PyOED: An Extensible Suite for Data Assimilation and Model-Constrained Optimal Design of Experiments

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This paper describes the first version (v1.0) of PyOED, a highly extensible scientific package that enables developing and testing model-constrained optimal experimental design (OED) for inverse problems. Specifically, PyOED aims to be a comprehensive *Python toolkit* for *model-constrained OED*. The package targets scientists and researchers interested in understanding the details of OED formulations and approaches. It is also meant to enable researchers to experiment with standard and innovative OED technologies with a wide range of test problems (e.g., simulation models). OED, inverse problems (e.g., Bayesian inversion), and data assimilation (DA) are closely related research fields, and their formulations overlap significantly. Thus, PyOED is continuously being expanded with a plethora of Bayesian inversion, DA, and OED methods as well as new scientific simulation models, observation error models, and observation operators. These pieces are added such that they can be permuted to enable testing OED methods in various settings of varying complexities. The PyOED core is completely written in Python and utilizes the inherent object-oriented capabilities; however, the current version of PyOED is meant to be extensible rather than scalable. Specifically, PyOED is developed to "enable rapid development and benchmarking of OED methods with minimal coding effort and to maximize code reutilization." This paper provides a brief description of the PyOED layout and philosophy and provides a set of exemplary test cases and tutorials to demonstrate how the package can be utilized.

Additional Key Words and Phrases: Optimal experimental design, OED, inverse problems, data assimilation

1 INTRODUCTION

Recently, interest has increased in developing scalable data assimilation (DA) and uncertainty quantification methodologies for solving large-scale inverse problems. An inverse problem refers to the retrieval of a quantity of interest (QoI) associated with or stemming from a physical phenomenon underlying partial noisy experimental or observational data of that physical system [7, 44, 51]. The QoI could be, for example, the model state, initial condition, or other physics quantity. Inverse problems are prominent in a wide spectrum of applications including power grids and atmospheric numerical weather prediction [26, 43]. In these problems, the prediction of the physical phenomena is often formulated as an initial value problem, while the initial condition of the simulator is corrected by fusing all available information. Algorithmic approaches for solving inverse problems seek either a single-point estimate of the target QoI or a full probabilistic description of the knowledge about the QoI given all available information. The underlying principle of these methods is that information collected from observational systems is fused into computational models, along with associated uncertainties, to produce an accurate estimate of the ground truth of the physical phenomena of interest. In the former approach seeking a single QoI estimate, the solution of an inverse problem is obtained by solving an optimization problem with an objective to minimize the mismatch between observational data and model simulations,

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possibly regularized by prior knowledge and uncertainty models. The latter approach, commonly known as Bayesian inversion, seeks to characterize the probability distribution of the QoI through the posterior formulated by applying Bayes' rule, that is, the probability distribution of the QoI conditioned by all available information.

DA methods [12–16, 18, 20, 26, 35, 43] aim to solve large- to extreme-scale inverse problems. They work by fusing information obtained from multiple sources, such as the dynamical model, prior knowledge, noisy and incomplete measurements, and error models, in order to better estimate the state and parameters of the physical system. This estimate improves the predictability of the simulation systems developed to make future predictions about the physical phenomena of interest.

The quality of DA systems, and hence the accuracy of their predictions, is heavily influenced by the extent to which the mathematical assumptions reflect reality and depends on the quality of the collected measurements. Optimal data acquisition is the problem of determining the optimal observational strategy, for example, from a large set of candidate observational schemes. This problem is widely formulated as an optimal experimental design (OED) problem [22, 39], where the design parameterizes and thus determines the observational configuration. In an OED problem, a design is defined to characterize a candidate configuration or a control, and the quality of the design is quantified by using a utility function. The optimal design is then defined as the one that maximizes this utility function or, equivalently, minimizes some OED criterion [9]. Since the aim of Bayesian inference is to estimate the QoI posterior, Bayesian OED seeks an observational configuration that, when combined with the underlying dynamics, would maximize information gain from the data or minimize the posterior uncertainty. Thus, an optimal design is found by solving an optimization problem with the objective to maximize a utility function that quantifies the quality of the design and its influence on the solution of the inverse problem. OED for inverse problems has experienced a recent surge in interest by the scientific computing community; see, for example, [2] and references therein.

Numerical testing and experiments are critical for developing efficient OED formulations and algorithms. This process is elementary for successful scientific research in general. Although statisticians have developed a plethora of mathematical formulations and algorithmic approaches for general-purpose OED algorithms, most of the available and publicly accessible OED software tools are limited to idealized formulations and specific applications such as finding optimal collocation points for regression problems or designing clinical experiments. In addition, they are written in the R programming language or MATLAB, thus limiting code reutilization and accessibility by a wider audience; see, for example, [24, 40, 41, 46, 52]. Unfortunately, these tools do not align well with the interests of the increasingly large computational science community for developing new OED formulations and algorithmic approaches for inverse problems, DA, and model-constrained OED [4, 8, 19, 23, 27, 28, 30, 37, 39]. As a first step in alleviating this limitation, we present and describe PyOED, a highly extensible open-source Python package written mainly to enable computational scientists to formulate and rapidly test OED—as well as DA—formulations and algorithmic approaches.

PyOED is unique in several ways. First, to the best of our knowledge, it is the first open-source package for scientific computing that allows implementing and testing the individual components of DA as well as OED systems in a unified and streamlined environment. Second, it is written in Python, which is arguably the most popular and adopted programming language for recent algorithmic developments in the computational science disciplines. It has a huge user-support community, and the learning curve is relatively smoother than that of other lower-level programming languages such as C/C++. Third, PyOED is designed in an object-oriented programming (OOP) fashion, which enables practitioners to reconfigure and reuse the individual building blocks. Moreover, it is easy to combine PyOED with

other user-defined routines, such as numerical integration of simulation models and optimization routines, which makes PyOED highly extensible and adaptable to a wide range of applications. Fourth, PyOED is not limited to a specific inverse problem formulation. Thus new DA and OED methods can be implemented and even interface with other inversion packages, for example, hIPPYlib [50]. Fifth, PyOED leverages best practices in software development, including detailed documentation with hands-on examples and robust unit-testing techniques.

The rest of this paper is organized as follows. Section 2 provides the mathematical formalism of inverse problems, DA, and OED. Section 3 describes the structure and the philosophy of the PyOED package. In Section 4 we provide a list of numerical experiments to demonstrate the general workflow and usage of PyOED. Concluding remarks are given in Section 5.

2 MATHEMATICAL BACKGROUND

In this section we provide a brief overview of the mathematical background of the PyOED core, which is important for approaching the OED problem for Bayesian inversion. In this presentation we focus on sensor placement for Bayesian inversion as a modal OED formulation. We start by discussing the forward problem in 2.1; then we introduce the inverse problem in 2.2 and the OED formalism in 2.3.

2.1 The forward problem

The forward problem maps the model parameters (e.g., the initial condition) onto the observation space. Consider the forward problem described by

$$y = \mathcal{F}(\theta) + \delta, \tag{1a}$$

where θ is the model parameter of interest, $\mathbf{y} \in \mathbb{R}^{N_{obs}}$ is the observation, and $\delta \in \mathbb{R}^{N_{obs}}$ is a noise term that accounts for the inaccuracy of the observational system. The forward operator \mathcal{F} is occasionally referred to as the "parameter-toobservable" map and generally represents a composition of a simulation/solution model S and an observation operator O. The simulation model S describes the evolution of the physical phenomena, for example, space-time advection and diffusion of a contaminant simulated over a predefined model grid. The observation operator O projects the simulated state onto the observational grid, for example, by interpolation or restriction to the observation grid. Thus, the forward problem (1a) can be rewritten as

$$\mathbf{y} = \mathbf{O} \circ \mathcal{S}(\theta) + \delta, \tag{1b}$$

where \circ is the composition operator, that is, $\mathbf{O} \circ \mathcal{S}(\theta) \equiv \mathbf{O}(\mathcal{S}(\theta))$.

It is impossible to find a simple unique formalism of the simulation model that accurately represents all possible dynamical systems. In this work and in the implementation of PyOED, we differentiate two types of simulation models: time-independent and time-dependent simulations. A wide range of time-dependent simulation models for dynamical systems governed by partial differential equations (PDEs) can be described as

$$\frac{\partial u}{\partial t} = f(u(x, t, \mu)), \tag{2}$$

where \boldsymbol{u} represents the prognostic variable(s) (e.g., physics), \boldsymbol{x} denotes the spatial coordinates, and μ defines the physics parameters of the model. To numerically solve the simulation model \boldsymbol{S} equations, we utilize spatial discretization and

temporal integration routines. If we follow a discretize-then-optimize approach, we can rewrite (2) in the form

$$\mathbf{u}_n \coloneqq \mathbf{u}(t_n) = \mathcal{S}_{t_{n-1} \to t_n}(\mathbf{u}_0, \mu), \tag{3}$$

where $\mathbf{u}_n := \mathbf{u}(t_n) \equiv \mathbf{u}(t_n, \mathbf{x}, \mu)$ is the model state at time instance t_n and $S_{t \to t+\Delta t}$ is a one-time step transition mapping that results from the application of a standard spatial discretization method (e.g., finite difference, finite volume, or finite element) and time integration scheme (e.g., Runge–Kutta routine) with a step size Δt . Thus, the prediction at time t_n can be related to the initial condition $\mathbf{u}(t_0)$ and the model parameters using the recursive application of the mapping S over a time interval $[t_0, t_n]$ as

$$\mathbf{u}_n = \mathcal{S}_{t_{n-1} \to t_n} \circ \dots \circ \mathcal{S}_{t_0 \to t_1}(\mathbf{u}_0, \mu) \,. \tag{4}$$

In space-time formulations, one can stack the model state in one long vector $\mathbf{u} := (\mathbf{u}_n^{\mathsf{T}}, \dots, \mathbf{u}_0^{\mathsf{T}})^{\mathsf{T}}$ and define the solution operator S as a block operator (e.g., a block matrix) that operates recursively on the the components of \mathbf{u} . This would enable unifying the formulation—to some extent—of the forward problem into the form (1a).

Since the observational measurements (e.g., sensory data) are not necessarily the same as the model state, we define the state-to-observable mapping $O_n(\cdot)$ to map the state u_n onto the observation space, for example, by restricting that state onto the observational grid points, as

$$\mathbf{y}(t_n) = \mathbf{O}_n(\mathbf{u}(t_n)), \tag{5}$$

which then can be used to construct a general observational vector $\mathbf{y} \in \mathbb{R}^{N_{obs}}$ representing spatiotemporal data, for example, by stacking observations at multiple time points.

Note that while we focused the discussion above on time-dependent problems, the case of time-independent simulations can be thought of as a special case of (4) where S maps, for example, the physics parameter μ to a model state **u** and the time index is dropped. In most inverse problem formulations, based on the application of interest, the inversion parameter θ stated in (1a) stands for the model physics μ , the model initial condition \mathbf{u}_0 , or both. Note also that we have omitted details including adaptive time stepping where Δt is adaptively adjusted to guarantee stability and accuracy of the time integration methodology. We intentionally remove such details from the discussion here to simplify the presentation and focus more on OED. In fact, the OED routines in PyOED are designed to solve OED problems where the utility function is regarded as a black box, thus abstracting the OED capabilities from the inverse problem definition. For these reasons, we take (1) to be an acceptable simplification that describes a forward problem setup that is general enough for our purposes in this paper.

Both the simulation model S and the observation operator O are imperfect and generally include sensory noise and representativeness errors characterizing imperfection of the map between the model space and observation space. The fact that model observations $\mathcal{F}(\theta)$ are not perfectly aligned with observational data (y) is modeled—assuming additive noise—by adding the noise term δ to the simulated observations $\mathcal{F}(\theta)$. In most applications, the observational noise follows a Gaussian distribution $\delta \sim \mathcal{N}(\mathbf{0}, \Gamma_{\text{noise}})$, where Γ_{noise} is the observation error covariance matrix that captures uncertainty stemming from sensory noise and representativeness errors. In this case, the data likelihood is

$$\mathbb{P}(\mathbf{y}|\boldsymbol{\theta}) \propto \exp\left(-\frac{1}{2} \left\|\mathcal{F}(\boldsymbol{\theta}) - \mathbf{y}\right\|_{\Gamma_{\text{noise}}^{-1}}^{2}\right),\tag{6}$$

where the matrix-weighted norm in (6) is defined as $\|\mathbf{x}\|_{\mathbf{A}}^2 = \mathbf{x}^T \mathbf{A} \mathbf{x}$ for a vector \mathbf{x} and a square symmetric matrix \mathbf{A} of conformable sizes.

2.2 The inverse problem

An inverse problem refers to the retrieval of the model parameter θ from noisy observation y, conditioned by the model dynamics. This can be achieved by finding a point estimate or by building a complete probabilistic description as discussed in Section 1. In the former, an optimization problem is solved to minimize the mismatch between the expected observations (through simulation models) and real data. This is typically employed in variational DA methods where the estimate of the true parameter is obtained by minimizing a regularized log-likelihood objective, where regularization is employed to enforce smoothness or background information on the parameter. In this case, a point estimate of the true θ is obtained by solving

$$\underset{\theta}{\arg\min} \mathcal{J}(\theta) \coloneqq \frac{1}{2} \left\| \mathcal{F}(\theta) - \mathbf{y} \right\|_{\Gamma_{\text{noise}}^{-1}}^2 + \frac{1}{2} \left\| \theta - \theta_{\text{pr}} \right\|_{\Gamma_{\text{pr}}^{-1}}^2, \tag{7}$$

where θ_{pr} is an initial guess of the unknown true value of θ . In general, the second term is added to enforce regularization or prior knowledge on the solution, for example, if the solution is assumed a priori to follow a Gaussian distribution $\theta \sim \mathcal{N}(\theta_{pr}, \Gamma_{pr})$.

Uncertainty envelopes around the single-point estimate obtained by solving (7) can be developed, for example, by using Laplacian approximation [47] where the posterior is approximated by a Gaussian distribution. This approach has been successfully employed in infinite-dimensional Bayesian inversion problems [44]. A fully Bayesian approach, on the other hand, aims to provide a consistent probabilistic description of the unknown parameter along with the associated uncertainties and is not limited to Gaussian distributions. This is achieved by describing the posterior, that is, the probability distribution of the model parameter θ conditioned by the available simulations and noisy data y, and is obtained by applying a form of Bayes' theorem

$$\mathbb{P}(\theta|\mathbf{y}) \propto \mathbb{P}(\mathbf{y}|\theta) \mathbb{P}(\theta), \qquad (8)$$

where $\mathbb{P}(\theta)$ is the prior, $\mathbb{P}(\mathbf{y}|\theta)$ is the data likelihood, and \propto indicates removal of a normalizing constant in the right-hand side of (8). For further details on Bayesian inversion see, for example, [43, 44]. Given the posterior (8), one can use the maximum a posteriori (MAP) point as an estimate of the true unknown QoI or follow a Monte Carlo approach to sample the posterior, thus building a complete probabilistic picture; see, for example, [16]. Both the variational and the Bayesian inference approaches provide a plethora of techniques for statistical data analysis in general, and specifically for solving inverse problems.

The Bayesian perspective provides a formal mathematical ground for estimating the physical QoI, for example, the model parameter θ , along with the associated uncertainties given the available sources of information. In many cases, however, this inversion is an intermediate step, and the goal QoI is a function of the model parameter, that is, $\rho := \mathcal{P}(\theta)$. A goal-oriented approach is followed in this case where one aims to inspect the posterior of the QoI conditioned by the available data [32, 33].

The ideal case: linear Gaussian problems. If the forward operator \mathcal{F} is linear (or linearized), and assuming Gaussian observational noise and a Gaussian prior $\mathcal{N}(\theta_{\text{pr}}, \Gamma_{\text{pr}})$, then the posterior is Gaussian $\mathcal{N}(\theta_{\text{post}}^{y}, \Gamma_{\text{post}})$ with

$$\Gamma_{\text{post}} = \left(\mathbf{F}^* \Gamma_{\text{noise}}^{-1} \mathbf{F} + \Gamma_{\text{pr}}^{-1} \right)^{-1}, \quad \theta_{\text{post}}^{\mathbf{y}} = \Gamma_{\text{post}} \left(\Gamma_{\text{pr}}^{-1} \theta_{\text{pr}} + \mathbf{F}^* \Gamma_{\text{noise}}^{-1} \mathbf{y} \right), \tag{9}$$

where $\mathbf{F} \equiv \mathcal{F}$ is the forward model and \mathbf{F}^* is the associated adjoint. Despite being simple, this setup (9) is of utmost importance in the Bayesian inversion and OED literature and is elementary for testing implementations of new DA and

OED approaches, mainly because the posterior can be formulated exactly. Moreover, in many large-scale applications, the posterior can be approximated, to an acceptable degree, by a Gaussian distribution obtained by linearizing the nonlinear operator \mathcal{F} around the MAP estimate. The linearized model is also known as the tangent linear model (TLM) obtained by differentiating \mathcal{F} .

As mentioned earlier, inversion for the parameter θ is often an intermediate stage, and the end-goal is to describe the posterior of a general QoI that is not the model parameter θ but rather a goal quantity ρ that depends on the inversion parameter θ . Specifically, goal-oriented inversion seeks the posterior $\mathbb{P}(\rho|\mathbf{y}) \propto \mathcal{L}(\mathbf{y}|\rho, \theta)\mathbb{P}(\rho)$, where $\mathbb{P}(\rho)$ is a prior on the goal QoI and $\mathcal{L}(\mathbf{y}|\theta) = \mathcal{L}(\mathbf{y}|\rho,\theta)$ is the data-likelihood (6), where ρ is determined completely based on θ . We focus the discussion here on the case of linear prediction operators **P**. That is, we consider prediction quantities of the form

$$\rho = \mathbf{P}\theta,\tag{10}$$

where **P** is a linear prediction operator. Within the Gaussian linear setting, the prior of the goal QoI ρ is $\mathcal{N}(\rho_{\text{pr}}, \Sigma_{\text{pr}})$ with

$$\rho_{\rm pr} = \mathbf{P}\theta_{\rm pr}, \qquad \Sigma_{\rm pr} = \mathbf{P}\Gamma_{\rm pr}\mathbf{P}^*, \tag{11}$$

where \mathbf{P}^* is the adjoint of the prediction operator \mathbf{P} . The posterior distribution of the prediction ρ , conditioned by the observations \mathbf{y} , is also Gaussian and is given by $\mathcal{N}(\rho_{\text{post}}, \Sigma_{\text{post}})$, where

$$\rho_{\text{post}} = \mathbf{P}\theta_{\text{post}}^{\mathbf{y}}, \qquad \Sigma_{\text{post}} = \mathbf{P}\Gamma_{\text{post}}\mathbf{P}^* = \mathbf{P}\left(\mathbf{F}^*\Gamma_{\text{noise}}^{-1}\mathbf{F} + \Gamma_{\text{pr}}^{-1}\right)\mathbf{P}^*.$$
(12)

Note that the goal-oriented Bayesian inversion falls back to the standard formulation of a Bayesian inverse problem if the prediction operator \mathcal{P} is an identity operator.

2.3 Optimal experimental design

Here we outline the basics of an OED problem for Bayesian inversion. An excellent review of recent advances on model-constrained OED can be found in [1]. An OED optimization problem takes the general form

$$\zeta^{\text{opt}} = \underset{\zeta}{\arg\max} \, \mathcal{U}(\zeta) \,, \tag{13}$$

where \mathcal{U} is a predefined utility function that quantifies the quality of the design ζ . The nature of ζ depends on the application at hand, and the utility function \mathcal{U} is chosen to enable defining what an "optimal" design is. The optimization problem (15) is often associated with an auxiliary sparsity-enforcing term $-\alpha \Phi(\zeta)$ to prevent dense designs and to reduce the cost associated with deploying observational sensors. The utility function can be rewritten as

$$\mathcal{U}(\zeta) = \Psi(\zeta) - \alpha \Phi(\zeta), \tag{14}$$

where $\Psi(\cdot)$ is an OED optimality objective, referred to hereafter as the "optimality criterion," which is defined based on the inverse problem at hand and on a chosen criterion (e.g., from the well-known OED alphabetic criteria). The function $\Phi(\zeta)$ asserts regularization or sparsity on the design. For example, this could be a resource constraint: $\sum_{i}^{n_s} \zeta_i = ||\zeta|| \le k$, or $\sum_{i}^{n_s} \zeta_i = ||\zeta|| = k$; $k \in \mathbb{Z}_+$, for example, an upper bound (or exact budget) on the number of sensors (in OED). It also could be a sparsifying (possibly nondifferentiable) function, for example, $||\zeta||_0$, $||\zeta||_1$.

Generally speaking, we seek a design that maximizes the utility function \mathcal{U} . Other formulations, however, involve minimization of an OED optimality criterion; see, for example, [8]. Both formulations are adopted in the OED literature

and in PyOED and often are even equivalent, as explained below. In inverse problems, a design can be associated with the observational configuration and thus can be used to optimally select an optimal observational policy. For example, a design can be defined to select sensor location or temporal observation frequency that can help provide accurate prediction with minimum uncertainty, or it can be defined to select an observational configuration that guarantees maximum information gain from the data.

OED for sensor placement. In sensor placement we associate a binary design variable ζ_i with the *i*th candidate sensor location with 1 meaning activating the sensor and deactivating it otherwise. This defines the design as a binary vector $\zeta \equiv \zeta^b \in \{0, 1\}^{n_s}$, which collectively define the observational configuration. In this case, the OED problem (13) takes the form

$$\boldsymbol{\zeta}^{\text{opt}} = \underset{\boldsymbol{\zeta} \in \{0,1\}^{n_{\text{s}}}}{\arg \max} \, \mathcal{U}(\boldsymbol{\zeta}) \coloneqq \Psi(\boldsymbol{\zeta}) - \alpha \Phi(\boldsymbol{\zeta}) \,. \tag{15}$$

In Bayesian OED for sensor placement, the observation covariance Γ_{noise} is replaced with a weighted version $W_{\Gamma}(\zeta)$, resulting in the weighted data-likelihood

$$\mathcal{L}(\mathbf{y}|\boldsymbol{\theta};\boldsymbol{\zeta}) \propto \exp\left(-\frac{1}{2} \|\mathbf{F}(\boldsymbol{\theta}) - \mathbf{y}\|_{\mathbf{W}_{\Gamma}(\boldsymbol{\zeta})}^{2}\right),\tag{16a}$$

where the weighted observation error covariance matrix takes the form

$$\mathbf{W}_{\Gamma}(\boldsymbol{\zeta}) := \left(\mathbf{W}(\boldsymbol{\zeta})\Gamma_{\text{noise}}\mathbf{W}(\boldsymbol{\zeta})\right)^{\mathsf{T}} = \mathbf{L}^{\mathsf{T}}(\boldsymbol{\zeta})\left(\mathbf{L}(\boldsymbol{\zeta})\left(\mathbf{W}(\boldsymbol{\zeta})\Gamma_{\text{noise}}\mathbf{W}(\boldsymbol{\zeta})\right)\mathbf{L}^{\mathsf{T}}(\boldsymbol{\zeta})\right)^{-1}\mathbf{L}(\boldsymbol{\zeta}), \tag{16b}$$

where \dagger denotes the Moore–Penrose (pseudo) inverse and $\mathbf{W}(\zeta) := \text{diag}(\zeta)$ is a diagonal matrix with the binary design $\zeta \in \{0, 1\}^{n_s}$ on its diagonal. $\mathbf{L}(\zeta)$ is a sparse matrix that extracts nonzero rows/columns from the design matrix \mathbf{W}_{Γ} ; see [9] for further details.

The utility function . In the case of linear Bayesian inversion, the posterior is Gaussian with the covariance being independent from the actual realizations of the data, as shown by (9) and (12). This fact enables designing observational policies before actually deploying the observational sensors. Specifically, in linear Bayesian OED, we set the objective to minimize a scalar summary of the posterior uncertainty, that is, the posterior covariance matrix. This is the underlying principle of the alphabetical criteria [38]. For example, an A-optimal design is the one that minimizes the trace of the posterior covariance matrix, and a D-optimal design is the one that minimizes its determinant (or equivalently the log-determinant). Note that in the case of a linear model F, the Fisher information matrix FIM is equal to the inverse of the posterior covariance matrix, that is, $FIM = \Gamma_{post}^{-1}(\zeta) = F^*W_{\Gamma}(\zeta)F + \Gamma_{pr}^{-1}$. Thus, in this case the utility function—discarding the penalty term—is set to $\mathcal{U}(\zeta) := \text{Tr}(FIM(\zeta))$ for A-optimal designs and $\mathcal{U}(\zeta) := \log \det(FIM(\zeta))$ for D-optimal designs, and then the utility function is maximized.

When the model \mathcal{F} is nonlinear, the FIM requires evaluating the TLM at the true parameter, that is, $\mathbf{F} = \partial \mathcal{F}|_{\theta = \theta_{true}}$. Thus, to obtain an optimal design, one can iterate over finding the MAP estimate of θ and solving an OED problem with Gaussian approximation around that estimate. Other utility functions employed in nonlinear OED problems or non-Gaussian distributions include the Kullback–Leibler divergence between the posterior and the prior [29].

Popular solution approaches. The OED problem (15) can be viewed as a mixed-integer program and can be solved by using branch-and-bound [25, 31]. However, this type of research has not yet been applied to model-constrained-OED. A

common approach to solving (15) is to replace the binary optimization with the following relaxation:

$$\boldsymbol{\zeta}^{\text{opt}} = \underset{\boldsymbol{\zeta} \in [0,1]^{n_{\text{s}}}}{\arg \max} \, \boldsymbol{\mathcal{U}}(\boldsymbol{\zeta}) \,, \tag{17}$$

where the design variables are relaxed to take any values in the interval [0, 1] rather than only the binary values $\{0, 1\}$. This approach, if carried out properly, has the effect of generating a continuous relaxation surface that connects the values of the objective evaluated at the binary designs; see [9] for further details. A gradient-based optimization approach is generally used to solve (17), which requires developing the gradient of both the optimality criterion Ψ and the penalty Φ with respect to the design ζ .

As mentioned earlier, the penalty term is generally chosen to promote sparsity on the design. A popular penalty function is based on the ℓ_0 norm to promote design sparsity and is thus nonsmooth and consequently is nondifferentiable. This difficulty can be alleviated, for example, by approximating the effect of ℓ_0 with a sequence of differentiable functions that converge in effect to the ℓ_0 ; see, for example, [3]. In order to guarantee continuity of the relaxation surface, the weighted precision matrix is defined in the general form

$$\mathbf{W}_{\Gamma}(\boldsymbol{\zeta}) := \left(\mathbf{W}(\boldsymbol{\zeta}) \odot \boldsymbol{\Gamma}_{\text{noise}}\right)^{\mathsf{T}},$$

$$\mathbf{W}_{i,j}(\boldsymbol{\zeta}) := \begin{cases} \omega_i \, \omega_j & ; i \neq j \\ 0 & ; \omega_i = 0 \\ \frac{1}{\omega_i^2} & ; \omega_i \neq 0 \end{cases}; \quad i, j = 1, 2, \dots, n_s,$$
(18)

where \odot is the Hadamard (Schur) product of matrices and $\omega_i \in [0, 1]$ is a weight calculated by using ζ_i , for example, $\omega_i := \zeta_i$; see [9] for additional details. The formulation (18) guarantees that for $\zeta_i \in [0, 1]^{n_s}$ it holds that $\lim_{\zeta \to \zeta^b} W_{\Gamma}(\zeta) = W_{\Gamma}(\zeta^b)$ for a binary design $\zeta^b \in \{0, 1\}^{n_s}$ and thus guarantees continuity of the relaxation surface. Thus, the solution of the relaxed OED optimization problem (17) is guaranteed to match the solution of the original binary OED optimization problem.

The A- and D-optimal design relaxed optimization problems (17) take the following respective forms:

$$\boldsymbol{\zeta}^{\text{A-opt}} = \underset{\boldsymbol{\zeta} \in [0,1]^{n_{\text{s}}}}{\arg\max} := \operatorname{Tr} \left(\mathbf{P} \left(\mathbf{F}^* \left(\boldsymbol{\Gamma}_{\text{noise}} \odot \mathbf{W}(\boldsymbol{\zeta}) \right)^{\dagger} \mathbf{F} + \boldsymbol{\Gamma}_{\text{pr}}^{-1} \right)^{-1} \mathbf{P}^* \right)^{-1} - \alpha \Phi(\boldsymbol{\zeta}),$$
(19a)

$$\boldsymbol{\zeta}^{\text{D-opt}} = \underset{\boldsymbol{\zeta} \in [0,1]^{n_{\text{s}}}}{\arg\max} := \log \det \left(\mathbf{P} \left(\mathbf{F}^* \left(\boldsymbol{\Gamma}_{\text{noise}} \odot \mathbf{W}(\boldsymbol{\zeta}) \right)^{\dagger} \mathbf{F} + \boldsymbol{\Gamma}_{\text{pr}}^{-1} \right)^{-1} \mathbf{P}^* \right)^{-1} - \alpha \Phi(\boldsymbol{\zeta}) \,. \tag{19b}$$

The most important piece of information for solving the relaxation (17) is the gradient of the utility function; see, for example, [9] for a detailed derivation of the gradients of the objective functions in (19). Gradient formulation, however, is mathematically involved and can be extremely computationally demanding because it requires numerous evaluations of the forward operator, the goal operator, and the corresponding adjoints. Moreover, the penalty function $\Phi(\cdot)$ is required to be differentiable.

A stochastic learning approach to binary OED has been recently presented in [10], to solve the binary optimization problem (15) without the need for relaxation. This approach does not require differentiability of the utility function \mathcal{U} .

In this approach the optimal design is defined as

$$\mathbf{p}^{\mathsf{opt}} = \underset{\mathbf{p} \in [0,1]^{n_{\mathsf{s}}}}{\arg\max} \mathbb{E}_{\boldsymbol{\zeta} \sim \mathbb{P}(\boldsymbol{\zeta} \mid \mathbf{p})} \Big[\mathcal{U}(\boldsymbol{\zeta}) - b \Big],$$
(20)

where $\mathbb{P}(\zeta | \mathbf{p})$ is a multivariate Bernoulli distribution with parameter \mathbf{p} specifying probabilities of success/activation of each entry of ζ , that is, $\mathbf{p}_i \in [0, 1]$. Here *b* is a constant "baseline" used to minimize variability of the stochastic estimate of the gradient; see [10] for further details. Algorithm 1 summarizes the procedure followed to solve (20).

Algorithm 1 Stochastic optimization for binary OED with the optimal baseline.

Input: Initial distribution parameter $\mathbf{p}^{(0)}$, step size schedule $\eta^{(n)}$, sample sizes N_{ens}, *m*, baseline batch size b_m Output: ζ^{opt} 1: initialize n = 02: while Not Converged do Update $n \leftarrow n + 1$ 3: Sample { $\boldsymbol{\zeta}[j]; j = 1, 2, \dots, N_{ens}$ } ~ $\mathbb{P}\left(\boldsymbol{\zeta}|\mathbf{p}^{(n)}\right)$ 4: Calculate $b = \text{OPTIMALBASELINE}(\mathbf{p}^{(n)}, \text{N}_{ens}, b_m)$ Calculate $\mathbf{g}^{(n)} = \frac{1}{N_{ens}} \sum_{j=1}^{N_{ens}} (\mathcal{J}(\boldsymbol{\zeta}[j] - b)) \sum_{i=1}^{n_s} \left(\frac{\boldsymbol{\zeta}_i[j]}{\mathbf{p}_i} + \frac{\boldsymbol{\zeta}[j]_i - 1}{1 - \mathbf{p}_i}\right) \mathbf{e}_i$ 5: 6: Update $\mathbf{p}^{(n+1)} = \mathbf{L} \left(\mathbf{p}^{(n)} - \eta^{(n)} g^{(n)} \right)$ 7: 8: end while Set $\mathbf{p}^{\text{opt}} = \mathbf{p}^{(n)}$ 9: Sample { $\zeta[j]$; j = 1, 2, ..., m} ~ $\mathbb{P}(\zeta|\mathbf{p}^{\text{opt}})$, and calculate $\mathcal{J}(\zeta[j])$ 10: 11: **return** ζ^{opt} : the design ζ with smallest value of \mathcal{J} in the sample. 12: **function** OptimalBaseline(θ , N_{ens}, b_m) Initialize $b \leftarrow 0$ 13: for $e \leftarrow 1$ to b_m do 14: **for** $j \leftarrow 1$ to N_{ens} **do** 15 $\begin{array}{l} \text{Sample } \zeta[j] \sim \mathbb{P}\left(\zeta|\mathbf{p}\right) \\ \text{Calculate } \mathbf{r}[j] = \sum_{i=1}^{n_s} \left(\frac{\zeta_i[j]}{\mathbf{p}_i} + \frac{\zeta[j]_i - 1}{1 - \mathbf{p}_i}\right) \, \mathbf{e}_i \end{array}$ 16: 17: end for 18: Calculate $\mathbf{d}[e] = \frac{1}{N_{\text{ens}}} \sum_{j=1}^{N_{\text{ens}}} \mathbf{r}[j]$, and $\mathbf{g}[e] = \frac{1}{N_{\text{ens}}} \sum_{j=1}^{N_{\text{ens}}} \mathcal{J}(\boldsymbol{\zeta}[j]) \mathbf{r}[j]$ Update $b \leftarrow b + (\mathbf{g}[e])^{\mathsf{T}} \mathbf{d}[e]$ 19: 20: end for 21: Update $b \leftarrow b \operatorname{N}_{ens} / \left(b_m \sum_{i=1}^{n_s} \frac{1}{\mathbf{p}_i - \mathbf{p}_i^2} \right)$ 22: 23: return b 24: end function

Note that we do not provide an exclusive set of formulations or solution approaches in this study. We provide here only an exemplary set of formulations and algorithms used to inspire the development of PyOED, which itself can be used to test further formulations and algorithmic approaches.

3 PYOED: STRUCTURE AND PHILOSOPHY

PyOED aims to provide a unified platform for implementing and testing model-constrained OED algorithmic approaches including formalisms (15), (17), (19), and (20). Solving model-constrained OED and inverse problems requires proper understanding and formulation of the underlying dynamical system, observational configuration, uncertainty models,

DA and inversion algorithms, and the OED objective [48] and the selected utility function. PyOED is a stand-alone, yet extensible, Python package that provides users and researchers in the computational science and engineering disciplines with a testing suite that effectively glues these components in an OOP fashion. For example, PyOED provides a variety of time-dependent and time-independent simulation models. These include systems governed by linear algebraic equations, ordinary differential equations, and PDEs. PyOED is also equipped with a set of classes implementing various observational operators, probabilistic uncertainty models, and DA and OED methods. A high-level overview of the PyOED major components and their coupling for solving DA and OED problems is provided in Figure 1. In Section 3.1 we briefly describe the main components of PyOED and outline the functionality they provide in correspondence with the diagram 1.

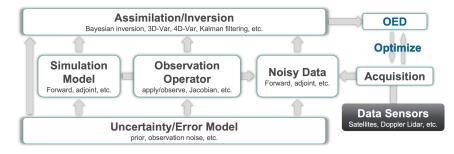


Fig. 1. High-level overview of the main components of PyOED.

3.1 Code structure

Figure 2 shows the main subpackages (ordered alphabetically) shipped with the current version of PyOED (v1.0). The rest of this section 3.1 provides a high-level description of the packages/subpackages of PyOED as displayed in Figure 2.

pyoed.models. Following the convention in the DATeS package [15], we use the word "model" to refer to three entities: *the simulation model, the observation model (or operator)*, and *the error models*.

The simulation model provides a prediction about the behavioral pattern of the physical phenomena of concern. In the current version of PyOED (v1.0) we provide various simulation models under the pyoed.models.simulation_models, including several versions of the Lorenz system [34] and advection-diffusion models. The structure of these prototypical simulation models should provide clear guidelines to practitioners willing to adopt PyOED for their particular applications.

The observation operator maps the model state onto the observation grid, thus providing a functional mapping between the model state and observational data. Two of the most prominent observation operators in experimental settings are the identity operator and an interpolator. PyOED provides implementations of several observation operators including these two, with an observational design properly incorporated to enable altering observational configurations at any point in the DA or OED solution process. Observation operators are provided in the pyoed.models.observation_operators subpackage.

The error models quantify the uncertainty associated with the model parameter, model state, and observational data. An experimental design can be associated with any of these pieces. For example, in sensor placement, an experimental

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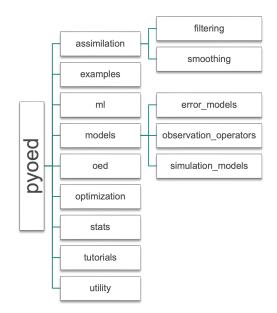


Fig. 2. Main subpackages (ordered alphabetically) available in the current version of PyOED (v1.0).

design is associated with the observational grid; thus, modifying the observational design affects the observational error model. For example, in the relaxation approach (19), the design weights scale the entries of the covariance matrix, and the stochastic approach (20) works by removing rows/columns of the observation error covariance matrix corresponding to zero design variables. PyOED provides various implementations of error models suitable for modeling priors, as well as observational errors in Bayesian inversion, where a design variable is consistently implemented to enable modifying the experimental design during any step of the DA and/or OED solution process. The current version of PyOED (v1.0) provides various error model implementations through the subpackage pyoed.models.error_models, including a Gaussian model and Laplacian model.

pyoed.assimilation. PyOED provides a set of DA tools that include algorithms for "filtering" and "smoothing." These two terms are widely used in the DA literature. The former algorithm solves inverse problems that involve time-independent or time-dependent simulation models, while the latter algorithm is restricted to time-dependent models. Filtering involves prediction (of observation) using the parameter-to-observable map, followed by a correction procedure to correct knowledge of the QoI given the observational data. In filtering for time-dependent simulations, the observational data is assimilated sequentially, with one observation time per assimilation window/cycle. Examples of filtering DA methods include three-dimensional variational DA, and Kalman filtering [6, 21]. Smoothing, on the other hand, is concerned with history matching; these algorithms try to find the QoI that best matches multiple spatiotemporal observations (a trajectory) and is usually defined as an initial value problem. Examples include space-time Bayesian inversion [45] and four-dimensional variational DA [6], for which vanilla implementations are provided in PyOED. Implementations of filtering DA algorithms are provided through pyoed.assimilation.filtering, and smoothing algorithms are provided in pyoed.assimilation.smoothing. pyoed.optimization. Numerical optimization routines are elementary for solving OED optimization problems, as well as the variational approaches for solving DA problems. A variety of optimization software packages can be used for solving numerical optimization problems including those described in this work. PyOED enables using external optimization packages, including Python's Scipy package, to solve DA and OED optimization problems. PyOED, however, provides specific implementations of optimization procedures not available in popular optimization packages, such as the stochastic algorithm described by Algorithm 1, various versions of the stochastic average approximation (SAA) algorithm, and robust optimization [11].

pyoed.ml. This subpackage is intended to provide implementations of machine learning algorithms useful for DA and OED applications. For example, the stochastic learning approach to OED (20) can be seen as a reinforcement learning (RL) approach to solving the OED problem. The module pyoed.ml.reinforcement_learning under this package provides implementation of RL components, including an agent, a policy, transition probability, actions, and utility functions.

pyoed.stats. This package aims to collect statistical procedures used by other parts of the package, such as sampling routines, and implementation of random variables and their probabilistic utility functions including density evaluation and log-probabilities. This version of PyOED (v1.0) provides an exemplary implementation of a multivariate Bernoulli distribution required by the RL algorithm 1. Since statistical tools are crucial for various DA and OED algorithms, we chose to keep the subpackage pyoed.stats rather than moving these implementations to other parts of the package. This approach is advantageous because we continuously extend the package with various statistical tools, for example, for randomized approximation methods for Bayesian inversion.

pyoed.oed. OED is the main component of PyOED that provides implementations of various algorithmic approaches for solving OED problems, including relaxation (19) and stochastic learning (20), as well as recent developments including robust OED [11]. Most implementations in this package take an inverse problem (DA object) as input and use it to access all the underlying components, thus gaining access to the simulation model, error models, and observation operator as well as the experimental design. This approach enables the user to modify an experimental design, solve the DA problem if needed, and solve the underlying OED optimization problem. The core OED functionalities in most PyOED routines, however, can be used with black-box utility functions, waiving the need for an inverse problem if needed.

pyoed.utility. This subpackage aims to collect implementations of general-purpose functionality, such as file I/O and visualization, as well as general mathematical and statistical procedures. The subpackage includes matrix-free implementations of expensive operations such as evaluating the trace and log-determinant of a matrix. It also provides routines to approximate matrix trace using statistical randomization [5, 42].

pyoed.examples. This subpackage provides various example scripts that users can follow to learn how to effectively use various pieces of the package. The modules in this subpackage explain how to load all pieces of the subpackage independently and explain how to properly coordinate these components to design a consistent DA and/or OED experiment.

pyoed.tutorials. Given the popularity of Jupyter Notebooks in the computational science community, we converted some of the examples in the subpackage pyoed.examples to Jupyter Notebooks and provided them in this subpackage pyoed.tutorials. We employ them in the test cases presented in Section 4. We can add more tutorials on reasonable demand.

3.2 PyOED utilization workflow

While the components of DA and OED problems can be used independently of each other, some level of ordering is mandatory for proper utilization. For example, an inverse problem (DA) object cannot be instantiated before a simulation model, an observation operator, and error model objects. Similarly, an OED problem for Bayesian inversion cannot be solved before creating an inverse problem. The general workflow for utilizing PyOED components is displayed in Figure 3. A practical guide that illustrates how to follow this simple workflow is described in Section 4.

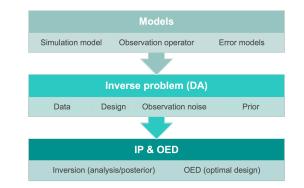


Fig. 3. Workflow describing initialization order and access level of PyOED components.

3.3 Extending and contributing to PyOED

PyOED is meant to be extensible. Thus, we continuously interface other software tools that provide efficient implementations of the components of DA and OED problems. For example, hIPPYlib [50] is a software package for solving high-dimensional inverse problems following an optimize-then-discretize approach. It has been employed to empirically verify several inversion and OED algorithmic developments recently. Instead of rebuilding the functionality of hIPPYlib and similar packages, we have interfaced with some of its components to show how easily and efficiently PyOED can extend other successful packages. For example, PyOED interfaces with finite-element (FE) implementations of advection-diffusion and Poisson models from hIPPYlib as well-as point observation operators. However, such extension does not hinder the functionality or limit the extensibility of PyOED. Specifically, interfacing with such external packages is optional and is not provided in the core of PyOED, mainly because the backbone of these packages is not guaranteed not to be quickly outdated or be unmaintained. Thus, these extensions (e.g., interfacing with hIPPYlib) are made optional during the import process of PyOED subpackages, and dependent functionality is used only when properly installed and available on the current architecture.

3.4 Code availability

The development version of PyOED is available from https://gitlab.com/ahmedattia/pyoed.

4 TEST CASES

PyOED comes with a set of prototypical test problems with increasing complexity for both DA and OED. An ideal case typically used in scientific publications is the linear Gaussian setup, where the simulation model and the observation operator are both linear and the error models (observation noise and the prior) are both Gaussian; see Section 2. In this case, the posterior is also a Gaussian; the solution of the inverse problem is unique—the posterior mean and mode (MAP) are identical; and posterior moments (mean and covariance) both have closed forms that can be obtained by applying the Kalman filter theory. Such a simplified setup can be used for testing new formulations in both DA and OED, and thus it is provided in PyOED. We discuss this formulation and in Section 4.1 show how it can be utilized. In Section 4.2 we discuss in further detail a standard experiment widely used in OED scientific research and offered by PyOED.

4.1 An ideal setup: linear Gaussian toy problem

Consider a time-dependent forward problem defined at time instances $t_0 + i\Delta t$, $i = 0, 1, ..., n_t$, for a fixed step size Δt , as follows:

$$\mathbf{u}_n = \mathbf{A} \, \mathbf{u}_{n-1} \,, \qquad \mathbf{y}_n = \mathbf{I} \mathbf{u}_n + \delta \,, \quad n = 1, 2, \dots, \tag{21}$$

where $\mathbf{u}_n \in \mathbb{R}^{N_{\text{state}}}$ is the discrete model state at time instance t_n , $\mathbf{A} \in \mathbb{R}^{N_{\text{state}} \times N_{\text{state}}}$ is a matrix representing model evolution over time interval $[t_{n-1}, t_n]$, and I is the identity observation operator/matrix. If we assume $\delta \sim \mathcal{N}(\mathbf{0}, \mathbf{R})$ and assume a Gaussian prior $\mathbf{u}_0 \sim \mathcal{N}(\mathbf{u}_0^{\text{pr}}, \Gamma_{\text{pr}})$, then the posterior is Gaussian $\mathcal{N}(\mathbf{u}_0^{\text{post}}, \Gamma_{\text{post}})$ with

$$\Gamma_{\text{post}} = \left(\mathbf{A}^{\mathsf{T}}\mathbf{R}^{-1}\mathbf{A} + \Gamma_{\text{pr}}^{-1}\right)^{-1}, \qquad \mathbf{u}_{0}^{\text{post}} = \Gamma_{\text{post}}\left(\Gamma_{\text{pr}}^{-1}\mathbf{u}_{0}^{\text{pr}} + \sum_{i=1}^{n_{t}}\mathbf{A}^{\mathsf{T}}\mathbf{R}^{-1}\mathbf{y}\right).$$
(22)

Since (22) is a closed form of the posterior, we can use it to test and debug new DA and OED implementations. This fact is highly utilized in the unit tests developed in PyOED. To create a proper experiment, we will follow the workflow described by Figure 3. In the rest of this section (4.1) we describe how to initialize an inverse problem in PyOED with the settings (22), and we provide a simple scheme that can be followed to initialize other experiments. The code summarized here is provided in the pyoed.examples.fourDVar_driver module with additional comments, details, and capabilities that can help the user understand the workflow for creating and solving an inverse problem. A Jupyter Notebook pyoed.tutorials.toy_linear is also available and can be used to regenerate the numerical results presented in this section (4.1).

Creating the models. Assuming PyOED is already in the Python path, the first step is to import/load the simulation model (that describes A), the observation operator (here an identity operator), and the error models to create the prior and the observation error model. This can be done as described in the code snippet 1.

1 from pyoed.models.simulation_models.toy_linear import ToyLinearTimeDependent

² from pyoed.models.observation_operators.identity import Identity

3 from pyoed.models.error_models.Gaussian import GaussianErrorModel

Snippet 1. Import essential modules to create the simulation model object, the observation operator, the prior, and the observation error model.

Note that we have imported only the classes we need in this example. However, PyOED provides several other implementations of the simulation models, observation operators, and error models. In order to create a simulation model, an object of ToyLinearTimeDepndent is instantiated as described by snippet 2. This generates an internal two-dimensional array of size 5×5 that represents the forward model **A**, which integrates the model state forward by a timestep dt = 0.1. That internal array can be reproduced by setting the random_seed parameter in the passed configurations dictionary.

n model = ToyLinearTimeDependent(configs={'nx':5, 'dt':0.1, 'random_seed':123})

Snippet 2. Instantiate the simulation model object.

Since each simulation model has its own configurations, many of which are assigned default values, we follow the strategy of DATeS [15] and use dictionaries to pass model arguments. PyOED aggregates and validates the passed dictionary against the default values and initiates the model accordingly. For example, in snippet 2 we specify a random_seed argument that guarantees reproducibility of any randomly generated data inside the model object. This is done by keeping an internal random state inside the model object that is independent from other objects and is initialized to the passed random seed. Thus, if no random seed is passed, each time the same model object is instantiated, completely random sequences will be generated if requested. Implementations of simulations model must provide an implementation of a class-level method get_default_configs that returns a dictionary with all default values used if not passed upon instantiation. In order to ensure that, all PyOED simulation models inherit the class pyoed.models.simulation_models.SimulationModel that guarantees enforcing the implementation of mandatory methods required for the seamless integration of various components in PyOED. The final configurations of a simulation model is a combination of those in the passed configurations dictionary and the default values, with precedence given to the passed configurations. The simulation model's configurations (a copy of it, in fact) can be accessed through the attribute configurations. We generally choose to return a copy to guarantee that all settings are validated before modification. For example, one cannot modify the time step dt without verifying whether the timestepping implementation is tied to that time step or not and updating dependencies accordingly.

The observation operator. Similar to simulation models, an observation operator is created by passing the settings in the configurations dictionary to the observation operator class constructor as shown in snippet 3. Thus, the observation operator has access to the model grid and other useful attributes to create and manipulate data structures (such as the model state) without having to provide any new implementations. This is mainly because observations in this case are the same as the corresponding model states (discarding observation noise).

obs_oper = Identity(configs={'model':model})

Snippet 3. Create an identity observation operator.

The prior and the data noise models. The error models (prior and observation noise) are created in this example as shown in snippet 4. Note that the random_seed configurations variable is used to set the random number generator for reproducibility. This enables us regenerate a set of experiments and generate proper benchmarks for a fair comparison between various implementations. As mentioned earlier, if no random seed is passed, each instance of the error model is assigned a randomly generated state that guarantees that each instance has its own different sequence of random numbers/vectors realizations.

prior = GaussianErrorModel(configs={'size':model.state_size, 'mean':1, 'variance':1, 'random_seed':1})
obs_noise = GaussianErrorModel(configs={'size':obs_oper.shape[0], 'variance':0.01, 'random_seed':1})

Snippet 4. Create the prior and the observation error model.

The inverse problem (DA) object. The next step is to put these models together in action and use them to create an inverse problem. We illustrate the utilization of a DA object to solve the inverse problem following a 4DVar formulation. The literature provides a plethora of variants of the general 4DVar scheme. PyOED provides a few implementations; however, the most basic (vanilla) implementation is used here for illustration. Two approaches are followed in PyOED for instantiating a DA object. The first is to pass all configurations (upon initialization) in the configurations dictionary configs similar to the case of simulation models, error models, and observation operators. The second approach is to use the proper registration methods associated with the created object after instantiation. The latter can be also used to update components of the DA object after initialization. For example, one might want to change the settings of the assimilation time window, register new observations or remove the old ones, or modify or even change the prior. Since the first approach has already been explained with the simulation and error models, we demonstrate the second approach here. Specifically, a 4DVar assimilation object is created as in snippet 5.

```
inverse_problem = VanillaFourDVar()
```

inverse_problem.register_model(model)

```
inverse_problem.register_observation_operator(obs_oper)
```

```
4 inverse_problem.register_prior_model(prior)
```

```
inverse_problem.register_observation_error_model(obs_noise)
```

Snippet 5. Create the inverse problem object with default settings, and then add (register) all the pieces created above, that is, the simulation model, the observation operator, the prior, and the observation error model.

The next step is to register observational data (along with observation times). A standard strategy in experimentation is to create synthetic data from a ground truth (known as a twin experiment). This is explained by snippet 6, where we define the assimilation timespan (window) to be the interval [0, 0.3], and the observations are taken at 3 time instances 0.1, 0.2, 0.3. The observational data is mimicked by adding random noise (using the observation error model) to the observed ground truth at the corresponding observation time instance.

```
# Set the assimilation/simulation time window
tspan = (0, 0.3)
inverse_problem.register_assimilation_window(tspan)

# Create truth (true initial state and trajectory)
true_IC = model.create_initial_condition()
checkpoints = [0.1, 0.2, 0.3]
, true_traject = model.integrate_state(true_IC, tspan=tspan, checkpoints=checkpoints)
```

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```
10 # Create synthetic data (perturbation to truth) and register them
11 for t, state in zip(checkpoints, true_traject):
12 obs = obs_noise.add_noise(obs_oper(state))
```

inverse_problem.register_observation(t=t, observation=obs)

Snippet 6. Create synthetic noisy observations, and register all observation time points and observational data to the inverse problem object.

The final step in the DA procedure is to solve the inverse problem and assess the quality of the solution. For this setup, we know the ground truth, and thus one can evaluate the root mean squared error (RMSE), which is a standard error metric in statistics in the DA literature. In order to solve the inverse problem, the solve_inverse_problem method of the 4DVar DA object is called (snippet 7). This method will raise an instructive error if any of the essential elements, for example, the simulation model, are not registered properly. Note that this function is flexible and allows the posterior covariance to be constructed if needed. It also allows waiving finding the MAP estimate, which can be advantageous in OED applications due to associated computational savings. For example, one might want to estimate the posterior covariance in the linear Gaussian case without evaluating the MAP.

i inverse_problem.solve_inverse_problem(init_guess=prior.mean, update_posterior=True)

Snippet 7. Solve the inverse problem. The optimization initial point is set by default to the prior mean; however, it can be modified if a better initial guess is known. Here, the posterior covariance is evaluated, and consequently the posterior is updated with both the mean and the covariance matrix.

PyOED provides several utility functions to evaluate statistics, such as the RMSE, which can be used to quantify the accuracy of the inverse problem solution. Snippet 8 shows how to call the utility function calculate_rmse and use it to evaluate the prior and the analysis (posterior) RMSE, which are then printed.

```
1 from pyoed import utility
```

```
2 prior_rmse = utility.calculate_rmse(true_IC, inverse_problem.prior.mean)
```

3 posterior_rmse = utility.calculate_rmse(true_IC, inverse_problem.posterior.mean)

```
4 print(f"Prior RMSE: {prior_rmse}")
```

```
5 print(f"Posterrior RMSE: {posterior_rmse}")
```

Snippet 8. Calculate and print the RMSE values associated with the prior mean (initial guess here) and the posterior mean.

The same procedure can be easily followed to inspect the RMSE results over the whole assimilation timespan as described by Snippet 9 with results plotted in Figure 4.

```
1 checkpoints, true_traject = model.integrate_state(true_IC, tspan=tspan)
2 _, prior_traject = model.integrate_state(inverse_problem.prior.mean, tspan=tspan)
3 _, posterior_traject = model.integrate_state(inverse_problem.posterior.mean, tspan=tspan)
4 prior_rmse = [utility.calculate_rmse(xp, xt) for xp, xt in zip(prior_traject, true_traject)]
5 posterior_rmse = [utility.calculate_rmse(xp, xt) for xp, xt in zip(posterior_traject, true_traject)]
```

Snippet 9. Generate RMSE over the whole assimilation window.

One can also analyze the posterior covariances, for example, by generating and plotting the posterior covariance matrix. Given the linear Gaussian settings in the present setup, one can validate the generated posterior covariance matrix against the exact formula (22). One way to construct the posterior covariance matrix is to invoke the posterior model as shown in snippet 10.

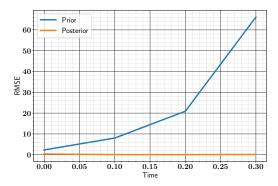


Fig. 4. RMSE results of the solution of the inverse problem presented in Section 4.1. The RMSE results of both the prior and the posterior trajectories plotted here are obtained by running the code in snippet 9.

post_cov = inverse_problem.posterior.covariance_matrix()

Snippet 10. Construct and retrieve the posterior covariance matrix

Note, however, that one should avoid constructing the covariance matrix for high-dimensional error models. Alternatively, matrix-free implementations of covariance (and precision) matrix-vector product should be used. For example, to multiply the prior covariance by state, one should call prior.covariance_matvec(state). The error models provide many attributes to efficiently access the statistics of the model, such as covariance diagonal, and trace. The posterior covariance matrix, constructed by employing the posterior functionality as in snippet 10 and the covariance matrix evaluated by applying (22) along with the mismatch errors are plotted in Figure 5.

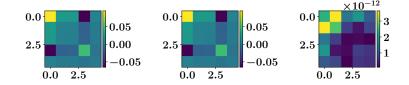


Fig. 5. Entries of the posterior covariance matrix and the associated errors. Left: the posterior covariance matrix generated by snippet 10. Middle: the closed-form posterior covariance matrix given by (22). Right: RMSE obtained by pointwise comparison of the covariance matrices obtained by solving the inverse problem (left) and by using the closed form (middle).

An OED experiment. The simulation model is instantiated with a model grid of size nx=5, and the observation operator copies the model state. In fact, one can inspect the model array representation **A** for this toy linear model by calling model.get_model_array(). Both the model state and the observation vector sizes here are 5. Thus, there are actually 5 candidate sensor locations (observation gridpoints), and one can try to find the optimal subset of sensors by using an OED implementation.

Here we briefly illustrate utilizing an OED object to find the A-optimal design for the toy linear example discussed above; see snippet 11. First, the proper OED module (here following [9]) is imported and is used to create the oed_problem instance. The A-optimality criterion is registered (which can be changed later by registering a proper OED criterion),

and the OED problem is then solved. The results of solving the OED problem, for example, the optimal observational design, are then stored in oed_result, which is an instance of (or derived from) the pyoed.oed.OEDResults class. This class provides access to various attributes of the OED problem and the solution process (such as the optimization trajectory and brute force solution if requested). This gives a taste of how simple it is to create and test DA and OED problems in PyOED. Further details on OED implementations in PyOED are discussed in the following section (4.2).

```
1 from pyoed.oed.relaxed_oed import RelaxedOED
```

```
2 oed_problem = RelaxedOED(inverse_problem=inverse_problem, problem_is_linear=True)
```

- 3 oed_problem.register_optimality_criterion('A-opt')
- oed_results = oed_problem.solve_oed_problem()

Snippet 11. Create an OED object, and solve the OED optimization problem for the toy linear model.

4.2 A standard model-constrained OED experiment

Parameter identification for an advection-diffusion (AD) model is the foundation of an experiment widely used in the model-constrained OED literature for validating theoretical developments; see, for example, [4, 8, 19, 30]. Comparing independent scientific OED developments is admittedly hard, mainly because of the lack of availability of open software packages developed for OED. This is one of the main goals and features of PyOED. Specifically, PyOED will enable OED researchers to compare the performance of new OED algorithmic approaches with other methods. Moreover, it enables comparison with solution by brute force search for small- to moderate-dimensional problems. In this section 4.2 we describe in detail the steps required to construct and solve an OED problem in PyOED with an AD simulation model. This problem has been utilized independently in several OED developments; see, for example, [4, 8–10, 19]. Here, we show how PyOED can be used to solve and benchmark this OED problem, thus providing a starting point for utilizing and developing multiple approaches for solving OED problems in general in PyOED. Following the same approach as in 4.1, we start by describing the components of the inverse problem and briefly show how they are initialized in PyOED; then we initialize and solve the OED problem using the efficient stochastic approach summarized by Algorithm 1. Additionally, we discuss the steps that should be modified to utilize other solution formulations and methods such as the relaxation approach (17).

The code summarized here is provided in the pyoed.examples.OED_AD_FE module with additional comments, details, and capabilities. A Jupyter Notebook pyoed.tutorials.OED_AD_FE is also available and can be used to regenerate the numerical results presented in this section (4.1).

The simulation model. The governing equation of the contaminant field $u = u(\mathbf{x}, t)$ is modeled by the following AD model equations with the associated boundary conditions:

$$u_{t} - \kappa \Delta u + \mathbf{v} \cdot \nabla u = 0 \quad \text{in } \mathcal{D} \times [0, T],$$

$$u(x, 0) = \theta \quad \text{in } \mathcal{D},$$

$$\kappa \nabla u \cdot \mathbf{n} = 0 \quad \text{on } \partial \mathcal{D} \times [0, T],$$
(23)

where $\kappa > 0$ is the diffusivity, *T* is the simulation final time and **v** is the velocity field. The domain is $\mathcal{D} := (0, 1) \times (0, 1)$ with two rectangular regions modeling two buildings inside the domain. The velocity field **v** is known exactly and is obtained by solving a steady Navier–Stokes equation, with the side walls driving the flow, as detailed in [9, 36].

To create a simulation model object implementing (23), ground truth of the initial condition, and plot the domain (with finite elements discretization) as well as the velocity field, one can use Snippet 12; the output is shown in Figure 6.

```
1 # Create the simulation model (AD with FE discretization)
2 from pyoed.models.simulation_models import fenics_models
3 model_timestep = 1.0
4 model = fenics_models.create_AdvectionDiffusion2D_model(dt=model_timestep)
5
6 # Ground truth of the inversion parameter (initial condition here)
7 true_model_state = model.create_initial_condition()
8
9 # Plot the domain
10 model.plot_domain()
11 model.plot_velocity_field()
```

```
Snippet 12. Create an object representing the simulation model (23).
```

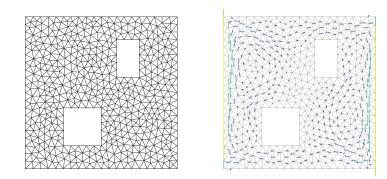


Fig. 6. Left: finite elements discretization of the domain $\mathcal D$ of the AD problem (23). Right: the velocity field v.

The prior. In this setup, following [8, 36, 49], we choose a Laplacian prior of the parameter θ is $\mathcal{N}(\theta_{\rm pr}, \Gamma_{\rm pr})$, with $\Gamma_{\rm pr}$ being a discretization of \mathcal{A}^{-2} , where \mathcal{A} is a Laplacian operator. In PyOED, a Laplacian prior can be created as described in snippet 13.

1	from pyoed.models.error_models import Laplacian
2	configs = dict(Vh=model.parameter_dof,
3	<pre>mean=model.parameter_vector(init_val=0.5),</pre>
4	gamma=1.0,
5	delta=16,
6	random_seed=123,)
7	prior = Laplacian.DolfinBiLaplacianErrorModel(configs)

Snippet 13. Create a Laplacian prior.

The observation operator. A common observational configuration is to consider uniformly distributed candidate sensor locations and solve an OED problem to choose the optimal subset of candidate sensor locations. A uniform observation operator can be created and incorporated in this problem as described in snippet 14.

20

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```
1 from pyoed.models.observation_operators.fenics_observation_operators import(
2     create_pointwise_observation_operator,
3 )
4 num_candidate_sensors = 10
5 obs_oper = create_pointwise_observation_operator(model=model, num_obs_points=num_candidate_sensors, )
```

Snippet 14. Create a uniform observation operator with 10 candidate locations.

Assuming Gaussian observational noise model, a Gaussian observation error model is created as described in 15

```
1 from pyoed.models.error_models.Gaussian import GaussianErrorModel
2 obs_noise = GaussianErrorModel(
3     configs={'size':obs_oper.shape[0], 'variance':0.1, 'random_seed':2345},
4 )
```

Snippet 15. Create a Gaussian noise model.

The inverse problem: 4DVar. As with the case of the toy linear problem described above in Section 4.1, the elements of the inverse problem here can be created as described by snippet 16. Similarly, synthetic observations (data) can be created as in snippet 17. Note that all steps followed so far in this example are similar to those followed in the case of the toy linear model discussed in Section 4.1.

```
import numpy as np
from pyoed.assimilation.smoothing import fourDVar
checkpoints = np.arange(0, model_timestep*(5.5), model_timestep)
DA_configs = dict(assimilation_window=(checkpoints[0], checkpoints[-1]),
model=model,
model=model,
prior_model=prior,
observation_operator=obs_oper,
observation_error_model=obs_noise, )
inverse_problem = fourDVar.VanillaFourDVar(configs=DA_configs)
```

Snippet 16. Create the DA object.

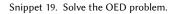
Snippet 17. Create synthetic observations, and associate them to the inverse problem object.

The OED problem. The discussion above is valid for all model-constrained OED approaches in PyOED. In what follows, we describe the steps needed to create an OED object that follows the stochastic approach (20). An OED object is created in PyOED by following the steps in snippet 18. Here, we seek to activate only 4 sensors out of the candidate 10, and we use the trace of the Fisher information matrix (FIM) as the utility function. To enforce the budget, we use an ℓ_0 penalty term as detailed in [10].

Snippet 18. Create an OED object implementing the stochastic approach 1.

The OED problem can be solved as described by snippet 19.

```
i oed_results = oed_problem.solve_oed_problem(
    oed_evaluation_method='randomized', # randomized approximation of FIM trace
    learning_rate=1e-10,
    batch_size=32,
    bruteforce=True, # To compare the solution to search by enumeration (bruteforce search)
    )
```



The resulting oed_results object can be used to generate several analysis plots as described by the code in snippet 20. This generates multiple standard plots, including the performance of the optimization algorithm over consecutive iterations in Figure 7(left), the optimal sensor locations generated by the optimization algorithm in Figure 7(middle), and comparison of the quality of the solution with respect to brute force search shown in Figure 7(right).

```
1 # Create standard plots of the OED results
```

```
oed_problem.plot_results(oed_results)
```

Snippet 20. Create standard plots for assessing the performance of the optimization routine and the quality of the generated design.

To use other OED formulations to solve the same problem, the user only needs to update the code in the snippet 18 with the proper OED implementation. For example, the relaxation approach (17) can be used as illustrated in the case of the linear toy model above in 4.1; see snippet 11. Specifically, the relaxation approach (17) can be used to solve the present optimal sensor placement problem by replacing the code in snippet 18 with the following code in snippet 21, which demonstrates the simplicity of PyOED interface. Results of snippet 21 are omitted from the presentation here for clarity and because the main goal here is to discuss usage of the approaches in PyOED rather than assessing the quality of the solution approach, which is left for interested users of the package and for future benchmarking research.

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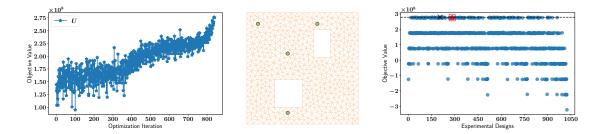


Fig. 7. Subset of the plots generated by running the code in snippet 20. Left: value of the utility (objective) function, i.e., the penalized OED criterion, over consecutive iterations of the optimization algorithm. Middle: optimal solution, showing optimal sensor locations in the domain. Right: value of the objective of the optimal solution (red star) returned by algorithm 1, compared with the global optimum solution (black *x* mark), and all possible solutions marked as blue circles; the x-axis shows the indexes of all possible binary designs from 1 to $2^{n_s=10} = 1024$, and the y-axis shows the corresponding values of the optimization objective.

```
1 # Formulate and solve using the relaxation approach

2 from pyoed.oed.relaxed_oed import PointwiseRelaxedOED

3 oed_problem = PointwiseRelaxedOED(inverse_problem=inverse_problem, problem_is_linear=True, )

4 oed_problem.register_optimality_criterion('A-opt')

5 ...

6 # Add penalty (differentiable function and gradient)

7 penalty_f_l2 = lambda design: np.power(np.sum(design)-budget, 2)

8 penalty_f_l2_grad = lambda design: 2 * (np.sum(design)-budget) * np.ones_like(design)

9 oed_problem.register_penalty_term(

10 penalty_weight=1,

11 penalty_function=penalty_f_l2,

12 penalty_function_gradient=penalty_f_l2_grad, )

13 ...

14 # Solve the OED problem

15 oed_results = oed_problem.solve_oed_problem(oed_evaluation_method='randomized', )
```

Snippet 21. Create an OED object implementing the relaxation approach (17).

Note, however, that we had to change the penalty function in snippet 21 because the ℓ_0 penalty function used in snippet 18 is non differentiable, while the relaxation approach requires the OED objective function to be differentiable. For details, see, for example, [10].

5 CONCLUDING REMARKS

This work describes PyOED, a highly extensible high-level software package for OED in inverse problems and DA. PyOED aims to be a comprehensive Python toolkit for model-constrained OED. The package targets scientists and researchers interested in understanding the details of OED formulations and approaches. It is also meant to enable researchers to experiment with standard and innovative OED technologies within external test problems (e.g., simulations). The mathematical formulations of OED, inverse problems, and DA overlap significantly, and thus, we plan to extend PyOED with a plethora of Bayesian inversion, DA, and OED implementations as well as new scientific simulation models, observation error models, and observation operators.

While we focused the discussions in this paper on specific OED approaches, the current version PyOED (v1.0) provides several other implementations and emphasizes implementing the essential infrastructure that enables combinining DA and OED elements with other parts of the package. The main limitation of the initial version of PyOED is scalability. Specifically, the concept is developed without parallelization capability. In future versions of PyOED, scalability will be achieved by adding message passing interface (MPI) support, for example using the mpi4py package, and by supporting PETSC [17]. Performance will also be enhanced by converting or rewriting suitable parts of the package in Cython.

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