal{U}}^{\text{bias}}(A) \|u^{\text{true}}\|$$

Furthermore, if  $\mathbf{y} = \boldsymbol{\ell}(u^{\text{true}}) + \boldsymbol{\epsilon}$  with  $\boldsymbol{\epsilon}_m \stackrel{\text{iid}}{\sim} (0, \sigma^2)$ , the mean-square error is bounded by

278 (3.6) 
$$\mathbb{E}\left[\|A(\mathbf{y}) - u^{\text{true}}\|^2\right] \leq \left(\Lambda_{\mathcal{U}}(A) \|\Pi_{\text{Im}(A)^{\perp}} u^{\text{true}}\| + \Lambda_{\mathcal{U}}^{\text{bias}}(A) \|u^{\text{true}}\|\right)^2 + \sigma^2 \operatorname{trace}\left(\mathbf{A}^T \mathbf{A}\right),$$

## 279 where A was introduced in Lemma 3.1.

*Proof.* Exploiting the definition of  $\Lambda_{\mathcal{U}}(A)$  and  $\Lambda_{\mathcal{U}}^{\text{bias}}(A)$ , we find

$$\begin{aligned} \|u - A_{\boldsymbol{\ell}}(u)\| &\leq \|(I - A_{\boldsymbol{\ell}})\Pi_{\mathrm{Im}(A)^{\perp}}u\| + \|(I - A_{\boldsymbol{\ell}})\Pi_{\mathrm{Im}(A)}u\| \\ &\leq \Lambda_{\mathcal{U}}(A)\|\Pi_{\mathrm{Im}(A)^{\perp}}u\| + \Lambda_{\mathcal{U}}^{\mathrm{bias}}(A)\|u\|. \end{aligned}$$

Then, we obtain (3.5):

$$\begin{aligned} \|A(\mathbf{y}) - u^{\text{true}}\| &\leq \|A\left(\mathbf{y} - \boldsymbol{\ell}(u^{\text{true}})\right)\| + \|A_{\boldsymbol{\ell}}(u^{\text{true}}) - u^{\text{true}}\| \\ &\leq \Lambda_2(A) \|\mathbf{y} - \boldsymbol{\ell}(u^{\text{true}})\|_2 + \Lambda_{\mathcal{U}}(A) \|\Pi_{\text{Im}(A)^{\perp}} u^{\text{true}}\| + \Lambda_{\mathcal{U}}^{\text{bias}}(A) \|u^{\text{true}}\|. \end{aligned}$$

To prove (3.6), we first define  $\mathbf{y}^{\text{true}} := \boldsymbol{\ell}(u^{\text{true}})$ ; then, if we exploit the definition of  $\mathbf{A}$ , we find

$$\mathbb{E}\left[\|A(\mathbf{y}) - u^{\text{true}}\|^{2}\right] \leq \mathbb{E}\left[\|A\left(\mathbf{y} - \mathbf{y}^{\text{true}}\right) + \left(A_{\boldsymbol{\ell}}(u^{\text{true}}) - u^{\text{true}}\right)\|^{2}\right]$$
$$= \mathbb{E}\left[\|A\left(\boldsymbol{\epsilon}\right)\|^{2}\right] + \|A_{\boldsymbol{\ell}}(u^{\text{true}}) - u^{\text{true}}\|^{2} = \sigma^{2}\text{trace}(\mathbf{A}^{T}\mathbf{A}) + \|A_{\boldsymbol{\ell}}(u^{\text{true}}) - u^{\text{true}}\|^{2}$$
$$\leq \sigma^{2}\text{trace}(\mathbf{A}^{T}\mathbf{A}) + \left(\Lambda_{\mathcal{U}}(A)\|\Pi_{\text{Im}(A)^{\perp}}u^{\text{true}}\| + \Lambda_{\mathcal{U}}^{\text{bias}}(A)\|u^{\text{true}}\|\right)^{2},$$

which is the thesis. In the second-to-last step we used the identity  $\mathbb{E}[\|A(\epsilon)\|^2] = \mathbb{E}[\|\mathbf{A}\epsilon\|_2^2]$ , and then we applied [22, Theorem C, Chapter 14.4].

Remark 3.3. Perfect algorithms. In [5], the authors restrict their attention to perfect algorithms, that is algorithms satisfying  $A_{\ell}(u) = u$  for all  $u \in \text{Im}(A)$ . Clearly, a linear algorithm A is perfect if and only if  $\Lambda_{\mathcal{U}}^{\text{bias}}(A) = 0$ . If A is perfect, estimate (3.5) reduces to

$$\|A(\mathbf{y}) - u^{\mathrm{true}}\| \le \Lambda_2(A) \|\mathbf{y} - \boldsymbol{\ell}(u^{\mathrm{true}})\|_2 + \|A_{\boldsymbol{\ell}}\|_{\mathcal{L}(\mathcal{U},\mathcal{U})} \|\Pi_{\mathrm{Im}(A)^{\perp}} u^{\mathrm{true}}\|$$

which is the error bound proved in [5]. We recall that in [5]  $\Lambda_2(A)$  is referred to as reconstruction operator norm, while  $\Lambda_{\mathcal{U}}(A)$  is called *quasi-optimality constant*. As observed in the next section, for  $\xi \in (0, \infty)$  PBDW is not perfect; therefore, the analysis in [5] cannot be applied. **3.1.2.** Application to Ridge regression. Before applying the error analysis to PBDW, we specialize our analysis to the recovery algorithm associated with the following optimization statement:

289 (3.7) 
$$\min_{u \in \mathcal{U}} \xi \|u\|^2 + \|\boldsymbol{\ell}(u) - \mathbf{y}\|_2^2.$$

We denote by  $A_{\xi}$  the recovery algorithm associated to (3.7). We remark that (3.7) has been widely studied in the context of spline smoothing and learning theory: more in detail, (3.7) is typically referred to as Ridge regression in the statistics literature, and as Tikhonov regularization in the inverse problem literature; we refer to [29] and to the references therein for a thorough discussion. We observe that  $\text{Im}(A_{\xi}) = \mathcal{U}_M$ ; furthermore, the constants in Proposition 3.2 are given by

$$\Lambda_2(A_{\xi}) = \max_{m=1,\dots,M} \frac{\sqrt{\lambda_m(\mathbf{K})}}{\xi + \lambda_m(\mathbf{K})}, \quad \Lambda_{\mathcal{U}}(A_{\xi}) = 1, \quad \Lambda_{\mathcal{U}}^{\text{bias}}(A_{\xi}) = 1 - \frac{\lambda_{\min}(\mathbf{K})}{\xi + \lambda_{\min}(\mathbf{K})}.$$

Since  $\Lambda_{\mathcal{U}}^{\text{bias}}(A_{\xi}) \neq 0$ , the algorithm does not belong to the class of methods studied in [5]. On the other hand, applying (3.5), we obtain the estimate:

$$\|A_{\xi}(\mathbf{y}) - u^{\text{true}}\| \leq \frac{1}{2\sqrt{\xi}} \|\mathbf{y} - \boldsymbol{\ell}(u^{\text{true}})\|_2 + \|\Pi_{\mathcal{U}_M^{\perp}} u^{\text{true}}\| + \left(1 - \frac{\lambda_{\min}(\mathbf{K})}{\xi + \lambda_{\min}(\mathbf{K})}\right) \|u^{\text{true}}\|,$$

where we used the identity  $\max_{x \in (0,\infty)} \frac{x}{\xi + x^2} = \frac{1}{2\sqrt{\xi}}$  to bound  $\Lambda_2(A_{\xi})$ . Note that in presence of noise the optimal value  $\xi^{\text{opt}}$  of  $\xi$  that minimizes the right-hand side of the error bound satisfies  $0 < \xi^{\text{opt}} < \infty$ .

**3.1.3.** Application to linear PBDW. We now specialize the analysis to the linear PBDW recovery algorithm,  $A^{\text{pbdw},\xi}$ . First, we observe that  $A^{\text{pbdw},\xi}$  satisfies:

$$\operatorname{Im}\left(A^{\operatorname{pbdw},\xi}\right) = \begin{cases} \mathcal{Z}_N \oplus \left(\mathcal{Z}_N^{\perp} \cap \mathcal{U}_M\right) & \xi \in [0,\infty) \\ \mathcal{Z}_N & \xi = \infty \end{cases}$$

Moreover, for all values of  $\xi$ ,  $(Id - A_{\ell}^{\text{pbdw},\xi})z = 0$  for all  $z \in \mathbb{Z}_N$ ; as a result, we can specialize (3.5) as

$$\begin{split} \|A^{\mathrm{pbdw},\xi}(\mathbf{y}) - u^{\mathrm{true}}\| &\leq \Lambda_2(A^{\mathrm{pbdw},\xi}) \|\mathbf{y} - \boldsymbol{\ell}(u^{\mathrm{true}})\|_2 \\ &+ \Lambda_{\mathcal{U}}(A^{\mathrm{pbdw},\xi}) \|\Pi_{\mathrm{Im}(A^{\mathrm{pbdw},\xi})^{\perp}} u^{\mathrm{true}}\| + \Lambda_{\mathcal{U}}^{\mathrm{bias}}(A^{\mathrm{pbdw},\xi}) \|\Pi_{\mathcal{Z}_N^{\perp} \cap \mathcal{U}_M} u^{\mathrm{true}}\| \;. \end{split}$$

We can further bound the latter as

$$\begin{split} \|A^{\mathrm{pbdw},\xi}(\mathbf{y}) - u^{\mathrm{true}}\| &\leq \quad \Lambda_2(A^{\mathrm{pbdw},\xi}) \|\mathbf{y} - \boldsymbol{\ell}(u^{\mathrm{true}})\|_2 \\ &+ \left(\Lambda_{\mathcal{U}}(A^{\mathrm{pbdw},\xi}) + \Lambda_{\mathcal{U}}^{\mathrm{bias}}(A^{\mathrm{pbdw},\xi})\right) \|\Pi_{\mathcal{Z}_N^{\perp}} u^{\mathrm{true}}\| \;. \end{split}$$

293 Therefore, we can interpret the sum  $(\Lambda_{\mathcal{U}} + \Lambda_{\mathcal{U}}^{\text{bias}})$  as the sensitivity to the model 294 mismatch<sup>2</sup>  $\|\Pi_{\mathcal{Z}_{\mathcal{V}}^{\perp}} u^{\text{true}}\|$ , and  $\Lambda_2$  as the sensitivity to experimental noise.

<sup>&</sup>lt;sup>2</sup> More precisely, as explained in [17, section 2.7],  $\|\Pi_{Z_N^{\perp}} u^{\text{true}}\|$  should be interpreted as the sum of a *nonparametric model error*  $\inf_{w \in \mathcal{M}^{\text{bk}}} \|u^{\text{true}} - w\|$  and of a *discretization error*  $\sup_{w \in \mathcal{M}^{\text{bk}}} \|\Pi_{Z_N^{\perp}} w\|$  associated with the compression of the solution manifold.

It is easy to show that  $\Lambda^{\text{bias}}_{\mathcal{U}}(A^{\text{pbdw},\xi}) \to 0$  as  $\xi \to 0^+$  and  $\Lambda^{\text{bias}}_{\mathcal{U}}(A^{\text{pbdw},\xi}) \to 1$ 295 as  $\xi \to \infty$ . For the model problems considered in section 4, we further empirically 296demonstrate that  $\Lambda_2(A^{\text{pbdw},\xi})$  is monotonic decreasing in  $\xi$ , while  $\Lambda_{\mathcal{U}}(A^{\text{pbdw},\xi})$  and 297 $\Lambda_{\mathcal{U}}^{\mathrm{bias}}(A^{\mathrm{pbdw},\xi})$  are monotonic increasing in  $\xi$ : this suggests that the optimal value of 298 $\xi$  should depend on the ratio  $\|\mathbf{y} - \boldsymbol{\ell}(u^{\text{true}})\|_2 / \|\Pi_{\boldsymbol{\mathcal{Z}}_N^{\perp}} u^{\text{true}}\|$ . In the numerical experi-299ments, we also find that  $\Lambda_2(A^{\text{pbdw},\xi})$  and  $\Lambda_{\mathcal{U}}(A^{\text{pbdw},\xi})$  increase as N increases while 300  $\|\Pi_{\mathcal{Z}_{N}^{\perp}} u^{\text{true}}\|$  decreases as N increases; as a result, the choice of N should also reflect 301 the amount of noise and the behavior of  $\|\Pi_{\mathcal{Z}_N^{\perp}} u^{\text{true}}\|$  with N. Since the noise level and 302  $\|\Pi_{\mathcal{Z}^{\perp}} u^{\text{true}}\|$  are typically unknown, the choice of  $\xi$  and N should be performed online 303 based on out-of-sample data. We anticipate that the constrained formulation is sig-304 nificantly less sensitive to the choice of N than the standard unconstrained approach; 305 on the other hand, both formulations are nearly equally sensitive to the choice of  $\xi$ . 306 We also emphasize that the present discussion for the choice of  $\xi$  is in good agreement 307 with the conclusions drawn in [24, 19]. 308

We further observe that the biasing constant satisfies:

$$\Lambda_{\mathcal{U}}^{\text{bias}}\left(A^{\text{pbdw},\xi}\right) = \begin{cases} 0 & \xi \in \{0,\infty\}, \\ \\ >0 & \xi \in (0,\infty), \end{cases}$$

and is continuous in  $[0, \infty)$ . Finally, we observe that for  $\xi = 0$  we can relate  $\Lambda_{\mathcal{U}}$  to the inf-sup constant  $\beta_{N,M} = \inf_{z \in \mathcal{Z}_N} \sup_{q \in \mathcal{U}_M} \frac{(z,q)}{\|z\| \|q\|}$  introduced in [18] to measure stability with respect to model mismatch for (2.4):

312 (3.8) 
$$\Lambda_{\mathcal{U}}(A^{\mathrm{pbdw},\xi=0}) = \frac{1}{\beta_{N,M}}.$$

Identity (3.8) implies that (3.5) reduces to the estimate proved in [6] for  $A = A^{\text{pbdw},\xi=0}$ and perfect measurements.

Proof. (Identity (3.8)) The state estimate  $\hat{u}_0 = A^{\text{pbdw},\xi=0}(\boldsymbol{\ell}(u)) \in \text{Im}(A) = \mathcal{Z}_N \oplus (\mathcal{Z}_N^{\perp} \cap \mathcal{U}_M)$  satisfies  $(\hat{u}_0, q) = (u, q)$  for all  $q \in \mathcal{U}_M$ . As a result, recalling standard results in Functional Analysis and Lemma 3.1, we find  $\Lambda_{\mathcal{U}}(A^{\text{pbdw},\xi=0}) = \frac{1}{\tilde{\beta}}$  where  $\tilde{\beta} = \inf_{w \in \text{Im}(A)} \sup_{q \in \mathcal{U}_M} \frac{(w,q)}{\|w\| \|q\|}$ . It remains to prove that  $\tilde{\beta} = \beta_{N,M}$ :

$$\tilde{\beta}^{2} = \inf_{\substack{(z,\eta)\in\mathcal{Z}_{N}\times(\mathcal{Z}_{N}^{\perp}\cap\mathcal{U}_{M})}} \left( \sup_{q\in\mathcal{U}_{M}} \frac{(z+\eta,q)}{\sqrt{\|z\|^{2}+\|\eta\|^{2}}\|q\|} \right)^{2}$$

$$\stackrel{(i)}{=} \inf_{\substack{(z,\eta)\in\mathcal{Z}_{N}\times(\mathcal{Z}_{N}^{\perp}\cap\mathcal{U}_{M})}} \frac{\|\Pi_{\mathcal{U}_{M}}(z)+\eta\|^{2}}{\|z\|^{2}+\|\eta\|^{2}}$$

$$\stackrel{(ii)}{=} \inf_{\substack{(z,\eta)\in\mathcal{Z}_{N}\times(\mathcal{Z}_{N}^{\perp}\cap\mathcal{U}_{M})}} \frac{\|\Pi_{\mathcal{U}_{M}}(z)\|^{2}+\|\eta\|^{2}}{\|z\|^{2}+\|\eta\|^{2}}$$

$$\stackrel{(iii)}{=} \inf_{z\in\mathcal{Z}_{N}} \frac{\|\Pi_{\mathcal{U}_{M}}(z)\|^{2}}{\|z\|^{2}} = \inf_{z\in\mathcal{Z}_{N}} \sup_{q\in\mathcal{U}_{M}} \left(\frac{(z,q)}{\|z\|\|q\|}\right)^{2} = \beta_{N,M}^{2}$$

where we used (i)  $\eta \in \mathcal{U}_M$ , (ii)  $(\eta, \Pi_{\mathcal{U}_M} z) = (\eta, z) = 0$  (which exploits the fact that  $\eta \in \mathcal{Z}_N^{\perp} \cap \mathcal{U}_M$ ), and (iii)  $\|\Pi_{\mathcal{U}_M} z\|^2 \le \|z\|^2$ .

317 **3.1.4. Optimality of PBDW algorithms.** In the next two Propositions, we 318 prove two optimality statements satisfied by PBDW for the limit cases  $\xi = 0$  and 319  $\xi = \infty$ . H. GONG ET AL.

The first result — which was proved in Theorem 2.9 of [6] — illustrates the connection between PBDW and the problem of optimal recovery ([20]), for perfect measurements. We recall that in [25, Chapter 2.2.2] a similar optimality statement is proved for the case  $\xi > 0$ . Note that another relevant result on the optimality of PBDW can be found in the recent work [8], where it is proven that the optimal affine algorithm that is possible to build among all state estimation algorithms can be expressed as a PBDW algorithm.

The second result shows that the algorithm  $\Pi_{\mathcal{Z}_N} A^{\text{pbdw},\xi} : \mathbf{y} \mapsto \hat{z}_{\xi} = \sum_{n=1}^{N} (\hat{\mathbf{z}}_{\xi})_n$   $\zeta_n \text{ for } \Phi_N = \mathbb{R}^N \text{ minimizes } \Lambda_2 \text{ for } \xi = \infty \text{ and } \Lambda_{\mathcal{U}} \text{ for } \xi = 0 \text{ over all linear algorithms}$   $A : \mathbb{R}^M \to \mathcal{Z}_N \text{ satisfying } \Lambda_{\mathcal{U}}^{\text{bias}}(A) = 0.$  As mentioned in the introduction, Proposition 3.5 has been proved in [5]. The proof of Proposition 3.4 is omitted, while the proof of Proposition 3.5 — which exploits a different argument from the one in [5] — is contained in Appendix B.

PROPOSITION 3.4. Given the space  $\mathcal{Z}_N = \operatorname{span}\{\zeta_n\}_{n=1}^N \subset \mathcal{U}$  and the set of linear observation functionals  $\boldsymbol{\ell} : \mathcal{U} \to \mathbb{R}^M$ , we introduce the compact set

$$\mathcal{K}_{N,M}(\delta, \mathbf{y}) := \left\{ u \in \mathcal{U} : \|\Pi_{\mathcal{Z}_N^{\perp}} u\| \le \delta, \ \boldsymbol{\ell}(u) = \mathbf{y} \right\}$$

where  $\delta > 0$  is a given constant. Then, for all  $\mathbf{y} \in \mathbb{R}^M$  and  $\delta > 0$  such that  $\mathcal{K}_{N,M}(\delta, \mathbf{y})$  is not empty, the linear PBDW algorithm  $A^{\text{pbdw},\xi=0} : \mathbb{R}^M \to \mathcal{U}$  satisfies

$$A^{\text{pbdw},\xi=0}(\mathbf{y}) = \arg \inf_{w \in \mathcal{U}} \sup_{u \in \mathcal{K}_{N,M}(\delta, \mathbf{y})} \|u - w\|$$

333 Note that the PBDW algorithm does not depend on the value of  $\delta$ .

334 PROPOSITION 3.5. Given the space  $\mathcal{Z}_N = \operatorname{span}\{\zeta_n\}_{n=1}^N \subset \mathcal{U}$ , and the set of linear 335 functionals  $\ell : \mathcal{U} \to \mathbb{R}^M$ , let A be a linear algorithm such that  $\operatorname{Im}(A) = \mathcal{Z}_N$  and 336  $\Lambda_{\mathcal{U}}^{\operatorname{bias}}(A) = 0$ . Then,

337 (3.9) 
$$\Lambda_2(A) \ge \Lambda_2(A^{\operatorname{pbdw},\xi=\infty}), \qquad \Lambda_{\mathcal{U}}(A) \ge \Lambda_{\mathcal{U}}\left(\Pi_{\mathcal{Z}_N}A^{\operatorname{pbdw},\xi=0}\right).$$

338 **3.2.** Analysis of nonlinear PBDW: a stability estimate. We here show 339 that if  $\Phi_N$  is convex the deduced background  $\hat{\mathbf{z}}_{\xi}$  associated with the (nonlinear) 340 PBDW solution satisfies the stability estimate  $\|\hat{\mathbf{z}}_{\xi}(\mathbf{y}_1) - \hat{\mathbf{z}}_{\xi}(\mathbf{y}_2)\|_2 \leq C \|\mathbf{y}_1 - \mathbf{y}_2\|_2$  for 341 some constant C and for any data  $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^M$ . Since the update is a linear function 342 of the residual  $\mathbf{y} - \mathbf{L}\hat{\mathbf{z}}_{\xi}$  (cf. Proposition 2.1), this implies that the whole PBDW 343 estimate depends continuously on data. Towards this end, we recall that the deduced 344 background  $\hat{\mathbf{z}}_{\xi} \in \mathbb{R}^N$  satisfies (cf. Proposition 2.1) (3.10)

345 
$$\hat{\mathbf{z}}_{\xi} \in \arg\min_{\mathbf{z}\in\Phi_{N}} \|\mathbf{L}\mathbf{z}-\mathbf{y}\|_{\mathbf{W}_{\xi}}^{2} = \arg\min_{\mathbf{z}\in\Phi_{N}} \frac{1}{2}\mathbf{z}^{T}\mathbf{Q}_{\xi}\mathbf{z}+\mathbf{z}^{T}\mathbf{c}_{\xi}, \text{ where } \begin{cases} \mathbf{Q}_{\xi} = \mathbf{L}^{T}\mathbf{W}_{\xi}\mathbf{L}, \\ \mathbf{c}_{\xi} = -\mathbf{L}^{T}\mathbf{W}_{\xi}\mathbf{y}. \end{cases}$$

346 Furthermore, we define the constant

347 (3.11) 
$$\Lambda_{\xi}^{\mathrm{nl}}(\Phi_N) = \left(\min_{\mathbf{z}_1, \mathbf{z}_2 \in \Phi_N, \, \mathbf{z}_1 \neq \mathbf{z}_2} \frac{\|\mathbf{z}_1 - \mathbf{z}_2\|_{\mathbf{Q}_{\xi}}^2}{\|\mathbf{z}_1 - \mathbf{z}_2\|_2^2}\right)^{-1}$$

Next Lemma lists a number of properties of  $\Lambda_{\mathcal{E}}^{nl}(\Phi_N)$ .

LEMMA 3.6. Let  $\{\zeta_n\}_{n=1}^N$  be an orthonormal basis of  $\mathcal{Z}_N$  and  $\mathbf{L} \in \mathbb{R}^{M,N}$  be full rank with  $M \geq N$ . Then, the constant  $\Lambda_{\mathcal{E}}^{\mathrm{nl}}(\Phi_N)$  (3.11) satisfies the following.

1. If 
$$\Phi_N \subset \Phi'_N$$
, then  $\Lambda^{\mathrm{nl}}_{\xi}(\Phi_N) \leq \Lambda^{\mathrm{nl}}_{\xi}(\Phi'_N)$ .

352 2. If 
$$\Phi_N = \mathbb{R}^N$$
, then  $\Lambda_{\xi}^{\mathrm{nl}}(\Phi_N) = \|\mathbf{Q}_{\xi}^{-1}\|_2$ . In particular, for  $\xi = 0$  (i.e.,  $\mathbb{Q}_{\xi} = \mathbf{L}^T \mathbf{K}^{-1} \mathbf{L}$ ), we have  $\Lambda_{\xi}^{\mathrm{nl}}(\Phi_N) = \Lambda_{\mathcal{U}}(A^{\mathrm{pbdw},\xi=0}) = \frac{1}{\beta_{N,M}}$ .

*Proof.* The first statement follows directly from the definition of minimum. On the other hand, for  $\Phi_N = \mathbb{R}^N$ ,  $\Lambda_{\xi}^{\text{nl}}$  can be rewritten as:

$$\Lambda_{\xi}^{\mathrm{nl}}(\mathbb{R}^N) = \left(\min_{\mathbf{z}\in\mathbb{R}^N} \frac{\|\mathbf{L}\mathbf{z}\|_{\mathbf{W}_{\xi}}^2}{\|\mathbf{z}\|_2^2}\right)^{-1} = \frac{1}{\lambda_{\min}(\mathbf{L}^T\mathbf{W}_{\xi}\mathbf{L})} = \|\mathbf{Q}_{\xi}^{-1}\|_2,$$

where in the second identity we exploited the relationship between eigenvalues of symmetric matrices and minimum Rayleigh quotients, and in the third identity we used a standard property of the  $\|\cdot\|_2$  norm of symmetric matrices. Finally, for  $\xi = 0$ exploiting [16, Lemma 3.3] and the fact that  $\{\zeta_n\}_{n=1}^N$  is an orthonormal basis, we find that  $\beta_{N,M} = \lambda_{\min}(\mathbf{L}^T \mathbf{K}^{-1} \mathbf{L})$ . Thesis then follows recalling (3.8).

Next Proposition motivates the definition of  $\Lambda_{\xi}^{nl}$ .

360 PROPOSITION 3.7. Let  $\Phi_N$  be convex, and let the hypotheses of Lemma 3.6 hold. 361 Given  $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^M$ , we denote by  $\hat{\mathbf{z}}_{\xi,i}$  the solution to (3.10) for  $\mathbf{y} = \mathbf{y}_i$ , for i = 1, 2. 362 Then, we have

363 (3.12) 
$$\|\hat{\mathbf{z}}_{\xi,2} - \hat{\mathbf{z}}_{\xi,1}\|_2 \le \|\mathbf{L}^T \mathbf{W}_{\xi}\|_2 \Lambda_{\xi}^{\mathrm{nl}}(\Phi_N) \|\mathbf{y}_1 - \mathbf{y}_2\|_2,$$

364 where  $\Lambda_{\xi}^{\text{nl}}$  is defined in (3.11).

In view of the proof, we state the following standard result (see, e.g., [10, Lemma 5.13]).

LEMMA 3.8. Let  $f : \mathbb{R}^N \to \mathbb{R}$  be convex and differentiable with gradient  $\nabla f$ , and let  $\Phi_N \subset \mathbb{R}^N$  be a closed convex set. Then,

$$\mathbf{z}^{\star} \in \arg\min_{\mathbf{z}\in\Phi_{N}} f(\mathbf{z}) \iff (\nabla f(\mathbf{z}^{\star}), \mathbf{h} - \mathbf{z}^{\star})_{2} \ge 0 \quad \forall \, \mathbf{h} \in \Phi_{N}$$

<sup>367</sup> where  $(\cdot, \cdot)_2$  denotes the Euclidean inner product.

*Proof.* (Proposition 3.7). For i = 1, 2, problem (3.10) for  $\mathbf{y} = \mathbf{y}_i$  can be restated as

$$\min_{\mathbf{z}\in\mathbb{R}^N} f_i(\mathbf{z}) := \frac{1}{2} \mathbf{z}^T \mathbf{Q}_{\xi} \mathbf{z} + \mathbf{z}^T \mathbf{c}_{\xi,i}, \qquad \mathbf{Q}_{\xi} = \mathbf{L}^T \mathbf{W}_{\xi} \mathbf{L}, \ \mathbf{c}_{\xi,i} = -\mathbf{L}^T \mathbf{W}_{\xi} \mathbf{y}_i.$$

Exploiting Lemma 3.8, we find for any  $\mathbf{h}_1, \mathbf{h}_2 \in \Phi_N$ 

$$(\mathbf{Q}_{\boldsymbol{\xi}}\hat{\mathbf{z}}_{\boldsymbol{\xi},i} + \mathbf{c}_{\boldsymbol{\xi},i}, \mathbf{h}_i - \hat{\mathbf{z}}_{\boldsymbol{\xi},i})_2 \ge 0, \qquad i = 1, 2.$$

If we consider  $\mathbf{h}_1 = \hat{\mathbf{z}}_{\xi,2}$  and  $\mathbf{h}_2 = \hat{\mathbf{z}}_{\xi,1}$  and we sum the two inequalities, we obtain

$$\begin{aligned} (\mathbf{Q}_{\xi}(\hat{\mathbf{z}}_{\xi,1} - \hat{\mathbf{z}}_{\xi,2}) + \mathbf{c}_{\xi,1} - \mathbf{c}_{\xi,2}, \, \hat{\mathbf{z}}_{\xi,2} - \hat{\mathbf{z}}_{\xi,1})_{2} &\geq 0 \\ \Rightarrow \|\hat{\mathbf{z}}_{\xi,1} - \hat{\mathbf{z}}_{\xi,2}\|_{\mathbf{Q}_{\xi}}^{2} &\leq (\mathbf{c}_{\xi,1} - \mathbf{c}_{\xi,2}, \hat{\mathbf{z}}_{\xi,2} - \hat{\mathbf{z}}_{\xi,1})_{2} \leq \|\mathbf{c}_{\xi,1} - \mathbf{c}_{\xi,2}\|_{2} \|\hat{\mathbf{z}}_{\xi,2} - \hat{\mathbf{z}}_{\xi,1}\|_{2} \\ \Rightarrow \|\hat{\mathbf{z}}_{\xi,1} - \hat{\mathbf{z}}_{\xi,2}\|_{2} &\leq \Lambda_{\xi}^{\mathrm{nl}}(\Phi_{N}) \,\|\mathbf{c}_{\xi,1} - \mathbf{c}_{\xi,2}\|_{2} \leq \Lambda_{\xi}^{\mathrm{nl}}(\Phi_{N}) \,\|\mathbf{L}^{T} \,\mathbf{W}_{\xi}\|_{2} \,\|\mathbf{y}_{1} - \mathbf{y}_{2}\|_{2} \end{aligned}$$

368 which is the thesis.

Remark 3.9. Comparison with linear PBDW. Recalling the properties of the constant  $\Lambda_{\xi}^{nl}$  (cf. Lemma 3.8), estimate (3.12) suggests that considering  $\Phi_N \subsetneq \mathbb{R}^N$  reduces the sensitivity of (3.10) to perturbations in the data. However, if we restrict the bound (3.12) to linear algorithms, we find

$$\|\hat{\mathbf{z}}_{\xi,2} - \hat{\mathbf{z}}_{\xi,1}\|_2 \leq \|\left(\mathbf{L}^T \mathbf{W}_{\xi} \mathbf{L}
ight)^{-1}\|_2 \|\mathbf{L}^T \mathbf{W}_{\xi}\|_2 \|\mathbf{y}_1 - \mathbf{y}_2\|_2,$$

which is clearly suboptimal compared to the optimal bound<sup>3</sup>

$$\|\hat{\mathbf{z}}_{\xi,2} - \hat{\mathbf{z}}_{\xi,1}\|_2 \le \|\left(\mathbf{L}^T \mathbf{W}_{\xi} \mathbf{L}\right)^{-1} \, \mathbf{L}^T \mathbf{W}_{\xi}\|_2 \, \|\mathbf{y}_1 - \mathbf{y}_2\|_2.$$

Although we cannot rigorously prove that reducing the admissible set  $\Phi_N$  for  $\hat{\mathbf{z}}_{\xi}$  always improves the stability of the formulation, several numerical results presented in the

improves the stability of the formulation, several numerical rest

next section confirm this intuition, and ultimately motivate the nonlinear approach.

**3.3. Selection of the observation functionals.** In [18], a greedy algorithm called SGreedy was proposed to adaptively select the observation centers<sup>4</sup>  $\{x_m\}_{m=1}^M \subset \Omega$  for functionals of the form

$$\ell_m(v) = C_m \int_{\Omega} \omega(\|x - x_m\|_2) v(x) \, dx,$$

where  $\omega : \mathbb{R}_+ \to \mathbb{R}_+$  is a suitable convolutional kernel associated with the physical transducer. A convergence analysis of the algorithm can be found in reference [7], which is a general study on greedy algorithms for the optimal sensor placement using reduced models.

SGreedy aims at maximizing the inf-sup constant  $\beta_{N,M}$ : recalling (3.8), maximizing  $\beta_{N,M}$  is equivalent to minimizing  $\Lambda_{\mathcal{U}}$  for  $\xi = 0$ . In [25, 19], a variant of the SGreedy algorithm is proposed: first, the SGreedy routine is executed until  $\beta_{N,M}$ exceeds a certain threshold, then the remaining points are chosen to minimize the fill distance  $h_M = \sup_{x \in \Omega} \min_{1 \le m \le M} ||x - x_m||_2$ , which is empirically found to be correlated with  $\Lambda_2$ .

While for perfect measurements and linear PBDW these Greedy routines are mathematically sounding and have been successfully tested, their performance for noisy measurement and nonlinear PBDW has not been fully investigated yet. In section 4, we present numerical results for two model problems. Our numerical results suggest that SGreedy is effective — if compared to standard *a priori* selections also in presence of noise for linear methods; on the other hand, the introduction of box constraints reduces the sensitivity of the method to measurement locations.

## 389 4. Numerical results.

393

## 390 4.1. A two-dimensional problem.

4.1.1. Problem statement. We first investigate the performance of PBDWusing the following two-dimensional advection-diffusion model problem:

$$(4.1) \qquad \begin{cases} -\Delta u_g(\mu) + \mathbf{b}(\mu) \cdot \nabla u_g(\mu) = x_1 x_2 + g_1 & x \in \Omega := (0, 1)^2 \\ u_g(\mu) = 4 x_2 (1 - x_2) (1 + g_2) & x \in \Gamma := \{0\} \times (0, 1) \\ \partial_n u_g(\mu) = 0 & x \in \partial\Omega \setminus \Gamma \end{cases}$$

14

<sup>&</sup>lt;sup>3</sup>The optimal bound can be trivially derived using (2.10a).

<sup>&</sup>lt;sup>4</sup> As explained in the original paper, SGreedy can also be used to choose  $\ell_1^o, \ldots, \ell_M^o$  from a dictionary of available functionals  $\mathcal{L} \subset \mathcal{U}'$ .

where  $\mathbf{b}(\mu) = \mu_1 [\cos(\mu_2), \sin(\mu_2)]$  with  $\mu = [\mu_1, \mu_2] \in \mathcal{P}^{bk} = [0.1, 10] \times [0, \pi/4]$ . We here define the bk manifold as

$$\mathcal{M}^{\mathrm{bk}} := \left\{ u^{\mathrm{bk}}(\mu) := u_{g=0}(\mu) : \quad \mu \in \mathcal{P}^{\mathrm{bk}} \right\}$$

and we consider

$$u^{\text{true}} = u_{g=(\bar{g}_1, \bar{g}_2)}(\mu^{\text{true}}) \quad \text{for some } \mu^{\text{true}} \in \mathcal{P}^{\text{bk}}, \quad \begin{cases} \bar{g}_1(x) = 0.2x_1^2\\ \bar{g}_2(x) = 0.1\sin(2\pi x_2). \end{cases}$$

The lack of knowledge of the value of  $\mu^{\text{true}}$  constitutes the anticipated parametric ignorance in the model, while uncertainty in g constitutes the unanticipated nonparametric ignorance.

We consider Gaussian observation functionals with standard deviation  $r_{\rm w} = 0.01$ :

398 (4.2) 
$$\ell_m(v) = \ell(v; x_m, r_w) = C(x_m) \int_{\Omega} \exp\left(-\frac{1}{2r_w^2} \|x - x_m\|_2^2\right) v(x) \, dx$$

where  $C(x_m)$  is a normalization constant such that  $\ell_m(1) = 1$ . To assess performance for imperfect observations, we pollute the measurements by adding Gaussian homoscedastic random disturbances  $\epsilon_1, \ldots, \epsilon_M$ :

$$y_m = \ell_m(u^{\text{true}}) + \epsilon_m$$
, where  $\epsilon_m \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ ,  $\sigma = \frac{1}{\text{SNR}} \operatorname{std}\left(\left\{\ell\left(u^{\text{true}}; \tilde{x}_j, r_w\right)\right\}_{j=1}^{100}\right)$ ,

for given signal-to-noise ratio SNR > 0 and uniformly-randomly chosen observation points  $\{\tilde{x}_j\}_j \subset \Omega$ .

We define the ambient space  $\mathcal{U} = H^1(\Omega)$  endowed with the inner product

$$(u,v) = \int_{\Omega} \nabla u \cdot \nabla v + u v \, dx.$$

Then, we generate the background space  $\mathcal{Z}_N$  using Proper Orthogonal Decomposition (POD, [27]) based on the  $\mathcal{U}$  inner product: we compute the solution to (4.1) for g = 0 for  $n_{\text{train}} = 10^3$  choices of the parameters  $\{\mu^i\}_{i=1}^{n_{\text{train}}}$  in  $\mathcal{P}^{\text{bk}}$ , then we use POD to build the background expansion  $\{\zeta_n\}_{n=1}^N$ . Furthermore, in view of the application of nonlinear PBDW ( $\Phi_N \subsetneq \mathbb{R}^N$ ), we set

$$a_n := \min_{i=1,\dots,n_{\text{train}}} \left( u^{\text{bk}}(\mu^i), \, \zeta_n \right), \quad b_n := \max_{i=1,\dots,n_{\text{train}}} \left( u^{\text{bk}}(\mu^i), \, \zeta_n \right), \quad n = 1,\dots, N.$$

401 The property of the POD construction (i.e., the decay rate of the POD eigenvalues)

402 gives some intuition of the fact that these bounds encode some valuable information.

# 403 **4.1.2. Results.**

Linear PBDW. Figure 1 shows the behavior of  $\Lambda_2$ ,  $\Lambda_{\mathcal{U}}$  and  $\Lambda_{\mathcal{U}}^{\text{bias}}$  with respect to the hyper-parameter  $\xi > 0$ , for several values of M and N. As anticipated in section  $\Lambda_{12}$  is monotonic decreasing in  $\xi$  and increases as N increases;  $\Lambda_{\mathcal{U}}$  is monotonic increasing in  $\xi$  and N, and decreases as M increases; finally,  $\Lambda_{\mathcal{U}}^{\text{bias}}$  is monotonic increasing in  $\xi$ , and weakly depends on M and N. We remark that we observed the same qualitative behavior for several other choices of M, N.

410 Figure 2 shows the behavior of the average relative error

(4.3)

411 
$$E_{\text{avg}}(\xi) = \frac{1}{K \times n_{\text{test}}} \sum_{j=1}^{n_{\text{test}}} \sum_{k=1}^{K} \frac{\|u^{\text{true}}(\mu^j) - \hat{u}_{\xi}^{(k,j)}\|_{L^2(\Omega)}}{\|u^{\text{true}}\|_{L^2(\Omega)}}, \quad \mu^j \stackrel{\text{iid}}{\sim} \text{Uniform}(\mathcal{P}^{\text{bk}}),$$



Fig. 1: two-dimensional problem. Behavior of  $\Lambda_2$ ,  $\Lambda_{\mathcal{U}}$  and  $\Lambda_{\mathcal{U}}^{\text{bias}}$  for several choices of N and M.

where K = 50,  $n_{\text{test}} = 10$ , and  $\hat{u}_{\xi}^{(k,j)}$  is the (linear) PBDW estimate associated with 412 the k-th realization of the random disturbance  $\epsilon$ , and the j-th true field  $u^{\text{true}}(\mu^j)$ 413 considered. To compute  $u^{\text{true}}(\mu^j)$ , we both consider the solution to (4.1) for  $g \equiv 0$ 414(unbiased) and  $g \neq 0$  (biased). We further consider two different signal-to-noise 415 levels,  $\text{SNR} = \infty$ , SNR = 10: the choice  $\text{SNR} = \infty$  corresponds to the case of perfect 416 measurements. As expected, for perfect measurements, the optimal value of  $\xi$  is equal 417 to zero, while for noisy measurements optimal performance is achieved for  $\xi = \infty$  in 418 the case of unbiased model, and for  $\xi \in (0, \infty)$  in presence of bias. These results are 419 in good qualitative agreements with the discussion in section 3, and with the results 420 in [24, 19]. 421



Fig. 2: two-dimensional problem. Behavior of  $E_{\text{avg}}$  for several values of  $\xi$  and three choices of N, M, for linear PBDW ( $\Phi_N = \mathbb{R}^N$ ).

Figure 3(a) shows the first M = N + 5 points selected by the SG reedy-procedure for N = 5, while Figures 3(b) and (c) show the behavior of the stability constants 424  $\Lambda_{\mathcal{U}}$  and  $\Lambda_2$  for different choices of the observation centers and  $\xi = 0$ . Figures 3(d)-425 (e)-(f) show analogous results for N = 15. We observe that for small values of M the 426 SGreedy procedure reduces the constants  $\Lambda_{\mathcal{U}}$  and  $\Lambda_2$  compared to a equispaced grid 427 of observations and to a grid associated with Gaussian quadrature nodes. We further 428 observe that the application of the variant SGreedy + approximation (with threshold 429 tol = 0.4) leads to more moderate values of  $\Lambda_2$  compared to the plain SGreedy, at the 430 price of a slight deterioration in  $\Lambda_{\mathcal{U}}$ .



Fig. 3: two-dimensional problem. Figures (a)-(d): location of the observation centers selected by SGreedy. Figures (b)-(e): behavior of  $\Lambda_{\mathcal{U}}$  with M for different choices of the observation centers. Figures (c)-(f): behavior of  $\Lambda_2$  with M for different choices of the observation centers.

Figure 4 shows the behavior of  $E_{\text{avg}}$  defined in (4.3) with N, for several choices of M. Observations are chosen using the SGreedy+approximation algorithm with threshold tol = 0.4. Here, the value of  $\xi$  is chosen using holdout validation based on I = M/2 additional measurements (see [24, 19] for further details). We observe that for noisy measurements the error reaches a minimum for an intermediate value of N, which depends on M and on the noise level. These results are consistent with the interpretation — stated in section 3 — of N as a regularization parameter.

438 **Nonlinear PBDW.** Figure 5 replicates the experiment of Figure 4 for the non-439 linear formulation. We observe that the nonlinear formulation is significantly more 440 robust to the choice of N compared to the linear formulation, particularly in the 441 presence of noise.

In Figures 6 and 7, we investigate the behavior of  $E_{\text{avg}}$  with N, for M = N + 3, for both linear and nonlinear formulations, and two noise levels. We consider three strategies for the selection of the observation centers: uniform points, Gaussian points, and adaptive points (based on SGreedy). For the problem at hand, the nonlinear formulation improves reconstruction performance, particularly in presence of noise and for non-adaptive selections of measurement locations.



Fig. 4: two-dimensional problem. Behavior of  $E_{\text{avg}}$  with N for several values of M, for linear PBDW ( $\Phi_N = \mathbb{R}^N$ ).



Fig. 5: two-dimensional problem. Behavior of  $E_{\text{avg}}$  with N for several values of M, for nonlinear PBDW  $(\Phi_N \subsetneq \mathbb{R}^N)$ .

# 448 **4.2.** A three-dimensional problem.



Fig. 6: two-dimensional problem. Behavior of  $E_{\text{avg}}$  with N for M = N + 3, for linear and nonlinear PBDW, and several choices of measurement locations (unbiased case).



Fig. 7: two-dimensional problem. Behavior of  $E_{\text{avg}}$  with N for M = N + 3, for linear and nonlinear PBDW, and several choices of measurement locations (biased case).

**4.2.1.** Problem statement. We consider the three-dimensional model prob-449 450lem:

451 (4.4) 
$$\begin{cases} -(1+\epsilon \mathbf{i})\Delta u_g(\mu) - (2\pi\mu)^2 u_g(\mu) = g \quad \text{in } \Omega;\\ \partial_n u_g(\mu) = 0 \qquad \qquad \text{on } \partial\Omega; \end{cases}$$

where  $\epsilon = 10^{-2}$ ,  $\Omega = (-1.5, 1.5) \times (0, 3) \times (0, 3) \setminus \Omega^{\text{cut}}$ ,  $\Omega^{\text{cut}} = (-0.5, 0.5) \times (0.25, 0.5) \times$ (0,1). Figure 8 shows the geometry; the same test case has been considered in [19]. We define the bk manifold  $\mathcal{M}^{bk} = \{u^{bk}(\mu) = u_{a^{bk}}(\mu) : \mu \in \mathcal{P}^{bk} = [0.1, 0.5]\}$ , and we define the true field as the solution to (4.4) for some  $\mu^{\text{true}} \in \mathcal{P}^{\text{bk}}$  and  $g = g^{\text{true}}$ , where

$$g^{\text{bk}}(x) = 10 e^{-\|x-p^{\text{bk}}\|_2^2}; \quad g^{\text{true}}(x) = 10 e^{-\|x-p^{\text{true}}\|_2^2}$$

and  $p^{\text{bk}} = [0, 2, 1], p^{\text{true}} = [-0.02, 2.02, 1]$ . Lack of knowledge of the input frequency 452 $\mu$  constitutes the anticipated ignorance in the system, while the incorrect location of 453the acoustic source (that is,  $p^{bk} \neq p^{true}$ ) constitutes unanticipated ignorance/model 454 error. Computations are based on a P2 Finite Element (FE) discretization with 455roughly  $\mathcal{N} = 16000$  degrees of freedom in  $\Omega$ .





Fig. 8: three-dimensional problem: computational domain.

As in the previous example, we model the synthetic observations by a Gaussian convolution with standard deviation  $r_{\rm w}$ , see (4.2). In order to simulate noisy observations, we add Gaussian homoscedastic disturbances

$$y_m = \ell_m(u^{\text{true}}) + \epsilon_m^{\text{re}} + i\epsilon_m^{\text{im}}, \text{ where } \epsilon_m^{\text{re}} \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma_{\text{re}}^2), \epsilon_m^{\text{im}} \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma_{\text{im}}^2),$$

with  $\sigma_{\rm re} = \frac{1}{\text{SNR}} \operatorname{std} \left( \{ \operatorname{Re} \{ \ell (u^{\rm true}; \tilde{x}_j, r_{\rm w}) \} \}_{j=1}^{100} \right), \sigma_{\rm im} = \frac{1}{\text{SNR}} \operatorname{std} \left( \{ \operatorname{Im} \{ \ell (u^{\rm true}; \tilde{x}_j, r_{\rm w}) \} \}_{j=1}^{100} \right) \right)$ 457 $\{\}_{i=1}^{100}\}$ , for given signal-to-noise ratio SNR > 0 and uniformly-randomly chosen ob-458servation points  $\{\tilde{x}_j\}_j \subset \Omega$ . Furthermore, we measure performance by computing the 459average relative  $L^2$  error  $E_{\text{avg}}$  (4.3) over  $n_{\text{test}} = 10$  different choices of the parameter 460  $\mu$  in  $\mathcal{P}^{bk}$ . 461

We consider the ambient space  $\mathcal{U} = H^1(\Omega)$  endowed with the inner product

$$(u,v) = \int_\Omega \nabla u \cdot \nabla \bar v \, + \, u \, \bar v \, dx,$$

where  $\bar{z}$  denotes the complex conjugate of  $z \in \mathbb{C}$ . On the other hand, the background 462

space  $\mathcal{Z}_N$  is built using the Weak-Greedy algorithm based on the residual, as in [17]. 463

Since the solution is complex, we compute the solution to the nonlinear formulation by solving the complex-valued counterpart of (2.11) as a 2*N*-dimensional real-valued quadratic problem for  $\hat{\mathbf{z}}_{\xi}^{\star} = [\operatorname{Re}\{\hat{\mathbf{z}}_{\xi}\}, \operatorname{Im}\{\hat{\mathbf{z}}_{\xi}\}]$  (see Remark 2.3). Given  $N \leq N_{\max} := 30$ , we estimate the constraints  $\{a_n, b_n\}_{n=1}^{2N}$  by evaluating a Galerkin Reduced Order Model (ROM) based on the reduced space  $\mathcal{Z}_{N_{\max}}$  for  $n_{\text{train}} = 10^3$ parameters  $\mu^1, \ldots, \mu^{n_{\text{train}}} \stackrel{\text{iid}}{\simeq}$  Uniform( $\mathcal{P}^{\text{bk}}$ ):

$$\begin{cases}
 a_n := \min_{i=1,\dots,n_{\text{train}}} \operatorname{Re} \left\{ \left( u_{N_{\max}}^{\text{bk}}(\mu^i), \zeta_n \right) \right\}, \\
 b_n := \max_{i=1,\dots,n_{\text{train}}} \operatorname{Re} \left\{ \left( u_{N_{\max}}^{\text{bk}}(\mu^i), \zeta_n \right) \right\}, \\
 a_{n+N} := \min_{i=1,\dots,n_{\text{train}}} \operatorname{Im} \left\{ \left( u_{N_{\max}}^{\text{bk}}(\mu^i), \zeta_n \right) \right\}, \\
 b_{n+N} := \max_{i=1,\dots,n_{\text{train}}} \operatorname{Im} \left\{ \left( u_{N_{\max}}^{\text{bk}}(\mu^i), \zeta_n \right) \right\},
\end{cases}$$

464 Here  $u_{N_{\text{max}}}^{\text{bk}}$  denotes the solution to the Galerkin ROM with  $N_{\text{max}}$  degrees of freedom. 465 We refer to the Reduced Basis literature for further details concerning the generation 466 and the evaluation of the ROM; we emphasize that by resorting to the low-dimensional 467 ROM — as opposed to the FE model — to estimate lower and upper bounds for the 468 background coefficients we significantly reduce the offline computational effort.

**4.2.2. Results.** Figure 9 shows the behavior of  $\Lambda_2$  and  $\Lambda_{\mathcal{U}}$  with N for M =469 N+2 and M=N+5, for two choices of the measurement locations: the SG reedy 470 adaptive algorithm, and a random uniform algorithm in which  $x_1, \ldots, x_M$  are sampled 471 uniformly in  $\Omega$  with the constraint that dist  $(x_m, \{x_{m'}\}_{m'=1}^{m-1}) \geq \delta = 0.02$ , for m =472 $1, \ldots, M$ . Results for the latter procedure are averaged over K = 10 independent 473 random choices of measurement locations. We observe that the Greedy algorithm 474leads to a reduction in both  $\Lambda_2$  and  $\Lambda_{\mathcal{U}}$  compared to the random uniform algorithm. 475Figures 10 and 11, show the behavior of the average relative error  $E_{\text{avg}}$  (4.3) with 476N for several fixed values of M, for two choices of the observation centers, for linear 477 and nonlinear PBDW, for two noise levels, and for both the biased and the unbi-478 479ased case. In all cases, the regularization hyper-parameter  $\xi$  is chosen using holdout validation, based on I = M/2 additional measurements. As for the previous model 480problem, we empirically find that the nonlinear formulation improves reconstruction 481 482 performance for noisy measurements and for non-adaptive selections of measurement locations. 483

5. Conclusions. In this paper, we provided theoretical and empirical investiga-484 tions of the performance of the PBDW approach. First, we presented a mathematical 485analysis of the PBDW formulation. For the linear case, we generalized the analysis 486 487 in [5] to obtain a complete *a priori* error analysis for noisy measurements, and we also presented two optimality results that motivate the approach. For the nonlinear 488 case, we showed a stability estimate that exploits a well-known result, first appeared 489 in the inverse problem literature. The latter estimate suggests that the nonlinear for-490491mulation should be more robust to measurement error. Second, we provided several numerical examples to compare the performance of linear PBDW with the perfor-492493 mance of nonlinear PBDW.

494 Results suggest that the box constraints for the entries of the background vector 495  $\hat{\mathbf{z}}_{\xi}$  improve the accuracy of the recovery algorithm, provided that measurements are 496 polluted by a non-negligible disturbance. As regards the choice of the observation 497 centers, the SG reedy method stabilizes the recovery algorithm for  $N \approx M$  and  $\Phi_N =$ 



Fig. 9: three-dimensional problem. Behavior of  $\Lambda_2$  and  $\Lambda_{\mathcal{U}}$  with N for M = N + 2 (Figures (a)-(b)) and M = N + 5 (Figures (c)-(d)).

498  $\mathbb{R}^N$ . On the other hand, at least for the numerical example considered in this work,

499 in presence of box constraints, SGreedy does not lead to substantial improvements. 500 Finally, we also empirically found that the nonlinear formulation is significantly less

sensitive to the choice of N, particularly for noisy measurements.

# 502 Appendix A. Proof of Proposition 2.1.

503 Proof. Given  $\eta \in \mathcal{U}$ , recalling the definition of  $\mathcal{U}_M$ , the Riesz theorem and the 504 projection theorem, we find that  $\mathcal{J}_{\xi}(\mathbf{z},\eta) = \mathcal{J}_{\xi}(\mathbf{z},\Pi_{\mathcal{U}_M}\eta) + \xi \|\Pi_{\mathcal{U}_M^{\perp}}\eta\|^2$ : therefore, the 505 optimal update  $\hat{\eta}_{\xi}$  belongs to  $\mathcal{U}_M$ . Using a similar argument, we can also prove that 506  $\hat{\eta}_0 \in \mathcal{U}_M$ .

Proof of (2.6b) is straightforward and is here omitted; we now focus on (2.6a). Towards this end, we introduce the eigendecomposition  $\mathbf{K} = \mathbf{U}\mathbf{D}\mathbf{U}^T$ ,  $\mathbf{D} = \operatorname{diag}(\lambda_1, \ldots, \lambda_M)$  and we observe that  $\mathbf{W}_{\xi} = (\xi\mathbf{Id} + \mathbf{K})^{-1}$  satisfies  $\mathbf{W}_{\xi} = \mathbf{U}\mathbf{D}_{\xi}\mathbf{U}^T$  with  $(\mathbf{D}_{\xi})_{m,m} = \frac{1}{\xi + \lambda_m(\mathbf{K})}$ . If we fix  $\mathbf{z} \in \mathbb{R}^N$ , it is easy to verify that the unique minimizer of  $\mathcal{J}_{\xi,\mathbf{z}}(\cdot) = \mathcal{J}_{\xi}(\mathbf{z}, \cdot)$  is given by

$$\eta(\mathbf{z}) = \sum_{m=1}^{M} (\boldsymbol{\eta}(\mathbf{z}))_m q_m, \text{ where } \boldsymbol{\eta}(\mathbf{z}) = \mathbf{W}_{\xi} \mathbf{y}^{\text{err}}(\mathbf{z}).$$

If we substitute the expression of  $\eta$  in (2.3), and we exploit the eigendecomposition of **K** and **W**<sub> $\xi$ </sub>, we find

$$\begin{aligned} \mathcal{J}_{\xi}(\mathbf{z},\eta(\mathbf{z})) &= \quad \left(\mathbf{y}^{\mathrm{err}}(\mathbf{z})\right)^{T} \left( \xi \mathbf{W}_{\xi} \mathbf{K} \mathbf{W}_{\xi} + \left(\mathbf{K} \mathbf{W}_{\xi} - \mathbf{Id}\right)^{T} \left(\mathbf{K} \mathbf{W}_{\xi} - \mathbf{Id}\right) \right) \, \mathbf{y}^{\mathrm{err}}(\mathbf{z}) \\ &= \quad \left(\mathbf{y}^{\mathrm{err}}(\mathbf{z})\right)^{T} \left(\mathbf{Id} - \mathbf{K} \mathbf{W}_{\xi}\right) \, \mathbf{y}^{\mathrm{err}}(\mathbf{z}) \\ &= \quad \left(\mathbf{y}^{\mathrm{err}}(\mathbf{z})\right)^{T} \left(\mathbf{Id} - \mathbf{K} \mathbf{W}_{\xi}\right) \, \mathbf{y}^{\mathrm{err}}(\mathbf{z}) \\ \end{aligned}$$

which implies (2.6a). Proof of (2.7) follows the exact same ideas and is here omitted.



Fig. 10: three-dimensional problem. Behavior of  $E_{\text{avg}}$  with N for several values of M, for linear and nonlinear PBDW and two noise levels (unbiased case).

We now prove (2.8). Given  $\mathbf{x} \in \mathbb{R}^M,$  exploiting the eigendecomposition of  $\mathbf{W}_{\xi}$  we find

$$\frac{1}{\xi + \lambda_{\max}(\mathbf{K})} \|\mathbf{x}\|_2^2 \le \|\mathbf{x}\|_{\mathbf{W}_{\xi}}^2 \le \frac{1}{\xi + \lambda_{\min}(\mathbf{K})} \|\mathbf{x}\|_2^2.$$



Fig. 11: three-dimensional problem. Behavior of  $E_{\text{avg}}$  with N for several values of M, for linear and nonlinear PBDW and two noise levels, (biased case).

By exploiting the latter, we obtain

$$\begin{split} \min_{\mathbf{z}\in\Phi_N} \|\mathbf{L}\mathbf{z}-\mathbf{y}\|_2^2 &\geq \quad (\xi+\lambda_{\min}(\mathbf{K}))\min_{\mathbf{z}\in\Phi_N} \|\mathbf{L}\mathbf{z}-\mathbf{y}\|_{\mathbf{W}_{\xi}}^2 \\ &= \quad (\xi+\lambda_{\min}(\mathbf{K}))\|\mathbf{L}\hat{\mathbf{z}}_{\xi}-\mathbf{y}\|_{\mathbf{W}_{\xi}}^2 \geq \frac{\xi+\lambda_{\min}(\mathbf{K})}{\xi+\lambda_{\max}(\mathbf{K})}\|\mathbf{L}\hat{\mathbf{z}}_{\xi}-\mathbf{y}\|_2^2, \end{split}$$

which is (2.8a). By observing that the generalized eigenvalues of  $\mathbf{W}_{\xi}^{1/2} \ \boldsymbol{\phi}_m = \lambda_m^{\text{gen}}$ 

$$\mathbf{K}^{-1/2}\boldsymbol{\phi}_m$$
 are given by  $\lambda_m^{\text{gen}} = \frac{\sqrt{\lambda_m(\mathbf{K})}}{\sqrt{\xi + \lambda_m(\mathbf{K})}}$  for  $m = 1, \dots, M$ , we obtain

$$\frac{\lambda_{\min}(\mathbf{K})}{\xi + \lambda_{\min}(\mathbf{K})} \|\mathbf{x}\|_{\mathbf{K}^{-1}}^2 \le \|\mathbf{x}\|_{\mathbf{W}_{\xi}}^2 \le \frac{\lambda_{\max}(\mathbf{K})}{\xi + \lambda_{\max}(\mathbf{K})} \|\mathbf{x}\|_{\mathbf{K}^{-1}}^2$$

and finally

$$\begin{split} \min_{\mathbf{z}\in\Phi_{N}} & \|\mathbf{L}\mathbf{z}-\mathbf{y}\|_{\mathbf{K}^{-1}}^{2} \geq \frac{\xi + \lambda_{\max}(\mathbf{K})}{\lambda_{\max}(\mathbf{K})} \min_{\mathbf{z}\in\Phi_{N}} \|\mathbf{L}\mathbf{z}-\mathbf{y}\|_{\mathbf{W}_{\xi}}^{2} \\ & = \frac{\xi + \lambda_{\max}(\mathbf{K})}{\lambda_{\max}(\mathbf{K})} \|\mathbf{L}\hat{\mathbf{z}}_{\xi} - \mathbf{y}\|_{\mathbf{W}_{\xi}}^{2} \geq \frac{\lambda_{\min}(\mathbf{K})}{\lambda_{\max}(\mathbf{K})} \left(\frac{\xi + \lambda_{\max}(\mathbf{K})}{\xi + \lambda_{\min}(\mathbf{K})}\right) \|\mathbf{L}\hat{\mathbf{z}}_{\xi} - \mathbf{y}\|_{\mathbf{K}^{-1}}^{2}, \end{split}$$

508 which is (2.8b).

Since  $(\hat{\mathbf{z}}_{\xi}, \hat{\eta}_{\xi})$  minimizes (2.3) over all  $(\mathbf{z}, \eta) \in \Phi_N \times \mathcal{U}$ , we have

$$\begin{aligned} &\xi \|\hat{\eta}_{\xi}\|^{2} \leq J_{\xi}(\hat{\mathbf{z}}_{\xi},\hat{\eta}_{\xi}) \leq J_{\xi}(\hat{\mathbf{z}}_{\infty},0) = \min_{\mathbf{z} \in \Phi_{N}} \|\mathbf{L}\mathbf{z} - \mathbf{y}\|_{2}^{2}; \\ &\|\boldsymbol{\ell}^{o}(\hat{\eta}_{\xi}) + \mathbf{L}\hat{\mathbf{z}}_{\xi} - \mathbf{y}\|_{2}^{2} \leq J_{\xi}(\hat{\mathbf{z}}_{\xi},\hat{\eta}_{\xi}) \leq J_{\xi}(\hat{\mathbf{z}}_{0},\hat{\eta}_{0}) = \xi \|\hat{\eta}_{0}\|^{2}. \end{aligned}$$

509 which is (2.9).

The fourth and fifth statements follow directly from the algebraic formulation of the PBDW statement, and from well-known results in convex optimization: we omit the details.

513 **Appendix B. Proof of Proposition 3.5**. We state upfront that the proof fol-514 lows the same idea of the well-known Gauss-Markov theorem ([2]) for linear unbiased 515 estimators.

516 *Proof.* Without loss of generality, we assume that  $\{\zeta_n\}_{n=1}^N$  is orthonormal; then, 517 we denote by  $\hat{\mathbf{z}}_{\xi}(\mathbf{y})$  the vector of coefficients associated with the basis  $\{\zeta_n\}_{n=1}^N$  and 518 the solution to the PBDW statement for  $\xi \in \{0, \infty\}$ , and we denote by  $\mathbf{z}_A(\mathbf{y})$  the 519 vector of coefficients associated with the algorithm A.

We first prove that  $\Lambda_2(A) \ge \Lambda_2(A^{\text{pbdw},\xi=\infty})$ . Since both PBDW and A are linear, recalling the definition of  $\mathbf{L}$ ,  $\mathbf{L}_{m,n} = \ell_m(\zeta_n)$ , we have that

$$\mathbf{z}_A(\mathbf{y}) = \hat{\mathbf{z}}_\infty(\mathbf{y}) \,+\, \mathbf{D}\,\mathbf{y}, \qquad \hat{\mathbf{z}}_\infty(\mathbf{y}) = \left(\mathbf{L}^T\mathbf{L}
ight)^{-1}\mathbf{L}^T\,\mathbf{y},$$

for a proper choice of  $\mathbf{D} \in \mathbb{R}^{N,M}$ . Since  $\Lambda_{\mathcal{U}}^{\text{bias}}(A) = 0$ , we must have  $\mathbf{z}_A(\mathbf{Lz}) = \mathbf{z}$  for all  $\mathbf{z} \in \mathbb{R}^N$ ; this implies that

$$\mathbf{z}_A(\mathbf{Lz}) = \mathbf{z} + \mathbf{D}\mathbf{Lz} \Rightarrow \mathbf{D}\mathbf{L} = 0.$$

Recalling (3.4), we shall prove that

$$s_{\max}\left(\left(\mathbf{L}^{T}\,\mathbf{L}\right)^{-1}\mathbf{L}^{T}\,+\,\mathbf{D}\right) \geq s_{\max}\left(\left(\mathbf{L}^{T}\,\mathbf{L}\right)^{-1}\,\mathbf{L}^{T}\right).$$

Towards this end, we observe that 5

$$\begin{aligned} \left(\Lambda_{2}(A)\right)^{2} &= \sup_{\mathbf{y}\in\mathbb{R}^{M}} \frac{\left\|\left(\left(\mathbf{L}^{T}\,\mathbf{L}\right)^{-1}\,\mathbf{L}^{T}\,+\,\mathbf{D}\right)\mathbf{y}\right\|_{2}^{2}}{\|\mathbf{y}\|_{2}^{2}} = \sup_{\mathbf{z}\in\mathbb{R}^{N}} \frac{\left\|\left(\mathbf{L}\left(\mathbf{L}^{T}\,\mathbf{L}\right)^{-1}\,+\,\mathbf{D}^{T}\right)\mathbf{z}\right\|_{2}^{2}}{\|\mathbf{z}\|_{2}^{2}} \\ &= \sup_{\mathbf{z}\in\mathbb{R}^{N}} \frac{\mathbf{z}^{T}\left(\left(\mathbf{L}^{T}\,\mathbf{L}\right)^{-1}\,+\,\left(\mathbf{L}^{T}\,\mathbf{L}\right)^{-1}\left(\mathbf{D}\mathbf{L}\right)^{T}\,+\,\mathbf{D}\mathbf{L}\,\left(\mathbf{L}^{T}\,\mathbf{L}\right)^{-1}\,+\,\mathbf{D}\mathbf{D}^{T}\right)\mathbf{z}}{\|\mathbf{z}\|_{2}^{2}} \\ &= \sup_{\mathbf{z}\in\mathbb{R}^{N}} \frac{\mathbf{z}^{T}\left(\left(\mathbf{L}^{T}\,\mathbf{L}\right)^{-1}\,+\,\mathbf{D}\mathbf{D}^{T}\right)\mathbf{z}}{\|\mathbf{z}\|_{2}^{2}} \geq \sup_{\mathbf{z}\in\mathbb{R}^{N}} \frac{\mathbf{z}^{T}\left(\left(\mathbf{L}^{T}\,\mathbf{L}\right)^{-1}\right)\mathbf{z}}{\|\mathbf{z}\|_{2}^{2}} \\ &= \left(\Lambda_{2}(A^{\mathrm{pbdw},\xi=\infty})\right)^{2}, \end{aligned}$$

which is the thesis. Note that in the second-to-last step we used the fact that  $\mathbf{DD}^T$ is semi-positive definite.

We now prove that  $\Lambda_{\mathcal{U}}(A) \geq \Lambda_{\mathcal{U}}(\prod_{\mathcal{Z}_N} A^{\text{pbdw},\xi=0})$ . As for the previous case, we observe that

$$\mathbf{z}_A(\mathbf{y}) = \hat{\mathbf{z}}_0(\mathbf{y}) + \mathbf{E}\mathbf{y}, \qquad \hat{\mathbf{z}}_0(\mathbf{y}) = \left(\mathbf{L}^T \mathbf{K}^{-1} \mathbf{L}\right)^{-1} \mathbf{L}^T \mathbf{K}^{-1} \mathbf{y},$$

where the matrix  $\mathbf{E} \in \mathbb{R}^{N,M}$  should satisfy  $\mathbf{EL} = 0$ . Exploiting Lemma 3.1, we find the desidered result:

$$\begin{split} \Lambda_{\mathcal{U}}(A) &= s_{\max}(\mathbf{A}\mathbf{K}^{1/2}) = \sup_{\mathbf{z} \in \mathbb{R}^{N}} \frac{\left\|\mathbf{K}^{1/2} \left(\mathbf{K}^{-1}\mathbf{L} \left(\mathbf{L}^{T}\mathbf{K}^{-1}\mathbf{L}\right)^{-1} + \mathbf{E}^{T}\right) \mathbf{z}\right\|_{2}}{\|\mathbf{z}\|_{2}} \\ &= \sup_{\mathbf{z} \in \mathbb{R}^{N}} \frac{\sqrt{\mathbf{z}^{T} \left(\left(\mathbf{L}^{T}\mathbf{K}^{-1}\mathbf{L}\right)^{-1} + \mathbf{E}\mathbf{K}\mathbf{E}^{T}\right) \mathbf{z}}}{\|\mathbf{z}\|_{2}} \geq \sup_{\mathbf{z} \in \mathbb{R}^{N}} \frac{\sqrt{\mathbf{z}^{T} \left(\mathbf{L}^{T}\mathbf{K}^{-1}\mathbf{L}\right)^{-1} \mathbf{z}}}{\|\mathbf{z}\|_{2}} \\ &= \Lambda_{\mathcal{U}} \left(\Pi_{\mathcal{Z}_{N}} A^{\text{pbdw}, \xi=0}\right). \end{split}$$

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<sup>5</sup> We recall that the maximum singular value of a matrix **B** is the square root of the maximum eigenvalue of  $\mathbf{B}^T \mathbf{B}$  or equivalently of  $\mathbf{B}\mathbf{B}^T$ .

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