Derivative-informed projected neural network for large-scale Bayesian optimal experimental design

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Abstract

We address the solution of large-scale Bayesian optimal experimental design (OED) problems governed by partial differential equations (PDEs) with infinite-dimensional parameter fields. The OED problem seeks to find sensor locations that maximize the expected information gain (EIG) in the solution of the underlying Bayesian inverse problem. Computation of the EIG is usually prohibitive for PDE-based OED problems. To make the evaluation of the EIG tractable, we approximate the (PDE-based) parameter-to-observable map with a derivative-informed projected neural network (DIPNet) surrogate, which exploits the geometry, smoothness, and intrinsic low-dimensionality of the map using a small and dimension-independent number of PDE solves. The surrogate is then

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deployed within a greedy algorithm-based solution of the OED problem such that no further PDE solves are required. We analyze the EIG approximation error in terms of the generalization error of the DIPNet, and demonstrate the efficiency and accuracy of the method via numerical experiments involving inverse scattering and inverse reactive transport.

**Keywords:** Bayesian optimal experimental design, Bayesian inverse problem, expected information gain, neural network, surrogate, greedy algorithm

## 1 Introduction

In modeling natural or engineered systems, uncertainties are often present due to the lack of knowledge or intrinsic variability of the system. Uncertainties may arise from sources as varied as initial and boundary conditions, material properties and other coefficients, external source terms, interaction and coupling terms, and geometries; for simplicity of exposition, we refer to all of these as *parameters*. Uncertainties in prior knowledge of these parameters can be reduced by incorporating indirect observational or experimental data on the system state or related quantities of interest into the forward model via solution of a Bayesian inverse problem. Prior knowledge can be incorporated through a prior distribution on the uncertain parameters. The data are typically noisy because of limited measurement precision, which induces a likelihood of the data conditioned on the given parameters. Uncertainties of the parameters are then reduced by the data and quantified by a posterior distribution, which is a joint distribution of the prior and the likelihood, given by Bayes’ rule.

Large amounts of informative data can reduce uncertainties in the parameters, and thus posterior predictions, significantly. However, the data are often sparse or limited due to the cost of their acquisition. In such cases it is critical to design the acquisition process or experiment in an optimal way so that as much information as possible can be gained from the acquired data, or the uncertainty in the parameters or posterior predictions can be reduced as much as possible. Experimental design variables can include what, when, and where to measure, which sources to use to excite the system, and under which conditions should the experiments be conducted. This is known as the optimal experimental design (OED) problem [1], or Bayesian OED in the context of Bayesian inference. OED problems arise across numerous fields including geophysical exploration, medical imaging, nondestructive evaluation, drug testing, materials characterization, and earth system data assimilation, to name just a few. For example, two notable uses of OED include optimal observing system
design in oceanography [2] and optimal sensor placement for tsunami early warning [3].

The challenges to solving OED problems in these and other fields are manifold. The models underlying the systems of interest typically take the form of partial differential equations (PDEs) and can be large-scale, complex, nonlinear, dynamic, multiscale, and coupled. The uncertain parameters may depend on both space and time, and are often characterized by infinite-dimensional random fields and/or stochastic processes. The PDE models can be extremely expensive to solve for each realization of the infinite-dimensional uncertain parameters. The computation of the OED objective involves high-dimensional (after discretization) integration with respect to (w.r.t.) the uncertain parameters, and thus require a large number of PDE solves. Finally, the OED objective will need to be evaluated numerous times, especially when the experimental design variables are high-dimensional or when they represent discrete decisions.

To address these computational challenges, different classes of methods have been developed by exploiting (1) sparsity via polynomial chaos approximation of parameter-to-observable maps [4–6], (2) Laplace approximation of the posterior [7–11], (3) intrinsic low dimensionality by low-rank approximation of (prior-preconditioned and data-informed) operators [7, 12–16], (4) decomposibility by offline (for PDE-constrained approximation)–online (for design optimization) decomposition [17, 18], and (5) surrogate models of the PDEs, parameter-to-observable map, or posterior distribution by model reduction [19, 20] and deep learning [21–23].

Here, we consider the Bayesian OED problem for optimal sensor placement governed by large-scale and possibly nonlinear PDEs with infinite-dimensional uncertain parameters. We use the expected information gain (EIG), also known as mutual information, as the optimality criterion for the OED problem. The optimization problem is combinatorial: we seek the combination of sensors, selected from a set of candidate locations, that maximizes the EIG. The EIG is an average of the Kullback–Leibler (KL) divergence between the posterior and the prior distributions over all realizations of the data. This involves a double integral: one integral of the likelihood function w.r.t. the prior distribution to compute the normalization constant or model evidence for each data realization, and one integral w.r.t. the data distribution. To evaluate the two integrals we adopt a double-loop Monte Carlo (DLMC) method that requires the computation of the parameter-to-observable map at each of the parameter and data samples. Since the likelihood can be rather complex and highly locally supported in the parameter space, the number of parameter samples from the prior distribution needed to capture the likelihood well with relatively accurate sample average approximation of the normalization constant can be extremely large. The requirement to evaluate the PDE-constrained
A parameter-to-observable map at each of the large number of samples leads to numerous PDE solves, which is prohibitive when the PDEs are expensive to solve. To tackle this challenge, we construct a derivative-informed projected neural network (DIPNet) [24–26] surrogate of the parameter-to-observable map that exploits the intrinsic low dimensionality of both the parameter and the data spaces. This intrinsic low dimensionality is due to the correlation of the high-dimensional parameters, the regularizing property of the underlying PDE solution, and/or redundant information contained in the data from all of the candidate sensors. In particular, the low-dimensional subspace of the parameter space can be detected by from derivatives of the parameter-to-observable map, such as the Jacobian, Gauss-Newton Hessian, or higher-order derivatives. This property has been observed and used in many uncertainty quantification problems such as model reduction for sampling and deep learning [27–29], optimization under uncertainty [30–32], Bayesian inverse problems [33–44], and Bayesian optimal experimental design [7, 15, 17, 18]. This intrinsic low-dimensionality of parameter and data spaces, along with smoothness of the parameter-to-observable map, allow us to construct an accurate (over parameter space) DIPNet surrogate with a limited and dimension-independent number of training data pairs, each requiring a PDE solve. Once trained, the DIPNet surrogate is deployed in the OED problem, which is solved without further PDE solution, resulting in very large reductions in computing time. Under suitable assumptions, we provide an analysis of the error propagated from the DIPNet approximation to the approximation of the normalization constant and the EIG. To solve the combinatorial optimization problem of sensor selection, we use a greedy algorithm developed in our previous work [17, 18]. We demonstrate the efficiency and accuracy of our computational method by conducting two numerical experiments with infinite-dimensional parameter fields: OED for inverse scattering (with an acoustic Helmholtz forward problem) and inverse reactive transport (with a nonlinear advection-diffusion-reaction forward problem).

The rest of the paper is organized as follows. The setup of the problems including Bayesian inversion, EIG, sensor design matrix, and Bayesian OED are presented in Section 2. Section 3 is devoted to presentation of the computational methods including DLMC, DIPNet and its induced error analysis, and the greedy optimization algorithm. Results for the two OED numerical experiments are provided in Section 4, followed by conclusions in Section 5.
2 Problem setup

2.1 Bayesian inverse problems

Let \( D \subset \mathbb{R}^{n_x} \) denote a physical domain in dimension \( n_x = 1, 2, 3 \). We consider the problem of inferring an uncertain parameter field \( m \) defined in the physical domain \( D \) from noisy data \( y \) and a complex model represented by PDEs. Let \( y \in \mathbb{R}^{n_y} \) denote the noisy data vector of dimension \( n_y \in \mathbb{N} \), given by

\[
y = F(m) + \varepsilon,
\]

which is contaminated by the additive Gaussian noise \( \varepsilon \sim \mathcal{N}(0, \Gamma_n) \) with zero mean and covariance \( \Gamma_n \subset \mathbb{R}^{n_y \times n_y} \). Specifically, \( y \) is obtained from observation of the solution of the PDE model at \( n_y \) sensor locations. \( F \) is the parameter-to-observable map which depends on the solution of the PDE and an observation operator that extracts the solution values at the \( n_y \) locations.

We consider the above inverse problem in a Bayesian framework. First, we assume that \( m \) lies in an infinite-dimensional real separable Hilbert space \( \mathcal{M} \), e.g., \( \mathcal{M} = L^2(D) \) of square integrable functions defined in \( D \). Moreover, we assume that \( m \) follows a Gaussian prior measure \( \mu_{pr} = \mathcal{N}(m_{pr}, C_{pr}) \) with mean \( m_{pr} \in \mathcal{M} \) and covariance operator \( C_{pr} \), a strictly positive, self-adjoint, and trace-class operator. As one example, we consider \( C_{pr}^{-1} = A^{-2} \), where \( A = -\gamma \Delta + \delta I \) is a Laplacian-like operator with prescribed homogeneous Neumann boundary condition, with Laplacian \( \Delta \), identity \( I \), and positive constants \( \gamma, \delta > 0 \); see [35, 45, 46] for more details. Given the Gaussian observation noise, the likelihood of the data \( y \) for the parameter \( m \in \mathcal{M} \) satisfies

\[
\pi_{\text{like}}(y|m) \propto \exp(-\Phi(m, y)),
\]

where

\[
\Phi(m, y) := \frac{1}{2} \| y - F(m) \|_{\Gamma_n^{-1}}^2
\]

is known as a potential function. By Bayes’ rule, the posterior measure, denoted as \( \mu_{\text{post}}(m|y) \), is given by the Radon-Nikodym derivative as

\[
\frac{d\mu_{\text{post}}(m|y)}{d\mu_{pr}(m)} = \frac{1}{\pi(y)} \pi_{\text{like}}(y|m),
\]

where \( \pi(y) \) is the so-called normalization constant or model evidence, given by

\[
\pi(y) = \int_{\mathcal{M}} \pi_{\text{like}}(y|m)d\mu_{pr}(m).
\]
This expression is often computationally intractable because of the infinite-dimensional integral, which involves a (possibly large-scale) PDE solve for each realization $m$.

### 2.2 Expected information gain

To measure the information gained from the data $y$ in the inference of the parameter $m$, we consider a Kullback–Leibler (KL) divergence between the posterior and the prior, defined as

$$D_{\text{KL}}(\mu_{\text{post}}(\cdot|y)\|\mu_{\text{pr}}) := \int_{\mathcal{M}} \ln \left( \frac{d\mu_{\text{post}}(m|y)}{d\mu_{\text{pr}}(m)} \right) d\mu_{\text{post}}(m|y),$$

which is random since the data $y$ is random. We consider a widely used optimality criterion, expected information gain (EIG), which is the KL divergence averaged over all realizations of the data, defined as

$$\Psi := \mathbb{E}_y \left[ D_{\text{KL}}(\mu_{\text{post}}(\cdot|y)\|\mu_{\text{pr}}) \right]$$

$$= \int_{\mathcal{Y}} \int_{\mathcal{M}} \ln \left( \frac{d\mu_{\text{post}}(m|y)}{d\mu_{\text{pr}}(m)} \right) d\mu_{\text{post}}(m|y) \pi(y) dy$$

$$= \int_{\mathcal{M}} \int_{\mathcal{Y}} \ln \left( \frac{\pi_{\text{like}}(y|m)}{\pi(y)} \right) \pi_{\text{like}}(y|m) dy d\mu_{\text{pr}}(m)$$

where the last equality follows Bayes’ rule (4) and the Fubini theorem under the assumption of proper integrability.

### 2.3 Optimal experimental design

We consider the OED problem for optimally acquiring data to maximize the expected information gained in the parameter inference. The experimental design seeks to choose $r$ sensor locations out of $d$ candidates $\{x_1, \ldots, x_d\}$ represented by a design matrix $W \in \mathbb{R}^{r \times d} \in \mathcal{W}$, namely, if the $i$-th sensor is placed at $x_j$, then $W_{ij} = 1$, otherwise $W_{ij} = 0$:

$$\mathcal{W} := \left\{ W \in \mathbb{R}^{r \times d} : W_{ij} \in \{0, 1\}, \sum_{i=1}^{r} W_{ij} \in \{0, 1\}, \sum_{j=1}^{d} W_{ij} = 1 \right\}.$$

Let $\mathcal{F}_d : \mathcal{M} \mapsto \mathbb{R}^d$ denote the parameter-to-observable map and $\epsilon_d \in \mathbb{R}^d$ denote the additive noise, both using all $d$ candidate sensors; then we have

$$\mathcal{F} = W \mathcal{F}_d \quad \text{and} \quad \epsilon = W \epsilon_d.$$
Then the likelihood (2) for a specific design $W$ is given by

$$\pi_{\text{like}}(y|m, W) \propto \exp\left(-\frac{1}{2}\|y - WF_d(m)\|_n^2\right),$$

and the normalization constant also depends on $W$ as

$$\pi(y, W) = \int_Y \pi_{\text{like}}(y|m, W) d\mu_{\text{pr}}(m).$$

From Section 2.2, we can see that the EIG $\Psi$ depends on the design matrix $W$ through the likelihood function $\pi_{\text{like}}(y|m, W)$. To this end, we formulate the OED problem to find an optimal design matrix $W^*$ such that

$$W^* = \arg\max_{W \in W} \Psi(W)$$

with the $W$-dependent EIG given by

$$\Psi(W) = \int_M \int_Y \ln\left(\frac{\pi_{\text{like}}(y|m, W)}{\pi(y, W)}\right) \pi_{\text{like}}(y|m, W) dy d\mu_{\text{pr}}(m).$$

### 2.4 Finite-dimensional approximation

To facilitate the presentation of our computational methods, we make a finite-dimensional approximation of the parameter field by using a finite element discretization. Let $M_n \subset M$ denote a subspace of $M$ spanned by $n$ piecewise continuous Lagrange polynomial basis functions $\{\psi_j\}_{j=1}^n$ over a mesh with elements of size $h$. Then the discrete parameter $m_h \in M_n$ is given by

$$m_h = \sum_{j=1}^n m_j \psi_j.$$  

The Bayesian inverse problem is then stated for the finite-dimensional coefficient vector $m = (m_1, \ldots, m_n)^T$ of $m_h$, with $n$ possibly very large. The prior distribution of the discrete parameter $m$ is Gaussian $N(m_{\text{pr}}, \Gamma_{\text{pr}})$ with $m_{\text{pr}}$ representing the coefficient vector of the discretized prior mean of $m_{\text{pr}}$, and $\Gamma_{\text{pr}}$ representing the covariance matrix corresponding to $C_{\text{pr}} = A^{-2}$, given by

$$\Gamma_{\text{pr}} = A^{-1}MA^{-1},$$

where $A$ is the finite element matrix of the Laplacian-like operator $A$, and $M$ is the mass matrix. Moreover, let $F_d : \mathbb{R}^n \to \mathbb{R}^d$ denote the discretized parameter-to-observable map corresponding to $F_d$, we have $F = WF_d$ as
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Then the likelihood function corresponding to (10) for the discrete parameter \(\mathbf{m}\) is given by

\[
\pi_{\text{like}}(\mathbf{y}|\mathbf{m}, \mathbf{W}) \propto \exp\left(-\frac{1}{2}\|\mathbf{y} - \mathbf{W}\mathbf{F}(\mathbf{m})\|_\Gamma^{-1}\right).
\]

(16)

3 Computational methods

3.1 Double-loop Monte Carlo estimator

To solve the OED problem (12), we need to evaluate the EIG repeatedly for each given design \(\mathbf{W}\). The double integrals in the EIG expression can be computed by a double-loop Monte Carlo (DLMC) estimator \(\Psi_{dl}\) defined as

\[
\Psi_{dl}(\mathbf{W}) := \frac{1}{n_{out}} \sum_{i=1}^{n_{out}} \log \left( \frac{\pi_{\text{like}}(\mathbf{y}_i|\mathbf{m}_i, \mathbf{W})}{\hat{\pi}(\mathbf{y}_i, \mathbf{W})} \right),
\]

(17)

where \(\mathbf{m}_i, i = 1, \ldots, n_{out}\), are i.i.d. samples from prior \(\mathcal{N}(\mathbf{m}_{pr}, \Gamma_{pr})\) in the outer loop and \(\mathbf{y}_i = \mathbf{F}(\mathbf{m}_i) + \mathbf{e}_i\) are the realizations of the data with i.i.d. noise \(\mathbf{e}_i \sim \mathcal{N}(\mathbf{0}, \Gamma_n)\). \(\hat{\pi}(\mathbf{y}_i, \mathbf{W})\) is a Monte Carlo estimator of the normalization constant \(\pi(\mathbf{y}_i, \mathbf{W})\) with \(n_{in}\) samples in the inner loop, given by

\[
\hat{\pi}(\mathbf{y}_i, \mathbf{W}) := \frac{1}{n_{in}} \sum_{j=1}^{n_{in}} \pi_{\text{like}}(\mathbf{y}_i|\mathbf{m}_{i,j}, \mathbf{W}),
\]

(18)

where \(\mathbf{m}_{i,j}, j = 1, \ldots, n_{in}\), are i.i.d. samples from the prior \(\mathcal{N}(\mathbf{m}_{pr}, \Gamma_{pr})\).

For complex posterior distributions, e.g., high-dimensional, locally supported, multi-modal, non-Gaussian, etc., evaluation of the normalization constant is often intractable, i.e., a prohibitively large number of samples \(n_{in}\) is needed. As one particular example, when the posterior of \(\mathbf{m}\) for data \(\mathbf{y}_i\) generated at sample \(\mathbf{m}_i\) concentrates in a very small region far away from the mean of the prior, the likelihood \(\pi_{\text{like}}(\mathbf{y}_i|\mathbf{m}_{i,j}, \mathbf{W})\) is extremely small for most samples \(\mathbf{m}_{i,j}\), which which leads to a requirement of a large number of samples to evaluate \(\hat{\pi}(\mathbf{y}_i, \mathbf{W})\) with relatively small estimation error. This is usually prohibitive, since one evaluation of the parameter-to-observable map, and thus one solution of the large-scale PDE model, is required for each of \(n_{out} \times n_{in}\) samples. This \(n_{out} \times n_{in}\) PDE solves are required for each design matrix \(\mathbf{W}\) at each optimization iteration.

3.2 Derivative-informed projected neural networks

Recent research has motivated the deployment of neural networks as surrogates for parametric PDE mappings [24, 47–53]. These surrogates can be
used to accelerate the computation of the EIG within OED problems. Specifically, to reduce the prohibitive computational cost, we build a surrogate for the parameter-to-observable map $F_d : \mathbb{R}^n \rightarrow \mathbb{R}^d$ at all candidate sensor locations by a derivative-informed projected neural network (DIPNet) [24–26]. Often, PDE-constrained high-dimensional parametric maps, such as the parameter-to-observable map $F_d$, admit low-dimensional structure due to the correlation of the high-dimensional parameters, the regularizing property of the underlying PDE solution, and/or redundant information in the data from all candidate sensors. When this is the case, the DIPNet can exploit this low-dimensional structure and parametrize a parsimonious map between the most informed subspaces of the input parameter and the output observables. The dimensions of the input and output subspaces are referred to as the “information dimension” of the map, which is often significantly smaller than the parameter and data dimensions.

For the input parameter dimension reduction, we use an active subspace (AS) [54], which is spanned by the generalized eigenvectors (input reduced basis) corresponding to the $r_M$ largest eigenvalues of the eigenvalue problem

$$\left[ \int_{\mathcal{M}_n} \nabla_m F_d(m)^T \nabla_m F_d(m) d\mu_{pr}(m) \right] v_i = \lambda_{i}^{AS} \Gamma_{pr}^{-1} v_i, \quad (19)$$

where the eigenvectors $v_i$ are ordered by the decreasing generalized eigenvalues $\lambda_{i}^{AS}, i = 1, \ldots, r_M$. For the output data dimension reduction, we use a proper orthogonal decomposition (POD) [55, 56], which uses the eigenvectors (output reduced basis) corresponding to the first $r_F$ eigenvalues of the expected observable outer product matrix,

$$\left[ \int_{\mathcal{M}_n} F_d(m) F_d(m)^T d\mu_{pr}(m) \right] \phi_i = \lambda_{i}^{POD} \phi_i, \quad (20)$$

where the eigenvectors $\phi_i$ are ordered by the decreasing eigenvalues $\lambda_{i}^{POD}, i = 1, \ldots, r_F$. When the eigenvalues of AS and POD both decay quickly, the mapping $m \mapsto F_d(m)$ can be well approximated when $m$ and $F_d$ are projected to the corresponding subspaces with small $r_M$ and $r_F$; this motivates the nonlinear neural network approximation between these subspaces [24, 26]. The neural network surrogate $\tilde{F}_d$ of the map $F_d$ then has the form

$$\tilde{F}_d(m, [w, b]) = \Phi_{r_F} f_r(V_{r_M}^T m, w) + b, \quad (21)$$

where $\Phi_{r_F} \in \mathbb{R}^{d \times r_F}$ represents the POD reduced basis for the output, $V_{r_M} \in \mathbb{R}^{n \times r_M}$ represents the AS reduced basis for the input, $f_r \in \mathbb{R}^{r_F}$ is the neural network mapping between the two bases parametrized by weights $w$ and bias $b$. The remaining difficulty is how to properly parametrize and train the
neural network mapping. Motivated by recent approximation theory for residual neural networks (ResNets) as approximations of sequentially minimizing control flows [57], we employ an adaptive algorithm for both the construction and training of a ResNet for the reduced basis nonlinear mapping, as shown in Fig. 1. This strategy adaptively constructs and trains a sequence of low-rank ResNet layers, where for convenience we take \( r = r_M = r_F \) or otherwise employ a restriction or prolongation layer to enforce dimensional compatibility. The ResNet hidden neurons at layer \( i + 1 \) have the form

\[
\begin{align*}
z_{i+1} = z_i + w_{i,2} \sigma(w_{i,1} z_i + b_i),
\end{align*}
\]

with \( z_{i+1}, z_i, b_i \in \mathbb{R}^r, w_{i,2}, w_{i,1}^T \in \mathbb{R}^{r \times k} \), where the parameter \( k < r \) is referred to as the layer rank. The ResNet weights \( \mathbf{w} = [(w_{i,2}, w_{i,1}, b_i)]_{i=0}^{\text{depth}} \) consist of all of the coefficient arrays in each layer. This architectural strategy is able to achieve high generalizability for few and (input-output) dimension-independent data, as shown in [26].

**Fig. 1** A schematic representation of the derivative-informed projected neural network using ResNet as the nonlinear mapping between the reduced subspace using active subspaces for input parameters and POD for output observables.

By removing the dependence of the input-to-output map on their high-dimensional and uninformed subspaces (complement to the low-dimensional and informed subspaces), we can construct a neural network of small input and output size that requires few training data. Since these architectures are able to achieve high generalization accuracy with limited training data for parametric PDE maps, they are especially well suited to scalable EIG approximation, since they can be efficiently queried many times at no cost in PDE solves, and require few high fidelity PDE solutions for their construction.
3.3 DLMC with DIPNet surrogate

We propose to train a DIPNet surrogate $\tilde{F}_d$ for the parameter-to-observable map $F_d$, so that $\hat{\pi}(y_i, W)$ can be approximated as

$$\hat{\pi}(y_i, W) = \frac{1}{n_{in}} \sum_{j=1}^{n_{in}} \exp \left( -\frac{1}{2} \| y_i - W \tilde{F}_d(m_{i,j}) \|^2_{\Gamma^{-1}_n} \right),$$

(23)

where we omitted a constant $\frac{1}{(2\pi)^{n_{out}/2} \det(\Gamma_n)^{1/2}}$ since it appears in both the numerator and denominator of the argument of the log in the expression for the EIG. To this end, we can formulate the approximate EIG with the DIPNet surrogate as

$$\Psi_{nn} := \frac{1}{n_{out}} \sum_{i=1}^{n_{out}} \log \left( \frac{\pi_{like}(y_i|m_i, W)}{\hat{\pi}(y_i, W)} \right)$$

(24)

$$= -\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} \frac{1}{2} \| W \varepsilon_{d,i} \|^2_{\Gamma^{-1}_n}$$

(25)

$$- \frac{1}{n_{out}} \sum_{i=1}^{n_{out}} \log \left( \frac{1}{n_{in}} \sum_{j=1}^{n_{in}} \exp \left( -\frac{1}{2} \| y_i - W \tilde{F}_d(m_{i,j}) \|^2_{\Gamma^{-1}_n} \right) \right),$$

(26)

where $\varepsilon_{d,i}$ are i.i.d. observation noise. Thanks to the DIPNet surrogate, the EIG can be evaluated at negligible cost (relating to PDE solver cost) for each given $W$, and does not require any PDE solves.

3.4 Error analysis

**Theorem 1** We assume that the parameter-to-observable map $F_d$ and its surrogate $\tilde{F}_d$ are bounded as

$$\mathbb{E}_{m \sim \mu_{pr}}[\|F_d(m)\|^2] < \infty \quad \text{and} \quad \mathbb{E}_{m \sim \mu_{pr}}[\|\tilde{F}_d(m)\|^2] < \infty.$$  

(27)

Moreover, we assume that the generalization error of the DIPNet surrogate can be bounded by $\varepsilon$, i.e.,

$$\mathbb{E}_{m \sim \mu_{pr}}[\|F_d(m) - \tilde{F}_d(m)\|^2] \leq \varepsilon^2.$$  

(28)

Then the error in the approximation of the normalization constant by the DIPNet surrogate can be bounded by

$$|\hat{\pi}(y_i, W) - \hat{\pi}(y_i, W)| \leq C_i \varepsilon,$$  

(29)

for sufficiently large $n_{in}$ and some constants $0 < C_i < \infty$, $i = 1, \ldots, n_{out}$. Moreover, the approximation error for the EIG can be bounded by

$$|\Psi_{dl}(W) - \Psi_{nn}(W)| \leq C \varepsilon$$  

(30)

for some constant $0 < C < \infty$. 


Proof For notational simplicity, we omit the dependence of \( \hat{\pi} \) and \( \bar{\pi} \) on \( W \) and write \( \mathbf{F} = \mathbf{W}_d \mathbf{F}_d \) and \( \mathbf{\bar{F}} = \mathbf{W}_d \mathbf{\bar{F}}_d \). Note that the bounds (27) and (28) also hold for \( \mathbf{F} \) and \( \mathbf{\bar{F}} \), since \( \mathbf{F} \) and \( \mathbf{\bar{F}} \) are selection of some entries of \( \mathbf{F}_d \) and \( \mathbf{\bar{F}}_d \). By definition of \( \hat{\pi} \) in (18) and \( \bar{\pi} \) in (23), and the fact that \( |e^{-x} - e^{-x'}| \leq |x - x'| \) for any \( x, x' > 0 \), we have

\[
|\hat{\pi}(y_i) - \bar{\pi}(y_j)|, \leq \frac{1}{n_{\text{in}}} \sum_{j=1}^{n_{\text{in}}} \frac{1}{2} \|y_i - \mathbf{F}(\mathbf{m}_{i,j})\|_{\Gamma_{n}^{-1}}^2 - \|y_i - \mathbf{\bar{F}}(\mathbf{m}_{i,j})\|_{\Gamma_{n}^{-1}}^2,
\]

\[
= \frac{1}{n_{\text{in}}} \sum_{j=1}^{n_{\text{in}}} \frac{1}{2} \left( 2y_i - \mathbf{F}(\mathbf{m}_{i,j}) - \mathbf{\bar{F}}(\mathbf{m}_{i,j}) \right)^T \Gamma_{n}^{-1} \left( \mathbf{F}(\mathbf{m}_{i,j}) - \mathbf{\bar{F}}(\mathbf{m}_{i,j}) \right),
\]

\[
\leq \frac{1}{n_{\text{in}}} \sum_{j=1}^{n_{\text{in}}} \|\Gamma_{n}^{-1}(2\|y_i\| + \|\mathbf{F}(\mathbf{m}_{i,j})\| + \|\mathbf{\bar{F}}(\mathbf{m}_{i,j})\|)\|\mathbf{F}(\mathbf{m}_{i,j}) - \mathbf{\bar{F}}(\mathbf{m}_{i,j})\|,
\]

\[
\leq C_i \left( \frac{1}{n_{\text{in}}} \sum_{j=1}^{n_{\text{in}}} \|\mathbf{F}(\mathbf{m}_{i,j}) - \mathbf{\bar{F}}(\mathbf{m}_{i,j})\|^2 \right)^{1/2},
\]

where we used the Cauchy–Schwarz inequality in the last inequality with \( C_i \) given by

\[
C_i = \|\Gamma_{n}^{-1}\| \left( 4\|y_i\|^2 + \left( \frac{1}{n_{\text{in}}} \sum_{j=1}^{n_{\text{in}}} \|\mathbf{F}(\mathbf{m}_{i,j})\|^2 \right)^{1/2} + \left( \frac{1}{n_{\text{in}}} \sum_{j=1}^{n_{\text{in}}} \|\mathbf{\bar{F}}(\mathbf{m}_{i,j})\|^2 \right)^{1/2} \right).
\]

For sufficiently large \( n_{\text{in}} \), we have that \( C_i < \infty \) by \( \|y_i\| < \infty \) and the assumption (27). Moreover, the error bound (29) holds by the assumption (28).

By the definition of the EIGs (17) and (24), we have

\[
|\Psi^{dl}(W) - \Psi^{nn}(W)| \leq \frac{1}{n_{\text{out}}} \sum_{i=1}^{n_{\text{out}}} |\log(\hat{\pi}(y_i, W)) - \log(\bar{\pi}(y_i, W))|. \quad (32)
\]

For sufficiently large \( n_{\text{in}} \), we have that the normalization constants \( \hat{\pi}(y_i, W) \) and \( \bar{\pi}(y_i, W) \) are bounded away from zero, i.e.,

\[
\hat{\pi}(y_i, W), \bar{\pi}(y_i, W) \geq c_i \quad (33)
\]

for some constant \( c_i > 0 \). Then we have

\[
|\Psi^{dl}(W) - \Psi^{nn}(W)| \leq \frac{1}{n_{\text{out}}} \sum_{i=1}^{n_{\text{out}}} \frac{1}{c_i} |\hat{\pi}(y_i, W) - \bar{\pi}(y_i, W)| \leq \frac{1}{n_{\text{out}}} \sum_{i=1}^{n_{\text{out}}} \frac{C_i}{c_i} \varepsilon \quad (34)
\]

where we used the bound (29), which implies the bound (30) with constant

\[
C = \frac{1}{n_{\text{out}}} \sum_{i=1}^{n_{\text{out}}} \frac{C_i}{c_i}. \quad (35)
\]

\[
3.5 \text{ Greedy algorithm}
\]

With the DIPNet surrogate, the evaluation of the DLMC EIG \( \Psi^{nn} \) defined in (26) does not involve any PDE solves. Thus to solve the optimization problem

\[
\mathbf{W}^{*} = \arg \max_{\mathbf{W} \in \mathcal{W}} \Psi^{nn}(\mathbf{W}), \quad (36)
\]
we can directly use a greedy algorithm that requires evaluations of the EIG, not its derivative w.r.t. $\mathbf{W}$. Let $S_d$ denote the set of all $d$ candidate sensors; we wish to choose $r$ sensors from $S_d$ that maximize the approximate EIG (approximated with the DIPNet surrogate). At the first step with $t = 1$, we select the sensor $v^* \in S_d$ corresponding to the maximum approximate EIG and set $S^* = \{v^*\}$. Then at step $t = 2, \ldots, r$, with $t - 1$ sensors selected in $S^*$, we choose the $t$-th sensor $v^* \in S_d \setminus S^*$ corresponding to the maximum approximate EIG evaluated with $t$ sensors $S^* \cup \{v^*\}$; see Algorithm 1 for the greedy optimization process, which can achieve (quasi-optimal) experimental design with an approximation guarantee under suitable assumptions on the incremental information gain of the additional sensor, see [58] and references therein. Note that at each step the approximate EIG can be evaluated in parallel for each sensor choice $S^* \cup \{v\}$ with $v \in S_d \setminus S^*$.

Algorithm 1 Greedy algorithm to solve (36)

Require: data $\{y_i\}_{i=1}^{N_s}$ generated from the prior samples $\{m_i\}_{i=1}^{N_s}$, $d$ sensor candidates set $S_d$, sensor budget $r$, optimal sensor set $S^* = \emptyset$

Ensure: optimal sensor set $S^*$

1: for $t = 1, \ldots, r$ do
2: $S \leftarrow S_d \setminus S^*$
3: for $v \in S$ do
4: $W_v$ is the design matrix of sensor choice $S^* \cup \{v\}$
5: evaluate $\Psi_{nn}(W_v)$
6: end for
7: $v^* \leftarrow \arg \max_{v \in S} \Psi_{nn}(W_v)$
8: $S^* \leftarrow S^* \cup \{v^*\}$
9: end for

4 Numerical results

In this section, we present numerical results for OED problems involving a Helmholtz acoustic inverse scattering problem and an advection-reaction-diffusion inverse transport problem to illustrate the efficiency and accuracy of our method. We compare the approximated normalization constant and EIG of our method with 1) the DLMC truth computed by a large number of Monte Carlo samples; and 2) the DLMC sampled at the same computational cost (number of PDE solves) as our method using DIPNet training.

Both PDE problems are discretized using the finite element library FEniCS [59]. The construction of training data and reduced bases (active subspace and
proper orthogonal decomposition) is implemented in hIPPYflow [60], a library for dimension reduced PDE surrogate construction, building on top of PDE adjoints implemented in hIPPYlib [61]. The DIPNet neural network surrogates are constructed in TensorFlow [62], and are adaptively trained using a combination of Adam [63], and a Newton method, LRSFN, which improves local convergence and generalization [26, 64, 65]. A TensorFlow implementation of LRSFN is available in hessianlearn [66].

4.1 Helmholtz problem

For the first numerical experiment, we consider an inverse wave scattering problem modeled by the Helmholtz equation with uncertain medium in the two-dimensional physical domain \( \Omega = (0, 3)^2 \)

\[
-\Delta u - e^{2m}k^2 u = f \quad \text{in } \Omega, \quad \text{(37a)}
\]

PML boundary condition on \( \partial \Omega \setminus \Gamma_{\text{top}} \),

\[
\nabla u \cdot n = 0 \quad \text{on } \Gamma_{\text{top}}, \quad \text{(37b)}
\]

\[
F_d(m) = [u(x_i, m)] \quad \text{at } x_i \in \Omega. \quad \text{(37d)}
\]

where \( u \) is the total wave field, \( k \approx 4.55 \) is the wavenumber, and \( e^{2m} \) models the uncertainty of the medium, with the parameter \( m \) a log-prefactor of the squared wavenumber. The right hand side \( f \) is a point source located at \( x = (0.775, 2.5) \). The perfectly matched layer (PML) boundary condition approximates a semi-infinite domain. The candidate sensor locations \( x_i \) are linearly spaced in the line segment between the edge points \((0.1, 2.9)\) and \((2.9, 2.9)\), as shown in Fig. 2. The prior distribution for the uncertain parameter \( m \) is Gaussian \( \mu_{\text{pr}} = N(m_{\text{pr}}, C_{\text{pr}}) \) with zero mean \( m_{\text{pr}} = 0 \) and covariance \( C_{\text{pr}} = (5.0I - \Delta)^{-2} \). The mesh used for this problem is uniform of size 64 \( \times \) 64. We use quadratic elements for the discretization of the wave field \( u \) and linear elements for the parameter \( m \), leading to a discrete parameter \( m \) of dimension 4225. A sample of the parameter field \( m \) and the PDE solution \( u \) is shown in Fig. 2 with all 50 candidate sensor locations marked in circles.

The neural network is trained adaptively using 4915 training samples, and 1228 validation samples. Using 512 independent testing samples, the DIPNet surrogate was 85.06\% \( \ell^2 \) accurate measured as a percentage by

\[
\ell^2 \quad \text{accuracy} = 100 \left( 1 - \frac{\| \tilde{F}_d - F_d \|_2}{\| F_d \|_2} \right). \quad \text{(38)}
\]

The network has 10 low-rank residual layers, each with a layer rank of 10. Due to the oscillatory nature of the Helmholtz solution we use \( r_M = 64 \) active subspace vectors for the reduced input; the ResNet then learns the mapping from
inputs to outputs in a 64 dimensional space. Since this is larger than the output dimension for this problem we use a restriction for the last layer (and thus use the entire POD basis for the output). For more details on this neural network architecture, see [26]. The computational cost of the 64 dimensional active subspace projector using 128 samples is equivalent to the cost of 1078 additional training data; since the problem is linear the additional linear adjoint computations are comparable to the costs of the training data generation. As we will see in the next example, when the PDE is nonlinear the additional active subspace computations are marginal. Thus for fair comparison with the same computational cost of PDE solves, we use 4915 + 1078 = 5993 samples for simple MC.

![Fig. 2](image_url) A random sample of the parameter field \( \mathbf{m} \) (left) and the corresponding solution \( \mathbf{u} \) with candidate observation sensor locations marked in circles (right) for the Helmholtz problem.

To test the efficiency and accuracy of our DIPNet surrogate, we first compute the log normalization constant \( \log \pi(\mathbf{y}) \) with our DIPNet surrogate for given observation data \( \mathbf{y} \) generated by \( \mathbf{y} = \mathbf{W} \mathbf{F}_d(\mathbf{m}) + \varepsilon \). \( \mathbf{m} \) is a random sample from the prior. We use in total 60000 random samples for Monte Carlo (MC) to compute the normalization constant as the ground truth. Fig. 3 shows the \( \log \pi(\mathbf{y}) \) comparison for three random designs \( \mathbf{W} \) that choose 15 sensors out of 50 candidates. We can see that DIPNet surrogate converges to a value close to the ground truth MC reference, while for the (simple) MC with 5993 samples, the approximated value indicated by the green star is much less accurate than the DIPNet surrogate using 60000 samples with similar cost in PDE solves. Note that the DIPNet training and evaluation cost for this small size neural network is negligible compared to PDE solves.

The left and middle figures in Fig. 4 illustrate the sample distributions of the relative approximation errors for the log normalization constant \( \log \pi(\mathbf{y}) \) and the EIG \( \Psi (n_{\text{out}} = 200) \) with (DIPNet MC with 60000 samples) and without (simple MC with 5993 samples) the DIPNet surrogate, compared to the
Fig. 3 The approximation of the log normalization constant with increasing numbers of samples without (true MC) and with (DIPNet MC) surrogate at 3 random designs. Green stars indicate 5993 samples (for simple MC), which is the same computational cost as DIPNet.

true MC with 60000 samples. These results show that using DIPNet surrogate we can approximate log $\pi(y)$ and $\Psi$ much more accurately with less bias compared to the simple MC. The sample distributions of EIG at 200 random designs compared to the design chosen by the greedy optimization using DIPNet surrogate for different number of sensors are shown in the right figure, from which we can see that our method can always chose better designs with larger EIG values than all the random designs.

Fig. 4 Sample distributions for 200 random designs of the relative approximation errors (compared to true MC) for the log normalization constant log $\pi(y)$ (left) and EIG $\Psi$ (middle) by DIPNet MC and simple MC with different number of sensors $r$. Right: Blue filled areas represent the sample distributions of the true DLMC EIG $\Psi^{dl}$ for 200 random designs. Pink crosses is the true DLMC EIG $\Psi^{dl}$ of designs chosen by the greedy optimization using DIPNet surrogates.

Fig. 5 gives approximate values of the EIG with increasing number of outer loop samples $n_{out}$ using: the DIPNet surrogate with inner loop $n_{in} = 60000$, simple DLMC with inner loop $n_{in} = 5993$, and the truth computed with inner loop $n_{in} = 60000$. We can see that the approximate values by the DIPNet surrogates are almost the same as the truth, while simple DLMC results are very inaccurate.
Fig. 5 EIG of true DLMC ($n_{in} = 60000$), DIPNet DLMC ($n_{in} = 60000$), and simple DLMC ($n_{in} = 5993$) with increasing number of outer loop samples $n_{out}$ at 3 random designs.

4.2 Advection-diffusion-reaction problem

For the second numerical experiment we consider an OED problem for an advection-diffusion-reaction equation with a cubic nonlinear reaction term. The uncertain parameter $m$ appears as a log-coefficient of the cubic nonlinear reaction term. The PDE is defined in a domain $\Omega = (0,1)^2$ as

$$-\nabla \cdot (k \nabla u) + \mathbf{v} \cdot \nabla u + e^m u^3 = f \quad \text{in } \Omega, \quad (39a)$$

$$u = 0 \quad \text{on } \partial \Omega, \quad (39b)$$

$$\mathcal{F}_d(m) = [u(x_i, m)] \quad \text{at } x_i \in \Omega. \quad (39c)$$

Here $k = 0.01$ is the diffusion coefficient. The volumetric forcing function $f$ is a smoothed Gaussian bump located at $x = (0.7, 0.7)$,

$$f(x) = \max \left( 0.5, e^{-25(x_1-0.7)^2-25(x_2-0.7)^2} \right) \quad (40)$$

The velocity field $\mathbf{v}$ is a solution of a steady-state Navier Stokes equation with shearing boundary conditions driving the flow (see the Appendix in [24] for more information on the flow). The candidate sensor locations are located in a linearly spaced mesh-grid of points in $(0.1, 0.9) \times (0.1, 0.9)$. The prior distribution for the uncertain parameter $m$ is a mean zero Gaussian with covariance $C_{pr} = (I - 0.1\Delta)^{-2}$. The mesh used for this problem is uniform of size $64 \times 64$. We use linear elements for both $u$ and $m$, leading to a discrete parameter of dimension 4225. Fig. 6 gives a prior sample of the parameter field $m$ and the solution $u$ with all 100 candidate sensor locations in white circles.

The neural network surrogate is trained adaptively using 409 training samples and 102 validation samples. Using 512 independent testing samples the DIPNet network was 94.40% $\ell^2$ accurate (see equation 38). The network has 20 low-rank residual layers, each with a layer rank of 10, the breadth of the network is again $r_M = r_F = 48$; for more details on this neural network architecture see [26]. The computational cost of the 48 dimensional active subspace projector using 256 samples is equivalent to the cost of 66 additional training samples.
data. As was noted before when the PDE is nonlinear the linear adjoint-based
derivative computations become much less of a computational burden. Thus
we use $409 + 66 = 475$ samples for simple MC for fair comparison.

We first examine the log normalization constant $\log \pi(y)$ computed with
our 409 PDE-solve-based DIPNet surrogate compared against the truth com-
puted with 60000 MC samples and the simple MC computed with 475 samples.
Fig. 7 shows the $\log \pi(y)$ comparison for three random designs that select 15
sensors out of 100 candidates. We can see that DIPNet MC converges to a
value close to the true MC curves, while the simple MC’s green star computed
with the same number of PDE solves (475) as DIPNet MC, has much worse
accuracy.

The left figure of Fig. 8 shows the relative errors for $\log \pi(y)$ computed with
the DIPNet surrogate and simple MC using 475 samples based on the true
MC with 60000 samples, for 200 random designs. We see again that DIPNet
gives better accuracy with less bias than simple MC.
Fig. 9 shows the EIG approximations of three random designs with increasing number of outer loop samples \( n_{\text{out}} \) using the DIPNet MC with 60000 (inner loop) samples, simple MC with 475 samples, and true MC with 60000 samples. We can see that the values of DIPNet MC are quite close to the true MC, while simple MC is far off. Relative errors of the EIG \( \Psi \) \((n_{\text{out}} = 100)\) computed with the DIPNet surrogate, the simple MC for 200 random designs is given in the middle figure of Fig. 8. With the DIPNet DLMC \( \Psi^{\text{nn}} \), we can use the greedy algorithm to find the optimal designs. The DIPNet greedy designs are presented as the pink crosses in the right figure of Fig. 8. We can see that the designs chosen by the greedy algorithm have much larger EIG values than all 200 random designs.

5 Conclusions

We have developed a computational method based on DIPNet surrogates for solving large-scale PDE-constrained Bayesian OED problems to
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determine optimal sensor locations (using the EIG criterion) to best infer infinite-dimensional parameters. We exploited the intrinsic low dimensionality of the parameter and data spaces and constructed a DIPNet surrogate for the parameter-to-observable map. The surrogate was used repeatedly in the evaluation of the normalization constant and the EIG. We presented error analysis for the approximation of the normalization constant and the EIG, showing that the errors are of the same order as the DIPNet RMS approximation error. Moreover, we used a greedy algorithm to solve the combinatorial optimization problem for sensor selection. The computational efficiency and accuracy of our approach are demonstrated by two numerical experiments. Future work will focus on gradient-based optimization also using the derivative information of the DIPNet w.r.t. both the parameter and the design variables, on the use of different optimality criteria such as A-optimality or D-optimality, and on exploring new network architectures for intrinsically high-dimensional Bayesian OED problems.

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