Abstract

We consider a weak adversarial network approach to numerically solve a class of inverse problems, including electrical impedance tomography and dynamic electrical impedance tomography problems. We leverage the weak formulation of PDE in the given inverse problem, and parameterize the solution and the test function as deep neural networks. The weak formulation and the boundary conditions induce a minimax problem of a saddle function of the network parameters. As the parameters are alternatively updated, the network gradually approximates the solution of the inverse problem. We provide theoretical justifications on the convergence of the proposed algorithm. Our method is completely mesh-free without any spatial discretization, and is particularly suitable for problems with high dimensionality and low regularity on solutions. Numerical experiments on a variety of test inverse problems demonstrate the promising accuracy and efficiency of our approach.

Keywords—Inverse Problem; Deep learning; Weak formulation; Adversarial network; Stochastic gradient.

1 Introduction

Inverse problems (IP) [5, 7, 11, 13, 16] are ubiquitous in a vast number of scientific disciplines, including geophysics [6, 58, 65], signal processing [17, 29], imaging [2, 21, 22, 23, 40, 57, 69, 70], computer vision [67], remote sensing [12, 63], control [10, 18, 71], statistics [43, 48], and machine learning [32]. Let \( \Omega \) be an open and bounded set in \( \mathbb{R}^d \), then an IP defined on \( \Omega \) can be presented in a general form as:

\[
\begin{align*}
A[u, \gamma] &= 0, \quad \text{in } \Omega \\
B[u, \gamma] &= 0, \quad \text{on } \partial \Omega
\end{align*}
\]

where \( A[u, \gamma] \) specifies a differential equation, in which \( u \) is the solution and \( \gamma \) the coefficient in the inverse medium problem or the source function in the inverse source problem. Equation \( A \) can be an ordinary differential equation (ODE), or a partial differential equation (PDE), or an integro-differential equation (IDE), that \( (u, \gamma) \) needs to satisfy (almost) everywhere inside the region \( \Omega \). The boundary value (and initial value if applicable) is given by \( B[u, \gamma] \) on \( \partial \Omega \). Depending on specific applications, partial information of \( u \) and/or \( \gamma \) may be available in the interior of \( \Omega \). Then IP (1) is to find \( (u, \gamma) \) that satisfies both (1a) and (1b).

To instantiate our approach, we mostly use the classical inverse conductivity problem in electrical impedance tomography (EIT) [15] as an example to present our main idea and the derivations in this paper. However, our methodology can be readily applied to other classes of IPs with modifications. An
example of dynamic EIT problem will be shown in Section 5. The goal of EIT is to determine the electrical conductivity distribution γ(x) of an unknown medium defined on Ω based on the voltage ̅u, the current −∇·(γ ̅u) − f = 0, in Ω

\[ u - u_b = 0, \quad γ - γ_b = 0, \quad ∇·u_n = 0, \quad \text{on } ∂Ω \]  

where ̅u_b is the measured voltage, γ_b is the conductivity near the surface of the object and u_n = ∇u·̅n with ̅n being the outer normal of ∂Ω. Note that our approach is not to estimate the Dirichlet-to-Neumann (DtN) map associated with the conductivity function as in classical methods specific to the EIT problem [19, 30, 47]. Instead, our goal is to directly solve a general class of IPs [1] numerically using the given data, with EIT problem (2) as a prototype example without exploiting its special structure (e.g., the DtN map). To make our presentation concise and focused, we only consider IPs with A[u, γ] characterized by PDEs in (1a), and assume that the given IP is well-defined and admits at least one (weak) solution.

Our approach is to train deep neural networks that can represent the solution (u, γ) of a given IP, with substantial improvement over classical numerical methods especially for problems with high dimensionality. More specifically, we leverage the weak formulation of the PDE (1a) and convert the IP into an operator norm minimization problem of u and γ. Then we parameterize both u, the unknown coefficient γ, and the test function φ as deep neural networks uθ, γθ, and φη respectively, with network parameters (θ, η), and form a minimax problem of a saddle function of the parameters (θ, η). Finally, we apply stochastic gradient descent method to alternately update the network parameters so that (uθ, γθ) gradually approximates the solution of the IP. The parameterization of (u, γ) using deep neural networks requires no discretization of the spatial and temporal domain, and hence is completely mesh free. This is a promising alternative compared to the classical finite difference method (FDM) and finite element methods (FEM) which suffer the issue of the so-called curse of dimensionality. Moreover, our approach combines the training of the weak solution (primal network) (u, γ) and the test function (adversarial network) φ governed by the weak formulation of the PDE, which requires less regularity of the solution (u, γ) and can be more advantageous in many real-world applications when the solution has singularities.

The remainder of this paper is organized as follows. We first review the recent work on deep learning based solutions to forward and inverse problems in Section 2. In Section 3, we provide the detailed derivation of our method and a series of theoretical results to support the validity of the proposed approach. We discuss several implementation techniques that can improve practical performance in Section 4. In Section 5, we conduct a series of numerical experiments to demonstrate the effectiveness of the proposed approach. Section 6 concludes this paper with some general remarks.

2 Related Work

The past few years have witnessed an emerging trend of using deep learning based methods to solve forward and inverse problems [3, 9, 14, 24, 25, 27, 36, 39, 42, 45, 50, 51, 54, 56, 59, 61, 64, 73]. These methods can be roughly classified into two categories. The first category includes methods that approximate the solution of a given problem based on supervised learning approaches. These methods require a large number of input-output pairs through numerical simulation and experiments to train the desired networks. In this category, deep neural networks are used to generate approximate intermediate results from measurement data for further refinement, or applied to improve the solution of classical numerical methods in the post-processing phase. For example, feed-forward neural networks are used to parameterize the coefficient functions and trained by minimizing the performance function in [20]. In [46], a neural network architecture called SwitchNet is proposed to solve the inverse scattering problem through the mapping between the scatterers and the scattered field. In [26], a deep learning approach specific to 2D and 3D EIT problems is developed to represent the DtN map by a compact neural network architecture. A mesh-free framework, called physics-informed neural networks (PINN), for solving both the forward and inverse problems using deep neural networks based on the strong

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formulation of PDEs is proposed in [59], where a constant coefficient function is considered for the inverse problem part. Solutions to IPs based on PINN with data given in problem domain are also considered in [54], where three neural networks, one for low-fidelity data and the other two for the linear and nonlinear functions for high-fidelity data, are used by following the PINN approach. The PINN with multi-fidelity network structure is also proposed for stochastic PDE cases, where polynomial chaotic expansions are used to express the solutions, i.e., as linear combination of random basis with coefficient functions to be learned [14]. In [8], the solution of an IP is parameterized by deep neural network and learned by minimizing a cost function that enforces the conditions of IP and additional regularization, where solutions to the PDE are required during the training.

Recently, meta-learning based approaches for forward problems are also considered [14, 27, 50]. In [27], the mapping from the coefficient of a differential operator to the pseudo-differential operator (e.g., the Green function) is learned by leveraging the compressed form of wavelet transform. In [50], a deep operator network consisting of a branch network and a trunk network is introduced. The network encodes the input function evaluated at a finite number of locations (branch-net) and the locations for the output function (trunk-net) and, the output function is given by the inner product of the two plus a bias. Learning network width and depth parameters are also considered using Bayesian optimization in [14].

Our approach to the IP follows our earlier work [73] for forward problems, which differs from the aforementioned existing methods in the use of weak formulation of PDEs. Weak formulation is a powerful approach for solving PDEs as it requires less regularity and allows for necessary singularities of the solutions, which is an important feature appreciated in many real-world applications such as imaging and abnormality detections. From the theoretical point of view, our method employs neural network parameterizations of both the solution (as the primal network) and the test function (as the adversarial network), and performs an adversarial training in a way that the test function criticizes on the solution network where the PDE is violated, and the solution network corrects itself at those spots until the PDE is satisfied (almost) everywhere in the domain. The adversarial training has a similar flavor as the one used in generative adversarial network [33], where an artificial discriminator network is created to evaluate the quality of samples produced by the generator network. However, the structure of weak solution versus test function in our work arises naturally from the weak formulation in the PDE theory, and enjoys numerous theoretical justifications and computational benefits for solving IPs for PDEs.

3 Weak Adversarial Network for Inverse Problems

The proposed weak adversarial network approach for IPs is inspired by the weak formulation of PDEs. To obtain the weak formulation of the PDE in (1a), we multiply both sides of (1a) by an arbitrary test function \( \varphi \in H^1_0(\Omega) \) and integrate over \( \Omega \):

\[
\langle A[u, \gamma], \varphi \rangle := \int_{\Omega} A[u, \gamma](x) \varphi(x) \, dx = 0. \tag{3}
\]

One of the main advantages of weak formulation (3) is that we can subsequently apply integration by parts to transfer certain gradient operator(s) in \( A[u, \gamma] \) to \( \varphi \), such that the requirement on the regularity of \( u \) (and \( \gamma \) if applicable) can be reduced. For example, in the case of inverse conductivity problem (2), the integration by parts and the fact that \( \varphi = 0 \) on \( \partial \Omega \) together yield

\[
\langle A[u, \gamma], \varphi \rangle = \int_{\Omega} (\gamma \nabla u \cdot \nabla \varphi - f \varphi) \, dx = 0, \tag{4}
\]

where \( \gamma \nabla u \) is not necessarily differentiable as in (2) in the classical sense anymore (we use \( \nabla \) to denote the gradient operator with respect to \( x \), and \( \nabla_\theta \) as the gradient with respect to \( \theta \) and so on in this paper). We call \( (u, \gamma) \) a weak solution (or generalized solution) of the inverse problem (1) if \( (u, \gamma) \) satisfies the boundary condition (1b) and (3) for all \( \varphi \in H^1_0(\Omega) \). Note that any classical (strong) solution of (1) is also a weak solution. In this work, we seek for weak solutions of inverse problem (1) so that we may be able to provide an answer to the problem even if it does not admit a solution in the classical sense.
Following the work \cite{73}, we consider the weak formulation of of the PDE \( A[u, \gamma] = 0 \) in (1). To cope with the unknown solution \( u \) and parameter \( \gamma \) of the PDE in an inverse problem, we parameterize both \( u \) and \( \gamma \) as deep neural networks, and consider \( A[u, \gamma] : H^1_0(\Omega) \to \mathbb{R} \) as a linear functional such that \( A[u, \gamma](\varphi) := \langle A[u, \gamma], \varphi \rangle \) as defined in (3). The operator norm of \( A[u, \gamma] \) induced by the \( L^2 \) norm is defined by

\[
\|A[u, \gamma]\|_{op} := \max_{\varphi \in H^1_0} \frac{\langle A[u, \gamma], \varphi \rangle}{\|\varphi\|_2},
\]

where \( \|\varphi\|_2 := (\int_\Omega |\varphi(x)|^2 \, dx)^{1/2} \). Therefore, \( (u, \gamma) \) is a weak solution of (1) if and only if \( \|A[u, \gamma]\|_{op} = 0 \) and \( B[u, \gamma] = 0 \) on \( \partial \Omega \). As \( \|A[u, \gamma]\|_{op} \geq 0 \), we know that a weak solution \( (u, \gamma) \) of (1) thus solves the following two equivalent problems in observation of (5):

\[
\min_{u, \gamma} \|A[u, \gamma]\|_{op}^2 \iff \min_{u, \gamma} \max_{\varphi \in H^1_0} \frac{|\langle A[u, \gamma], \varphi \rangle|^2}{\|\varphi\|_2^2},
\]

among all \( (u, \gamma) \in H^1(\Omega) \times L^2(\Omega) \) and attains minimal value 0. This result is summarized in the following theorem, the proof is provided in Appendix A.1.

**Theorem 1.** Suppose that \((u^*, \gamma^*)\) satisfies the boundary condition \( B[u^*, \gamma^*] = 0 \), then \((u^*, \gamma^*)\) is a weak solution of (1) if and only if \((u^*, \gamma^*)\) solves the problems in (6) and \( \|A[u^*, \gamma^*]\|_{op} = 0 \).

Theorem 1 implies that, to find the weak solution of (1), we can instead seek for the optimal solution \((u^*, \gamma^*)\) that satisfies \( B[u^*, \gamma^*] = 0 \) and meanwhile minimizes (6). In other words, \((u^*, \gamma^*)\) is a weak solution of the problem (1) if and only if both \( \|A[u^*, \gamma^*]\|_{op} \) and \( \|B[u^*, \gamma^*]\|_{L^2(\partial \Omega)} \) vanish. Therefore, we can solve for \((u^*, \gamma^*)\) from the following minimization problem which is equivalent to (1):

\[
\min_{u, \gamma} \|A[u, \gamma]\|_{op}^2 + \beta \|B[u, \gamma]\|_{L^2(\partial \Omega)}^2,
\]

where \( \beta > 0 \) is a weight parameter that balances the two terms in the minimization. Note that both terms of the objective function in (7) are nonnegative and vanish simultaneously only at the weak solution(s) \((u, \gamma)\) of (1).

A promising alternative to classical numerical methods for high-dimensional PDEs is the use of deep neural networks since they do not require domain discretization and are completely mesh free. Deep neural networks are compositions of multiple simple functions (called layers) so that they can approximate rather complicated functions. Consider a simple multi-layer neural network \( u_\theta \) as follows:

\[
u_\theta(x) = w_K^T l_{K-1} \circ \cdots \circ l_0(x) + b_K,
\]

where the \( k \)th layer \( l_k : \mathbb{R}^{d_k} \to \mathbb{R}^{d_{k+1}} \) is given by

\[
l_k(z) = \sigma_k(W_k z + b_k),
\]

and the network parameters of all layers are collectively denoted by \( \theta \) as follows,

\[
\theta := (w_K, b_K, W_{K-1}, b_{K-1}, \ldots, W_0, b_0).
\]

That is, \( l_k \) is a composition of a componentwise activation function \( \sigma_k \) and an affine function with weight \( W_k \in \mathbb{R}^{d_{k+1} \times d_k} \) and bias \( b_k \in \mathbb{R}^{d_{k+1}} \) for \( k = 0, 1, \ldots, K - 1 \). Throughout, all vectors in this paper are column vectors by default. In \cite{8}, \( x \in \Omega \) is the input of the network, \( d_0 = d \) is the problem dimension of (1) (also known the size of input layer), \( w_K \in \mathbb{R}^{d_K} \) and \( b_K \in \mathbb{R} \) are parameters in the last, \( K \)th layer (also called the output layer). The activation functions \( \sigma_k \) are critical as they introduce nonlinearities into \( \theta \) to generate highly complicated nonlinear function \( u_\theta \). Typical choices of \( \sigma_k \) include sigmoid function \( \sigma(z) = (1 + e^{-z})^{-1} \), hyperbolic tangent (tanh) function \( \sigma(z) = (e^z - e^{-z})/(e^z + e^{-z}) \), and rectified linear unit (ReLU) function \( \sigma(z) = \max(0, z) \). Note that these activation functions are applied componentwisely. We do not apply activation in the output layer in \cite{8} unless there is certain constraint such as positivity on the output. The training of deep neural networks refers to the process of optimizing \( \theta \) using available data.
or constraints such that the function \( u_\theta \) can approximate the (unknown) target function. If the activation functions \( \sigma_k \) also have parameters to be determined, then they can be added to \( \theta \) in (10) for training as well.

Despite of the simple structures like (5), deep neural networks are capable to approximate rather complicated continuous function (and its derivatives if needed) uniformly on a compact support \( \bar{\Omega} \). This significant result, known as the universal approximation theorem [38], is the foundation of deep learning, which we restate as follows.

**Theorem 2** (Universal Approximation Theorem). For any \( u \in H^p(\Omega) \cap C(\bar{\Omega}) \) and \( \epsilon > 0 \), there exists a neural network \( u_\theta \) in the form of (4) with parameter \( \theta \), such that \( |\partial^\alpha u_\theta - \partial^\alpha u| \leq \epsilon \) for all \( x \in \Omega \) and multi-indices \( \alpha = (\alpha_1, \ldots, \alpha_d) \) with \( |\alpha| \leq p \).

**Remark.** The original universal approximation theorem states that a single-layer (but possibly very large width \( d_1 \)) neural network can approximate a given continuous function \( u \) uniformly with a prescribed accuracy \( \epsilon > 0 \). Due to the compactness of \( \bar{\Omega} \) and that \( \partial^\alpha u \in C(\bar{\Omega}) \) if \( |\alpha| \leq p \), this result immediately implies the version of Theorem 2. Therefore we use the statement of Theorem 2 here as it is directly applicable to our problem.

The expressive power of neural networks ensured by the universal approximation theorem above suggests a promising mesh-free parametrization of the weak solution \( (u, \gamma) \) of (1). In what follows, we select sufficiently deep neural network structures of form (8) for both \( u \) and \( \gamma \). Specific structures, i.e., layer number \( K \) and sizes \( \{d_1, \ldots, d_{K-1}\} \), used in our numerical experiments will be provided in Section 5. Note that \( u \) and \( \gamma \) are two separate networks, but we use a single letter \( \theta \) to denote their network parameters rather than \( \theta_u \) and \( \theta_\gamma \) to simplify notations. That is, we parameterize \( (u, \gamma) \) as deep neural networks \( (u_\theta, \gamma_\theta) \), and attempt to find the parameter \( \theta \) such that \( (u_\theta, \gamma_\theta) \) solves (7). To this end, the test function \( \varphi \) in the weak formulation (3) is also parameterized as a deep neural network \( \varphi_\eta \) in a similar form of (8) and (10) with parameter denoted by \( \eta \). With the parameterized \( (u_\theta, \gamma_\theta) \) and \( \varphi_\eta \), we follow the inner product notation in (3) and define

\[
E(\theta, \eta) := |\langle A[u_\theta, \gamma_\theta], \varphi_\eta \rangle|^2. \tag{11}
\]

Instead of normalizing \( E(\theta, \eta) \) by \( \|\varphi_\eta\|_2^2 \) as in the original definition of (squared) operator norm (5), we approximate (up to a constant scaling of) the squared operator norm in (5) by the following loss function of \( \theta \):

\[
L_{\text{int}}(\theta) = \max_{|\eta|^2 \leq 2B} E(\theta, \eta) \tag{12}
\]

where \( B > 0 \) is a prescribed bound to constrain the magnitude of network parameter \( \eta \). Here \( |\eta|^2 = \sum_k \sum_{ij} (||W_k||_{ij}^2 + ||b_k||_{j}^2) \), and \( |M|_{ij} \in \mathbb{R} \) stands for the \((i, j)\)th entry of a matrix (or vector) \( M \). This bound constraint on \( \eta \) plays the role of regularization and ensures that the stochastic gradient used in numerical optimization later has bounded variance, which is a requirement for the stochastic gradient descent method to converge. Furthermore, we define the loss function associated with the boundary condition (1b) by

\[
L_{\text{bdry}}(\theta) = \|B[u_\theta, \gamma_\theta]\|_{L^2(\partial\Omega)}^2 = \int_{\partial\Omega} |B[u_\theta, \gamma_\theta]|^2 \, dS(x). \tag{13}
\]

For instance, if the boundary condition of \( (u, \gamma) \) is given in (2b) with known boundary value \( (u_b, \gamma_b) \), then

\[
L_{\text{bdry}}(\theta) = \int_{\partial\Omega} |u_\theta(x) - u_b(x)|^2 + |\gamma_\theta(x) - \gamma_b(x)|^2 + |\partial_n(x)u_\theta(x) - u_n(x)|^2 \, dS(x).
\]

Finally, we define the total loss function of \( \theta \) and set the minimization problem to recover \( \theta \):

\[
\min_{\theta} L(\theta), \quad \text{where} \quad L(\theta) = L_{\text{int}}(\theta) + \beta L_{\text{bdry}}(\theta), \tag{14}
\]

where we also constrain on the magnitude of the parameter \( \theta \) such that \( |\theta|^2 \leq 2B \) for the same \( B \) to simplify notation. Note that here both \( \theta \) and \( \eta \) are finite dimensional vectors, and \( L_{\text{int}}(\theta), L_{\text{bdry}}(\theta), E(\theta, \eta) \in \mathbb{R}_+ \), hence it is possible to apply numerical optimization algorithms to find the minimizer of \( L(\theta) \).

In this work, we opt to the commonly used (stochastic) gradient descent method to minimize (14). Namely, we iterate the gradient descent step as follows:

\[
\theta \leftarrow \Pi(\theta - \tau \nabla \theta L(\theta)), \tag{15}
\]
where \( \Pi(\theta) = \min(\sqrt{2B}, |\theta| \cdot (\theta/|\theta|)) \) is the projection of \( \theta \) to the ball centered at origin with radius \( \sqrt{2B} \), and \( \tau > 0 \) is the step size. As we can see, the main ingredient of the gradient descent \( (15) \) is the computation of the gradient \( \nabla_\theta L(\theta) = \nabla_\theta L_{\text{int}}(\theta) + \beta \nabla_\theta L_{\text{bdry}}(\theta) \). The computation of \( \nabla_\theta L_{\text{bdry}}(\theta) \) is straightforward as shown later. The loss \( L_{\text{int}}(\theta) \), however, is defined as a maximization problem \( (12) \), and we need to write its gradient as a function of \( \theta \) first. To this end, we have the following lemma to compute the gradient \( \nabla_\theta L_{\text{int}}(\theta) \), whose proof is available in Appendix A.2.

**Lemma 3.** Suppose \( L_{\text{int}}(\theta) \) is defined in \( (12) \). Then the gradient \( \nabla_\theta L_{\text{int}}(\theta) \) at any \( \theta \) is given by \( \nabla_\theta L_{\text{int}}(\theta) = \partial_\theta E(\theta, \eta(\theta)) \), where \( \eta(\theta) \) is a solution of \( \max_{|\eta|^2 \leq 2B} E(\theta, \eta) \) for the specified \( \theta \).

**Remark.** Lemma 3 suggests that, to obtain \( \nabla_\theta L_{\text{int}}(\theta) \) at any given \( \theta \), we can first take the partial derivative of \( E \) with respect to \( \theta \) with \( \eta \) untouched, and then evaluate the partial derivative using \( \theta \) and any solution \( \eta(\theta) \) of the maximization problem \( (12) \).

The exact gradients of \( L_{\text{int}}(\theta) \) and \( L_{\text{bdry}}(\theta) \) require integrations of functions parameterized by deep neural networks over \( \Omega \) and \( \partial \Omega \), which are computationally intractable in practice. Therefore, we consider their stochastic gradients obtained by evaluations at sample collocation points. To this end, we need the following result on the approximation of integrals using samples, whose proof is provided in Appendix A.3.

**Lemma 4.** Suppose \( \Omega \subset \mathbb{R}^d \) is bounded, and \( \rho \) is a probability density defined on \( \Omega \) such that \( \rho(x) > 0 \) for all \( x \in \Omega \). Given a function \( \psi \in L^2(\Omega) \), denote \( \Psi = \int_\Omega \psi(x) \, dx \). Let \( x^{(1)}, \ldots, x^{(N)} \) be \( N \) independent samples drawn from \( \rho \). Consider the following estimator \( \hat{\Psi} \) of \( \Psi \):

\[
\hat{\Psi} = \frac{1}{N} \sum_{i=1}^{N} \frac{\psi(x^{(i)})}{\rho(x^{(i)})}.
\]

Then the first and second moments of \( \hat{\Psi} \) are given by

\[
\mathbb{E}[\hat{\Psi}] = \Psi \quad \text{and} \quad \mathbb{E}[\hat{\Psi}^2] = \frac{N-1}{N} \Psi^2 + \frac{1}{N} \int_\Omega \frac{\psi(x)^2}{\rho(x)} \, dx.
\]

Hence the variance of \( \hat{\Psi} \) is \( N^{-1} \cdot (\int_\Omega (\psi^2/\rho) \, dx - (\int_\Omega \psi \, dx)^2) \). In particular, with the uniform distribution \( \rho(x) = 1/|\Omega| \), the variance of \( \hat{\Psi} = (|\Omega|/N) \cdot \sum_i \psi(x^{(i)}) \) is \( N^{-1} \cdot (|\Omega| \int_\Omega \psi^2 \, dx - (\int_\Omega \psi \, dx)^2) \).

**Remark.** We have several remarks regarding Lemma 4:

- **The estimator** \( \hat{\Psi} \) of the integral \( \Psi \) is unbiased.
- **The variance of** \( \hat{\Psi} \) **shown above decreases at the rate of** \( O(1/N) \) **in the number** \( N \) **of sample collocation points. By Hölder’s inequality and that** \( \rho \) **is a probability density, we know**

\[
\left| \int_\Omega \psi \, dx \right| \leq \int_\Omega |\psi| \, dx = \int_\Omega \frac{|\psi|}{\sqrt{\rho}} \sqrt{\rho} \, dx \leq \left( \int_\Omega \frac{|\psi|^2}{\rho} \, dx \right)^{1/2} \left( \int_\Omega \rho \, dx \right)^{1/2} = \left( \int_\Omega \frac{|\psi|^2}{\rho} \, dx \right)^{1/2},
\]

**which also verifies that** \( V(\hat{\Psi}) \geq 0 \). **More importantly, the equalities hold if** \( \psi \) **does not change sign and** \( \rho \propto |\psi| \). **Therefore, we can set** \( \rho \) **as close to** \( |\psi| \) **(up to a normalizing constant) as possible to reduce the variance, but meanwhile ensure** \( \rho \) **is easy to sample from and evaluate as required in** \( (16) \). **This is closely related to the concept of importance sampling.**

- **The result** \( (16) \) **and** \( (17) \) **in Lemma 4 can be easily extend to the case with unbounded domain** \( \Omega \), **provided that** \( \psi/\sqrt{\rho} \in L^2(\Omega) \).

Lemma 4 provides a feasible approach to compute the stochastic gradient of \( L(\theta) \) for \( (15) \). For instance, to compute \( \nabla_\theta L_{\text{bdry}}(\theta) \), we can take gradient of \( (13) \) with respect to \( \theta \), sample \( N_b \) collocation points \( \{x_b^{(i)} : 1 \leq i \leq N_b\} \) on the boundary \( \partial \Omega \) and approximate \( \nabla_\theta L_{\text{bdry}}(\theta) \) by summation of function evaluations at
the sample points. If we take \( B[u, \gamma] = (u - u_b, \gamma - \gamma_b, \partial \eta u - u_n) \) and uniformly sample \( x_b^{(i)} \), the estimate becomes

\[
\nabla_\theta L_{\text{bdry}}(\theta) = 2 \int_{\partial \Omega} \left( (u_\theta - u_b) \nabla_\theta u_\theta + (\gamma_\theta - \gamma_b) \nabla_\theta \gamma_\theta + (\partial \eta u_\theta - u_n) \nabla_\theta \nabla u \cdot \vec{n} \right) dS(x)
\]

\[
\approx 2\frac{\partial \Omega}{N_b} \sum_{i=1}^{N_b} \left( (u_\theta(x_b^{(i)}) - u_b(x_b^{(i)})) \nabla_\theta u_\theta(x_b^{(i)}) + (\gamma_\theta(x_b^{(i)}) - \gamma_b(x_b^{(i)})) \nabla_\theta \gamma_\theta(x_b^{(i)}) \right)
\]

\[
+ (\partial \eta u_\theta(x_b^{(i)}) - u_n(x_b^{(i)})) \nabla_\theta \nabla u_\theta x_b^{(i)} \cdot \vec{n} x_b^{(i)} .
\]

Similarly, we can compute the stochastic gradient of \( \nabla_\theta L_{\text{int}}(\theta) \). In the case of taking \( A[u, \gamma] = \nabla \cdot (\gamma \nabla u) - f \) in \( \Omega \) with \( f \) given, and uniformly sampling \( N_r \) collocation points \( \{ x_r^{(i)} : 1 \leq i \leq N_r \} \) inside the region \( \Omega \), \( \nabla_\theta L_{\text{int}}(\theta) \) can be estimated by

\[
\nabla_\theta L_{\text{int}}(\theta) = 2 I(\theta) \int_{\Omega} \left( \nabla_\theta \gamma_\theta(\nabla u_\theta \cdot \nabla \varphi_{\eta}(\theta)) + \gamma_\theta(\nabla_\theta \nabla u_\theta \cdot \nabla \varphi_{\eta}(\theta)) \right) dS(x)
\]

\[
\approx 2\frac{\partial \Omega}{N_r} \sum_{i=1}^{N_r} \left( \nabla_\theta \gamma_\theta(x_r^{(i)})(\nabla u_\theta(x_r^{(i)}) \cdot \nabla \varphi_{\eta}(\theta)(x_r^{(i)})) + \gamma_\theta(x_r^{(i)})(\nabla_\theta \nabla u_\theta(x_r^{(i)}) \cdot \nabla \varphi_{\eta}(\theta)(x_r^{(i)})) \right)
\]

where \( I(\theta) \) and its estimator \( \tilde{I}(\theta) \) are given by

\[
I(\theta) = \int_{\Omega} \gamma_\theta(\nabla u_\theta \cdot \nabla \varphi_{\eta}(\theta)) \ dx,
\]

\[
\tilde{I}(\theta) = \frac{\partial \Omega}{2} \sum_{i=1}^{N_r} \gamma_\theta(x_r^{(i)})(\nabla u_\theta(x_r^{(i)}) \cdot \nabla \varphi_{\eta}(\theta)(x_r^{(i)})),
\]

and \( \varphi_{\eta}(\theta) \) is a solution of the maximization problem \([12]\) according to Lemma \(3\). All integrals in the gradients can be approximated in a similar way. These approximated gradients are in fact stochastic gradients, which are unbiased and have bounded variances due to the boundedness of the network parameters. With these ingredients, the stochastic gradient descent algorithm \([15]\) ensures convergence to a local stationary point of \([14]\). Since \([14]\) is constrained, the gradient mapping, defined by \( G(\theta) := \tau^{-1}[\theta - \Pi(\theta - \tau \nabla_\theta L(\theta))] \), is used as the convergence criterion of \( \theta \) \([21][39][60]\). Note that the definition of gradient mapping takes the normalization of step size \( \tau \) into consideration. Moreover, without the projection \( \Pi \), the gradient mapping reduces to \( G(\theta) = \nabla_\theta L(\theta) \), whose magnitude is an evaluation criterion for local stationary points (i.e., \( |\nabla_\theta L(\theta)| = 0 \)) for unconstrained case. This result is stated in the following theorem, and the proof is given in Appendix A.4

**Theorem 5.** For any \( \varepsilon > 0 \), let \( \{ \theta_j \} \) be a sequence of the network parameter in \((u_\theta, \gamma_\theta)\) generated by the gradient descent algorithm \([15]\) with integrals in \( \nabla_\theta L(\theta) \) approximated by sample averages as in \([16]\) with sample complexities \( N_r, N_b = O(\varepsilon^{-1}) \) in each iteration, then \( \min_{1 \leq j \leq J} \mathbb{E}[|G(\theta_j)|^2] \leq \varepsilon \) after \( J = O(\varepsilon^{-1}) \) iterations.

**Remark.** Theorem \(5\) establishes the convergence and iteration complexity of \([15]\) to the so-called \( \varepsilon \)-solution of the problem. The result is based on the expected magnitude of the gradient mapping, which is a standard convergence criterion in nonconvex constrained stochastic optimization. However, this only ensures approximation to a stationary point (not necessarily a local or global minimizer) on expectation. In theory, one can apply additional global optimization techniques to \([17]\) in order to find a global minimizer (possibly only with high probability at best) with substantially higher computational cost. However, we will not exploit this issue further in this work. In the numerical experiments, we find that stochastic gradient descent method (or its variants) is effective in finding the target solutions for a variety of tests.

Now we summarize the steps of our algorithm for solving IPs using weak adversarial networks. To simplify the presentation, we introduce the following notation to indicate a stochastic gradient descent (SGD) procedure:

\[
\theta \leftarrow \text{SGD}(G(\theta), X, \tau, J),
\]

(20)
which means the output is the result after we execute the (projected) SGD scheme with step size $\tau$ as follows for $J$ iterations:

$$
\theta \leftarrow \Pi(\theta - \tau \hat{G}(\theta; X)).
$$

Here $X = \{x^{(i)}: 1 \leq i \leq N\}$ is the set of $N$ sampled collocation points, and $\hat{G}(\theta; X)$ stands for the stochastic approximation of $G(\theta)$ where the integrals are estimated as in (16) using the sampled collocation points $X$. Therefore, each iteration of our algorithm consists two steps: Given $\theta$, we solve the maximization problem with objective $E(\theta, \eta)$ with $J_\eta$ SGD steps to obtain an approximate solution $\eta$, and then update $\theta$ by one SGD step on $\nabla_b L(\theta) = \partial_b E(\theta, \eta) + \beta \nabla_b L_{bdry}(\theta)$. Hence, our objective function is $E(\theta, \eta) + \beta L_{bdry}(\theta)$, for which we seek for the optimal point $(\theta^*, \eta^*)$ via a min-max optimization $\min_{\theta} \max_{\eta} E(\theta, \eta) + \beta L_{bdry}(\theta)$. This procedure is referred to Inverse Problem Solver using Weak Adversarial Network (IWAN) and summarized in Algorithm 1.

### 4 Implementation Details

In this section, we discuss several implementation details and modifications regarding Algorithm 1. First, to avoid spending excessive time in solving the inner maximization problem (12), we only apply a few iterations $J_\eta$ to compute $\eta$ before updating $\theta$ in Algorithm 1. In fact, we can employ two separate test functions $\varphi_\eta$ and $\bar{\varphi}_\eta$ (we again use the same $\eta$ for notation simplicity). In each iteration $j$, we alternately update $(u_\theta, \varphi_\eta, \gamma_\eta, \bar{\varphi}_\eta)$ in order, each with one or a few SGD steps (21). We will specify the numbers of steps for these networks for our experiments in Section 5.

During the derivations in Section 3, we require bounded network parameters $\theta$ and $\eta$, where the bound $B$ can be arbitrarily large, to ensure finite variances of the integral estimators using samples so that the SGD is guaranteed to converge. An alternative way to handle the boundedness constraints is to add $|\theta|^2$ and $|\eta|^2$ as regularization terms to the objective function in (7). One can also use the original formulation of operator norm (5) where the integral $\|\varphi_\eta\|_2^2$ can be approximated by sample averages similarly as in (16), which is also adopted in our implementation.

A test function $\varphi_\eta$ is required to vanish on $\partial \Omega$ in the weak formulation (3). One simple technique to ensure this is to precompute a function $\varphi_0 \in C(\Omega)$ such that $\varphi_0(x) = 0$ if $x \in \partial \Omega$ and $\varphi_0(x) > 0$ if $x \in \Omega$ (e.g., a distance function to $\partial \Omega$ would work). Then we seek for a parameterized network $\varphi_\eta'$ with no constraint on its arbitrary boundary, and set the test function $\varphi_\eta$ to $\varphi_0 \varphi_\eta'$ which still takes zero value on $\partial \Omega$.

We implemented our algorithm using TensorFlow 2 (Python version 3.7), a state-of-the-art deep learning framework that can efficiently employ GPUs for parallel computing. The gradients with respect to network parameters ($\theta$ and $\eta$) and input ($x$) are computed by the TensorFlow built-in auto-differentiation module. During training, we can also substitute the standard SGD optimizer by many of its variants, such as AdaGrad, RMSProp, Adam, Nadam etc. In our experiments, we use AdaGrad supplied by the TensorFlow package, which appears to provide better performance than other optimizers in most of our tests. All other parameters, such as the network structures (numbers of layers and neurons), step sizes (also known as the learning rates), number of iterations, will be specified in Section 5.
Relative error of $\gamma$ have main spatial variations are shown (same for the other test results below).

Figure 1: Test 1 result on (2) with smooth $\gamma^*$ and problem dimension $d = 5$.

5 Numerical Experiments

5.1 Experiment Setup

In this section, we conduct a set of numerical experiments to show the practical performance of Algorithm 1 in solving inverse problems. To quantitatively evaluate the accuracy of an approximate solution $\gamma$, we use the $L^2$ relative error of $\gamma$ to the ground truth $\gamma^*$, defined by $\|\gamma - \gamma^*\|_2/\|\gamma^*\|_2$, where $\|\gamma\|_2^2 := \int_\Omega |\gamma(x)|^2 \, dx$.

In practice, we compute $\|\gamma\|_2^2 = (|\Omega|/N) \cdot \sum_{i=1}^N |\gamma(x(i))|^2$ by evaluating $\gamma$ on a fixed set of $N$ mesh grid points $\{x(i) \in \Omega : 1 \leq i \leq N\}$ in $\Omega$. More specifically, we used a regular mesh grid of size 100 x 100 for $(x_1, x_2)$, and sampled one point $x$ for each of these grid points, i.e., for each grid point $(x_1, x_2)$, randomly draw values of the other coordinates within the domain $\Omega$ such that $N = \Omega^d$. These points were sampled in advance and then used for all comparison algorithms to compute their test relative error. Note that these points are different from those sampled for training in these methods.

In all of our experiments, we parameterize each of $(u_\theta, \varphi_\gamma, \gamma_\theta, \tilde{\varphi}_\gamma)$ as a 9-layer fully connected neural network with 20 neurons per layer as in [5] unless otherwise noted. We set $\sigma_k$ to $\text{tanh}$ for $k = 1, 2$, $\text{softplus}$ for $k = 4, 6, 8$, $\text{sinc}$ for $k = 3, 5, 7$ in $u_\theta$, and $\text{tanh}$ for $k = 1, 2, 4, 6$, $\text{elu}$ for $k = 3, 5$, and $\text{sigmoid}$ for $k = 7, 8$ in $\gamma_\theta$ (we also use $\text{elu}$ in the output layer of $\gamma_\theta$ to ensure positivity). In parallel, we set $\sigma_k$ to $\text{tanh}$ for $k = 1, 2$ and $\text{sinc}$ for $k \geq 3$ in $\varphi_\gamma$ and $\tilde{\varphi}_\gamma$. Unless otherwise noted, we apply one SGD update with step size $\tau_\eta = 0.01$ to both of $u_\theta$ and $\gamma_\theta$, and two SGD updates with step size $\tau_\eta = 0.008$ to both of $\varphi_\gamma$ and $\tilde{\varphi}_\gamma$. We set the weight $\beta = 10,000$ for the boundary loss function $L_{\text{bdry}}(\theta)$ in (7), but also set a weight $\beta'$ to $L_{\text{int}}(\theta)$ and specify its value in the experiment. Other parameters will also be specified below. All the experiments are implemented, trained, and tested in the TensorFlow framework [1] on a machine equipped with Intel 2.3GHz CPU and an Nvidia Tesla P100 GPU and 16GB of graphics card memory.

5.2 Experimental Results on Inverse Conductivity Problems

Test 1: Inverse conductivity problem with smooth $\gamma$. We first test our method on the inverse conductivity problem (2) with a smooth conductivity distribution $\gamma$. In this test, we set $\Omega = (-1, 1)^d \subset \mathbb{R}^d$ with problem dimension $d = 5$, ground truth conductivity distribution $\gamma^*(x) = 2(\exp(-|x - c_1|^2_{\Sigma_1}) + \exp(-|x - c_2|^2_{\Sigma_2}))$, where $\Sigma_1 = \text{diag}(1.25, 5, 0, 0, 0)$, $\Sigma_2 = \text{diag}(5, 1.8, 0, 0, 0)$, $c_1 = (-0.5, 0.5, 0, 0, 0)$, $c_2 = (0.5, -0.5, 0, 0, 0)$, and $|x|_2^2 := x^T \Sigma x$. We set the boundary condition as $u_\theta(x) = \cos(|x|^2)$ on $\partial \Omega$, $u_\eta(x) = -2\sin(|x|)(x_1, x_2, \ldots, x_d) \cdot \bar{n}$, and $f = 8 \sum_{i=1}^2 \sum_{j=1}^2 (\Sigma_{ij})_{ii}(x_i - c_{ij}) x_i \sin(|x|^2) \exp(-|x - c_{ij}|^2_{\Sigma_{ij}}) + 2(\exp(-|x - c_{ij}|^2_{\Sigma_{ij}}) + |x|^2 \cos(|x|^2))$ in $\Omega$, where $\Sigma_{ij}$ and $c_{ij}$ stand for the $(i, j)$-th entry of the matrix $\Sigma$ and $j$th component of the vector $c$, respectively. We set $N_r = 100,000$ and $N_p = 100d$, $\beta' = 10$, and run Algorithm 1 for 20,000 iterations. The true $\gamma^*$ and the recovered conductivity distribution $\gamma_\theta$ (with relative error 2.54%) are shown in Figure 1a. The progress of the $L^2$ relative error of $\gamma_\theta$ versus iteration number is shown in Figure 1b. For the demonstration purpose, only the $(x_1, x_2)$ cross sections that have main spatial variations are shown (same for the other test results below).

Test 2: Inverse conductivity problem with nearly piecewise constant $\gamma$. We consider (2) with a
less smoothly, nearly piecewise constant conductivity $\gamma$. In this test, we set $\Omega = (-1, 1)^d$, define $\Omega_0 = \{x \in \Omega : |x - c|^2 \leq 0.6^2\}$ where $\Sigma = \text{diag}(0.81, 0.09, \ldots, 0.09)$ and $c = (0.1, 0.3, 0, \ldots, 0)$, and set $\gamma^*$ to 2 in $\Omega_0$ and 0.5 in $\Omega^c$. We slightly smooth $\gamma^*$ as follows: we set the true conductivity $\gamma^*(x) = 0.5 + (2 - 0.5)/(1 + \delta(x))$ where $\delta(x) = \exp((|x - c|^2 - 0.6^2)/\lambda)$ with $\lambda = 0.02$. Note that, for small $\lambda$, $\delta(x)$ approaches $\infty$ (0 resp.) quickly as $x$ gets outside (inside resp.) of the ellipse described by $|x - c|^2 = 0.6^2$, and hence $\gamma^*$ is approximately 0.5 outside (2 inside) of the ellipse, with smoothed change near its boundary. This smoothed $\gamma^*$ also allows us to derive an explicit expression of $f$ for our test. We then set the boundary condition as $u_0(x) = |x|^2$ on $\partial\Omega$, $u_{\eta}(x) = (2x_1, x_2, \ldots, x_d) \cdot \vec{n}$, and define $f(x) = \frac{4(2-0.5)(x-c) \Sigma x}{\lambda(1+(\delta_1(x)+\delta_2(x)))^2} - 2d\gamma$. Then we solve the inverse problem \( \gamma \) with dimensionality $d = 5, 10, 20$. We set $N_r = 20,000d$ and $N_b = 100d$, and $\beta = 10, 1, 0.005$ for $d = 5, 10, 20$ respectively. In each case, we run Algorithm \( 1 \) for 20,000 iterations, and obtain relative errors 1.16%, 1.43%, 2.29% for $d = 5, 10, 20$, respectively. The recovery results are shown in Figure 2. Figure 2a shows the ground truth $\gamma^*$ (left) and the progress of relative errors versus iteration number for different $d$ (right). The recovered conductivity functions $\gamma_0$ and the pointwise absolute error $|\gamma_0 - \gamma^*|$ for these dimensions are shown in Figure 2b and 2c respectively.

**Test 3:** **Inverse conductivity problem with noisy measurements.** Under the same experiment setting as Test 2, we solve the inverse problem \( \gamma \) where the measurement data are perturbed by random noise for the $d = 5$ case. Specifically, we scale every measurement data value by $1 + 5\%e, 1 + 10\%e, 1 + 20\%e$ where $e$ is drawn independently from the standard normal distribution every time, followed by a truncation into interval $[-100, 100]$. We do not perturb $f$. The results are given in Figure 3 in parallel to the noiseless case above, where Figure 3a shows the ground truth conductivity $\gamma^*$ (left) and the progress of relative error of $\gamma_0$ versus iteration number (right). The recovered $\gamma_0$ after 20,000 iterations and the pointwise absolute error $|\gamma_0 - \gamma^*|$ with noise levels 5%, 10%, 20% are shown in Figure 3b and 3c. We observe that the progress becomes more oscillatory due to the random measurement noise in Figure 3a and the final reconstruction error is larger for higher noise level in Figure 3c as expected.

**Test 4:** **Inverse conductivity problem with different features in $\gamma$.** We consider several cases with more challenging ground truth conductivity $\gamma^*$. The first case has $\gamma^*$ with two disjoint modes. We define $\Omega = (-1, 1)^5$, and set $\Omega_1 = \{x : |x - c_1|^2 \leq 0.4^2\}$ and $\Omega_2 = \{x : |x - c_2|^2 \leq 0.4^2\}$, where $c_1 = (-0.5, -0.5, 0, 0, 0)$, $c_2 = (0.5, 0.5, 0, 0, 0)$, $\Sigma_1 = \text{diag}(0.81, 0.09, 0.09, 0.09, 0.09)$, and $\Sigma_2 = \text{diag}(0.81, 0.09, 0.09, 0.09)$. We set the conductivity $\gamma^*$ to 4 in $\Omega_1$, 2 in $\Omega_2$, and 0.5 in $(\Omega_1 \cup \Omega_2)^c$. We also smooth $\gamma^*$ using a Gaussian kernel. Specifically, we set the ground truth $\gamma^*(x) = 0.5 + (2-0.5)/(1+\delta_1(x)) + (2-0.5)/(1+\delta_2(x))$ where $\delta_1(x) = \exp((|x - c_1|^2 - 0.4^2)/\lambda)$ and $\delta_2(x) = \exp((|x - c_2|^2 - 0.4^2)/\lambda)$ with $\lambda = 0.02$. We set the boundary condition as $u_0(x) = |x|^2$ on $\partial\Omega$, $u_{\eta}(x) = (2x_1, x_2, \ldots, x_d) \cdot \vec{n}$, and $f(x) = \frac{4(2-0.5)(x-c) \Sigma x}{\lambda(1+(\delta_1(x)+\delta_2(x)))^2} - 2d\gamma$ in $\Omega$. We set $N_r = 200,000, N_b = 100d$, $\beta = 10$, and run Algorithm \( 1 \) for 20,000 iterations. Figure 4a shows the ground truth $\gamma^*$ (left) and the recovered conductivity $\gamma_0$ with relative error 1.77% (right). Figure 4b plots the progress of relative error of $\gamma_0$ versus iteration number. In the second case, we follow the same setting but define $\Omega_1 = \{x : |x_1 + 0.5| \leq 0.15, |x_2| \leq 0.6\}$ (which has sharp corner) and $\Omega_2 = \{x : |x - c|^2 \leq 0.4^2\}$ where $c = (0.55, 0, 0, 0, 0)$, $\Sigma = \text{diag}(1.4, 0, 0, 0, 0)$, and set $\gamma^* = 2$ in $\Omega_1 \cup \Omega_2$ and 0.5 in $(\Omega_1 \cup \Omega_2)^c$. We again smooth $\gamma^*$ such that $\gamma^*(x) = 0.5 + (2-0.5)/(1+\delta_1(x)) + (2-0.5)/(1+\delta_2(x))$ where $\delta_1(x) = \exp((|x - c_1|^2 - 0.4^2)/\lambda)$, $\delta_2(x) = \exp((|x_1 + 0.5| - 0.15)/\lambda)$ and $\delta_3(x) = \exp(|x - 0.6|/\lambda)$ with $\lambda = 0.02$. We set $u_0(x) = |x|^2$ on $\partial\Omega$, $u_{\eta}(x) = (2x_1, x_2, \ldots, x_d) \cdot \vec{n}$, and $f(x) = \frac{4(2-0.5)(x-c) \Sigma x}{\lambda(1+(\delta_1(x)+\delta_2(x)))^2} - 2d\gamma$ in $\Omega$. We set $\beta = 1$ and again run Algorithm \( 1 \) for 20,000 iterations. The recovered $\gamma_0$ (with relative error 1.15%) and the progress of relative error are shown in Figure 4e and 4d respectively. Lastly, we consider a non-convex shaped $\gamma$, and show the recovered $\gamma_0$ (with relative error 1.57%) and the progress of relative error in Figure 4f and 4e respectively. We set the domain $\Omega = (-1, 1)^5$ and define $\Omega_1 = \{x \in \Omega : \sum_{i=1}^2 |x_1 - c_1(i)| \leq r_1(x)\}$, $j = 1, 2, 3$, where $c_1 = (-0.5, 0), c_2 = (-0.1, 0.6), c_3 = (-0.1, -0.6)$ and $r_1 = (0.15, 0.8), r_2 = r_3 = (0.55, 0.2)$. We set $\gamma^* = 4$ in $\Omega_1 \cup \Omega_2 \cup (\Omega_1 \cup \Omega_3)$ and 2 in $\Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \Omega_0$ and 0.5 in $(\Omega_1 \cup \Omega_2 \cup \Omega_3)^c$. We defined $\gamma = 0.5 + \sum_{j=1}^3 |x_j - c_j|/(1+\delta_1(x)+\delta_2(x))$ where $\delta_1(x) = \exp((|x_1 - c_1(1) - r_1(1)|/\lambda), \delta_2(x) = \exp(|x_2 - c_2(2)| - r_j(2))/\lambda)$, $j = 1, 2, 3$ with $\lambda = 0.02$. We set the boundary condition $u_{\eta}(x) = (2x_1, x_2, \ldots, x_d) \cdot \vec{n}$, $u_{\eta}(x) = |x|^2$ on $\partial\Omega$ and $f(x) = 2(2-0.5)\sum_{j=1}^3 \frac{|x_1 - c_1(j)|\delta_1(x) + |x_2 - c_2(j)|\delta_2(x)}{\lambda(1+\delta_1(x)+\delta_2(x))^2} - 2d\gamma$.

**Test 5:** **EIT problem.** We consider an artificial 5D EIT problem \( \gamma \) on $\Omega = (0, 1)^5$ but replace \( \partial \Omega \) with a different boundary condition given by $\gamma \nabla u \cdot \vec{n}$ on $\partial\Omega$, where $\vec{n}$ is the outer normal vector at the
boundary point. We define $\Gamma_1 = \{ x \in \partial \Omega : x_1 = 0, 1 \}$ and $\Gamma_2 = \partial \Omega \setminus \Gamma_1$. We set ground truth $\gamma^*(x) = \pi^{-1} \exp\{(d-1)\pi^2(x_1 - x_1^2)/2\}$ and $u^*(x) = \exp\{(d-1)\pi^2(x_2 - x_2^2)/2\} \cdot \prod_{i=2}^d \sin(x_i)$, and compute the corresponding boundary value as our input data. We set $f = 0$ in (2), $N_r = 100,000, N_b = 100d, \beta' = 10$, and run Algorithm 1 for 20,000 iterations. The $x_1$ cross section of the recovered $\gamma_\theta$ and the progress of relative error versus iteration number are shown in Figure 5a and 5b, respectively.

Test 6: Inverse thermal conductivity problem involving time. We consider an inverse thermal
conductivity problem of (1) with temporally varying $u(x,t)$ as follows,

$$\partial_t u - \nabla \cdot (\gamma \nabla u) - f = 0, \quad \text{in } \Omega_T = \Omega \times [0,T] \quad (22a)$$

$$u - u_i = 0, \quad \text{in } \Omega \times \{0\} \quad (22b)$$

$$\nabla u \cdot \vec{n} - u_n = 0, \quad u - u_b = 0, \quad \gamma - \gamma_b = 0, \quad \text{on } \partial\Omega \times [0,T] \quad (22c)$$

where $\Omega = (0,1)^5 \subset \mathbb{R}^5$ and $T = 1$, where $\vec{n}$ is the unit outer normal vector of $\partial\Omega$, $u_i(x)$ for $x \in \Omega$ is the given initial value, and $u_n(x,t), u_b(x,t), \gamma_b(x,t)$ for $(x,t) \in \partial\Omega \times [0,T]$ are given boundary values. In this problem, we would like to recover the thermal conductivity $\gamma(u)$ which is a function of $u$ in the standard setting, but we simply treat $\gamma(x,t) := \gamma(u(x,t))$ as a function of $(x,t)$ in our experiment here. We set the
We consider the case with problem dimension $d = 5$, and set $N_r = 100,000$, $N_b = 100d$, $\beta = 1$, and $\beta' = 1$ and $\beta = 1,000$. The results are shown in Figure 4, where Figure 4a plots the sampled values of recovered $(\gamma_0, \gamma')$ in comparison with the ground truth relation $\gamma^* = k_1 + k_2u^*$, and Figure 4b shows the progress of $L^2$ relative error of $\gamma_0$ versus iteration number for the three different noise levels. The reconstructions of $\gamma_0$ are all faithful, while higher noise levels decreases the accuracy and make convergence to true solution more
Test 5: Result on artificial 5D EIT problem with boundary condition on $\gamma \nabla u \cdot \vec{n}$.

(a) True $\gamma^*$ vs recovered $\gamma_\theta$.

(b) $L_2$ relative error vs iteration.

Figure 5: Test 5 result on artificial 5D EIT problem with boundary condition on $\gamma \nabla u \cdot \vec{n}$.

Test 6: Result on inverse thermal conductivity problem with dimension $d = 5$ and noise levels 0%, 10% and 20%. Ground truth relation between $u^*$ and $\gamma^*$ is $\gamma^* = k_1 + k_2 u^*$ where $k_1 = 1.5$ and $k_2 = 0.6$.

(a) Recovered $(u_\theta, \gamma_\theta)$.

(b) $L^2$ relative error of $\gamma_\theta$.

Figure 6: Test 6 result on inverse thermal conductivity problem with dimension $d = 5$ and noise levels 0%, 10% and 20%.

Test 7: Comparison with PINN.

We compare the proposed method with a state-of-the-art method called physics-informed neural networks (PINNs) [59]. PINN is also a deep-learning based method designed for solving forward problem as well as inverse problem for PDEs. PINN is based on the strong form of the PDEs, where the loss function in the minimization problem of PINN consists of the sum of squared errors in the violation of the PDE and the boundary condition at points sampled inside $\Omega$ and on $\partial \Omega$, respectively. In contrast, our method is based on the weak form of PDE which employs a test function and yields a min-max problem to better tackle singularities of the problem. We first compare the proposed method and the PINN method in the problem in Test 1. Note that PINN was only applied to inverse conductivity problem with constant conductivity in [59], it is straightforward to extend this method to nonconstant conductivity by also parameterizing the conductivity $\gamma$ as an additional deep neural network. In this problem, we take $N_r = 10,000, N_b = 100 \times d$ with $d = 5$. For the PINN method, we also parameterize $u(x)$ as a 9-layer fully-connected network with 20 neurons in each hidden layer and tanh as activations in all hidden layers. For $\gamma$, we parameterized it by using the same network structure as that used for the proposed method in Test 1. We let the weight of the boundary term in the loss function is 1.0 and use the built-in Adam optimizer of TensorFlow with learning rate 0.001 to update the network parameters in PINN. For fair comparison, we also use the Adam optimizer with learning rate 0.001 for updating $\theta$ and $\eta$ in the proposed method. The results after 20,000 iterations of both methods are given in Figure 7. In Figure 7a, we can see the error of $\gamma$ obtained by IWAN is much lower than that by PINN. This can also be seen from Figure 7b, where the error decays very fast for the proposed IWAN. We tried a variety of network structures and parameter settings of...
PINN and obtain similar results.

We also compared the proposed method and PINN on the inverse conductivity problem in Test 2, where the ground truth conductivity $\gamma^*$ is less smooth and nearly piecewise constant. We use the same parameter settings for both methods as above except for the network structure of $\gamma$, which follows the one in Test 2. The conductivity $\gamma$ recovered by PINN and IWAN and the progress of their relative error versus computation time (in seconds) are given in Figures 7c and 7d, respectively. From Figure 7d, it appears that PINN cannot get close to the ground truth $\gamma^*$ within 20,000 iterations. Therefore, we rerun PINN for 100,000 iterations, and plot the relative error versus computation time in Figure 7f from which it seems that PINN still cannot converge to the desired solution. However, the result obtained by PINN does satisfy the PDE closely, as shown in Figure 7e, the difference between the two sides of PDE (left), i.e., $|−\nabla(\gamma \nabla u) − f|$, is much smaller than $|f|$ (right), but PINN cannot capture the irregularities and singularities of the solution since it is based on the strong form of the PDE. In contrast, IWAN can overcome this issue and recover the weak solution properly. We also show the objective function value of PINN and IWAN in Figures 7g and 7h respectively (Note that the objective function $L(\theta, \eta)$ in IWAN is defined as $E(\theta, \eta) + \beta L_{bdry}(\theta)$ for min-max optimization, and the objective function of PINN is for minimization only and hence different from IWAN).

**Test 8: Efficiency improvement using important sampling.** As shown in Lemma 4, adaptive sampling may reduce the variance of the sample-based approximation of integrals, which in turn can improve the convergence of stochastic gradient descent. To demonstrate this, we consider the inverse conductivity problem on $\Omega = (-1,1)^d \subset \mathbb{R}^d$ with problem dimension $d = 5$, ground truth conductivity distribution $\gamma^*(x) = 2 \exp(-|x - c|_{\Sigma}^2/2)$, where $\Sigma = \text{diag}(4.0, 100.0, 0.0, 0.0, 0.0)$, $c_1 = (-0.2, 0.2, 0, 0, 0)$. We set $u_n(x) = -2 \sin(|x|^2)(x_1, x_2, \ldots, x_d)$, $u_0 = \cos(|x|^2)$ on $\partial \Omega$ and $f(x) = 8 \sum_{i=1}^d \Sigma_{ii} (x_i - c_i) x_i \sin(|x|^2) \exp(-|x - c|_{\Sigma}^2/2) + 2 \exp(-|x - c|_{\Sigma}^2/2) \ast (2d \sin(|x|^2) + 4|x|^2 \cos(|x|^2))$. For the parameter setup, we use the same setup as that in Test 7. Then we solve this inverse problem using the proposed method IWAN with points in the domain $\Omega$ sampled from the uniform distribution as above and also a multivariate normal distribution respectively. Specifically, to obtain multivariate normal samples, we first sample $N$ points of $(x_1, x_2)$ from the multivariate normal distribution with mean value $\mu = (-0.2, 0.2)$ and inverse covariance matrix $\Sigma = \text{diag}(1.0, 25.0)$ (points outside of $\Omega$ is discarded), and then draw each of the remaining coordinates randomly from interval $(-1, 1)$ independently. The result was shown in the figure 8. The progress of relative error versus computation time (in second) for 20,000 iterations is shown in Figure 8 which shows that the convergence using adaptive multivariate normal distribution is faster than that with uniform distribution.

**5.3 Empirical Robustness Analysis**

We conduct a series of experiments to evaluate the robustness of Algorithm 1 in terms of network structure (number of layers and neurons) and the number of sampled collocation points.

**Test 9: Network structure.** In this experiment, we test the performance of Algorithm 1 with different network structures, i.e., the layer number (network depth) $K$ and the per-layer neuron number (network width) $d_k$. We test different combinations of $K$ and $d_k$ (in each combination we set $d_k = d'_k$ for all $k = 1, \ldots, K$). More specifically, we apply Algorithm 1 to the inverse conductivity problem (2) in Test 2 above with problem dimension $d = 5$ and a total of 16 combinations $(K, d')$ with $K = 5, 7, 9, 11$ and $d' = 5, 10, 20, 40$. For each combination $(K, d')$, we run Algorithm 1 for 20,000 iterations and record the relative error of $\gamma_\theta$ in Table 7. Based on Table 7, it seems that deeper (larger $K$) and/or wider (larger $d'$) neural networks yield lower reconstruction error (but at the expense of higher per-iteration computational cost). For fixed layer number $K = 9$, we show the progress of relative error versus iteration number with varying per-layer neuron number $d'$ in Figure 9a. Similarly, for fixed per-layer neuron number $d' = 10$, we also show the progress of relative error versus iteration number with varying layer number $K$ in Figure 9b. These figures also suggest that larger $K$ and $d'$ yield better accuracy, although the per-iteration computational cost also increases and it may take more iterations to converge.

**Test 10: Number of sampled collocation points.** In Section 3 we showed that the number $N$ of sampled collocation points affects the variance of the integral estimator, so that the variance reduces at the order of $O(1/N)$. In this experiment, we test the empirical effect of the collocation point numbers $N_r$ in the region $\Omega$ and $N_b$ on the boundary $\partial \Omega$ in Algorithm 1 for the same inverse conductivity problem (2) of dimension $d = 5$ in Test 2 above. We choose different combinations of $(N_r, N_b)$ for $N_r = 25K, 50K, 100K, 200K$ (K=1,000)
Figure 7: Test 7 on the comparison of IWAN and PINN on the recovery smooth ((a) and (b)) and less smooth ((c)–(h)) conductivity \( \gamma^* \). (a) Pointwise absolute error \( |\gamma - \gamma^*| \) with \( \gamma \) obtained by PINN (left) and the proposed method IWAN (right) for smooth \( \gamma^* \). (b) Relative error versus time in seconds for smooth \( \gamma^* \). (c) Pointwise absolute error \( |\gamma - \gamma^*| \) with \( \gamma \) obtained by PINN (left) and the proposed method IWAN (right) for less smooth, nearly piecewise constant \( \gamma^* \). (d) Relative error versus time in seconds for 20,000 iterations for less smooth, nearly piecewise constant \( \gamma^* \). (e) \( |f| \) (left) and \( \| - \nabla(\gamma \nabla u) - f \| \) by the PINN (right) for the less smooth \( \gamma^* \). (f) Relative error versus time in seconds for 100,000 iterations for less smooth, nearly piecewise constant \( \gamma^* \). (g) Objective function value versus iteration number by PINN for nearly piecewise constant \( \gamma^* \). (h) Objective function value versus iteration number by the proposed IWAN for nearly piecewise constant \( \gamma^* \).
Figure 8: Test 8 result on the difference of relative errors versus computation time (s) using collocations points \( \{ x_r(i) \in \Omega : i \in [N_r] \} \) sampled from uniform distribution (orange) and adaptive multivariate normal distribution (blue).

Table 1: Test 9 result on \( L^2 \) relative error of recovered conductivity \( \gamma_\theta \) using various combinations of \((K, d')\), where \( K \) is the layer number and \( d' \) is the per-layer neuron number.

| \( d' \) | \( K = 5 \) | \( K = 7 \) | \( K = 9 \) | \( K = 11 \) |
|------|------|------|------|------|
| 5    | 0.060347 | 0.040950 | 0.014905 | 0.019489 |
| 10   | 0.053842 | 0.029382 | 0.013325 | 0.011165 |
| 20   | 0.017955 | 0.016862 | 0.010916 | 0.011490 |
| 40   | 0.012390 | 0.010213 | 0.004422 | 0.005309 |

and \( N_b = (10 \times 2d, 20 \times 2d, 40 \times 2d, 80 \times 2d) \), and keep all other parameters in Test 2 unchanged. We run Algorithm 1 for 20,000 iterations, and record the final relative error of \( \gamma_\theta \) in Table 2. We also plot the progress of relative error of \( \gamma_\theta \) versus iteration number for fixed \( N_r = 25K \) and varying \( N_b \) in Figure 10a and that for fixed \( N_b = 20 \times 2d = 100 \) and varying \( N_r \) in Figure 10b. The results in Table 2 and Figure 10 show that larger amounts of collocation points can generally improve accuracy of the reconstruction, e.g., in Figure 10a. However, the improvement may be saturated after certain point, for instance, the accuracy does not seem to improve when \( N_r \) increases from 100K to 200K in Figure 10b. One possible reason is that the iterates using \( N_r = 200K \) may be trapped to a local minimizer as the problem is highly nonconvex due to the deep neural network parametrization. This issue will be exploited in our future work.

6 Concluding Remarks

We have presented a weak adversarial network approach to solve a class of inverse problems numerically. We leverage the weak formulation of PDEs in the inverse problems, and parameterize the unknown solution as primal neural network and the test function as adversarial network. The weak formulation and the boundary conditions yield a saddle function in the parameters of the primal network and adversarial network, which only rely on the inverse problem itself but not any other training data. These parameters are alternately updated until convergence. We provide a series of theoretical justifications on the convergence of our proposed algorithm. Our method does not require any spatial discretization, and can be applied to a large class of inverse problems, especially those with high dimensionality and less regularity on solutions. Numerical experiments have been conducted by applying the proposed method to a variety of challenging inverse problems. The results suggest promising accuracy and efficiency of our approach.
Figure 9: Test 9 result on the effect of network structure. (a) $L^2$ relative error of $\gamma_\theta$ versus iteration number with fixed layer number $K = 9$ and varying per-layer neuron number $d' = 5, 10, 20, 40$; (b) $L^2$ relative error of $\gamma_\theta$ versus iteration number with fixed per-layer neuron number $d' = 10$ and varying layer number $K = 5, 7, 9, 11$.

Table 2: Test 10 result on $L^2$ relative error of recovered conductivity $\gamma_\theta$ with various combination of $(N_r, N_b)$ for problem dimension $d = 5$, where $N_r$ is the number of sampled collocation points inside the region $\Omega$ and $N_b$ is the number of those on the boundary $\partial\Omega$.

| $N_b$   | $N_r = 25K$ | $N_r = 50K$ | $N_r = 100K$ | $N_r = 200K$ |
|---------|-------------|-------------|-------------|-------------|
| $10 \times 2d$ | 0.019023    | 0.020007    | 0.020898    | 0.012208    |
| $20 \times 2d$ | 0.013999    | 0.012920    | 0.009681    | 0.010050    |
| $40 \times 2d$ | 0.010668    | 0.012292    | 0.012053    | 0.010385    |
| $80 \times 2d$ | 0.006061    | 0.009207    | 0.010200    | 0.007267    |

Figure 10: Test 10 result on the different numbers of collocation points $N_r$ and $N_b$. (a) $L^2$ relative error of $\gamma_\theta$ versus iteration number with fixed $N_r = 25K$ and varying $N_b$; (b) $L^2$ relative error of $\gamma_\theta$ versus iteration number with fixed $N_b = 100$ and varying $N_r$.

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A Appendix: Proofs

A.1 Proof of Theorem 1

For ease of presentation, our proof of Theorem 1 here is based on the problem formulation 2. However, it can be easily modified for the PDEs in many other inverse problems.

Proof. For any fixed \( u \in H^1(\Omega) \cap C(\bar{\Omega}) \) and \( \gamma \in C(\Omega) \), the maximum of \( \langle A[u, \gamma], \varphi \rangle \) is achievable over \( Y := \{ \varphi \in H_0^1(\Omega) : ||\varphi||_2 = 1 \} \) since \( \langle A[u, \gamma], \cdot \rangle \) is continuous and \( Y \) is closed in \( H_0^1(\Omega) \). Define \( h(u, \gamma) = \max_{\varphi \in Y} \langle A[u, \gamma], \varphi \rangle \), then \( h(u, \gamma) = \| A[u, \gamma] \|_{op} \), due to the definition of operator norm in 3. On the other hand, since \( \mathcal{X} = \{ (u, \gamma) \in H^1(\Omega) \times C(\Omega) : B(u, \gamma) = 0 \} \) is also closed in \( H^1(\Omega) \times C(\Omega) \), we know the minimum of \( h(u) \) over \( X \) can be attained. Hence the minimax problem 4 is well-defined.

Now we show that \( (u^*, \gamma^*) \) satisfying \( B[u^*, \gamma^*] = 0 \) is the solution of the minimax problem 6 if and only if it is a weak solution of the problem 1. Suppose \( (u^*, \gamma^*) \) is a weak solution of the problem 1, namely \( (\hat{u}, \hat{\gamma}) \) satisfies 3 for all \( \varphi \in \mathcal{Y} \), then \( \langle A[u^*, \gamma^*], \varphi \rangle \equiv 0 \) for all \( \varphi \in \mathcal{Y} \). Therefore, \( \| A[u^*, \gamma^*] \|_{op} = 0 \), and \( (u^*, \gamma^*) \) is the solution of the minimax problem 6. On the other hand, suppose a weak solution \( (\hat{u}, \hat{\gamma}) \) of 1 exists. Assume that \( (u^*, \gamma^*) \) is a minimizer of the problem 6, i.e., \( (u^*, \gamma^*) = \arg \min_{(u, \gamma) \in H^1 \times C} h(u, \gamma) \), but not a weak solution of the problem 1, then there exists \( \varphi^* \in \mathcal{Y} \) such that \( \langle A[u^*, \gamma^*], \varphi^* \rangle > 0 \). Therefore \( h(\hat{u}, \hat{\gamma}) = 0 \) for all \( \varphi \in \mathcal{Y} \), which contradicts to the assumption that \( (u^*, \gamma^*) \) is the minimizer of 6. Hence \( (u^*, \gamma^*) \) must also be a weak solution of 1, i.e., \( (u^*, \gamma^*) \) satisfies 3.

\( \square \)

A.2 Proof of Lemma 3

Proof. Due to the definition of \( L_{int}(\theta) \) in 12 and the optimality of \( \eta(\theta) \), we know that \( L_{int}(\theta) = E(\theta, \eta(\theta)) \). Therefore, we have

\[
\nabla_{\theta} L_{int}(\theta) = \partial_\theta E(\theta, \eta(\theta)) + \partial_\eta E(\theta, \eta(\theta)) \nabla_\theta \eta(\theta).
\]

Now we form the Lagrange function \( L(\theta, \eta, \mu) = E(\theta, \eta) + \mu(\frac{1}{2}||\eta||^2 - B) \) for the maximization problem \( \max_{||\eta||^2 \leq 2B} E(\theta, \eta) \). Then the Karush-Kuhn-Tucker (KKT) condition of \( \eta(\theta) \) is given by

\[
\begin{align*}
\partial_\theta L(\theta, \eta, \mu) &= \partial_\theta E(\theta, \eta(\theta)) + \mu(\theta) \eta(\theta) = 0, \\
\mu(\theta) ((1/2) \cdot ||\eta(\theta)||^2 - B) &= 0, \\
\mu(\theta) \geq 0, \quad ||\eta(\theta)||^2 \leq 2B.
\end{align*}
\]

The complementary slackness condition \( 24b \) implies that

\[
\nabla_\theta \mu(\theta) ((1/2) \cdot ||\eta(\theta)||^2 - B) + \mu(\theta) \eta(\theta) \nabla_\theta \eta(\theta) = 0
\]

If \( \mu(\theta) = 0 \), then we know \( \partial_\eta E(\theta, \eta(\theta)) = 0 \) due to \( 24a \) and hence \( 23 \) reduces to \( \nabla_\theta L_{int}(\theta) = \partial_\theta E(\theta, \eta(\theta)) \).

If \( \mu(\theta) > 0 \), then \( ||\eta(\theta)||^2 = 2B \) due to \( 24b \), and hence \( 23 \) implies \( \mu(\theta) \eta(\theta) \nabla_\theta \eta(\theta) = 0 \). Thus multiplying \( 24a \) by \( \nabla_\theta \eta(\theta) \) yields \( \partial_\theta E(\theta, \eta(\theta)) \nabla_\theta \eta(\theta) = 0 \), from which we can see \( 23 \) also reduces to \( \nabla_\theta L_{int}(\theta) = \partial_\theta E(\theta, \eta(\theta)) \).

\( \square \)

A.3 Proof of Lemma 4

Proof. The first moment, i.e., expectation of \( \hat{\Psi} \), can be computed as follows:

\[
\mathbb{E}[\hat{\Psi}] = \mathbb{E}[\hat{\Psi} / \rho] = \int_\Omega \rho \hat{\Psi} \rho d\rho = \int_\Omega \hat{\Psi} d\rho = \Psi.
\]

To compute the second moment of \( \hat{\Psi} \), we first observe that the variance of \( \hat{\Psi} \) is

\[
V(\hat{\Psi}) = V \left( \frac{1}{N} \sum_{i=1}^N \frac{\psi(x^{(i)})}{\rho(x^{(i)})} \right) = \frac{1}{N} V \left( \frac{\psi}{\rho} \right).
\]
Note that the variance of $\psi/\rho$ is

$$V\left(\frac{\psi}{\rho}\right) = E\left[\left(\frac{\psi}{\rho}\right)^2\right] - \left(E\left[\frac{\psi}{\rho}\right]\right)^2 = \int_{\Omega} \frac{\psi^2}{\rho} \, dx - \left(\int_{\Omega} \psi \, dx\right)^2 = \int_{\Omega} \frac{\psi^2}{\rho} \, dx - \Psi^2$$

Hence the second moment of $\hat{\Psi}$ is

$$E[\hat{\Psi}^2] = V(\hat{\Psi}) + E[\hat{\Psi}]^2 = \frac{1}{N} \left( \int_{\Omega} \frac{\psi^2}{\rho} \, dx - \Psi^2 \right) + \Psi^2 = \frac{N-1}{N} \Psi^2 + \frac{1}{N} \int_{\Omega} \psi(x)^2 \, dx,$$

which completes the proof.

### A.4 Proof of Theorem 5

**Proof.** Due to the parameterization of $(u_\theta, \gamma_\theta)$ using finite-depth neural network [6] and the compactness of $\Theta := \{ \theta : |\theta| \leq \sqrt{2B} \}$, we know $\partial^2 u_\theta$ and $\gamma_\theta$ have Lipschitz continuous gradient with respect to $\theta$ for all $|\alpha| \leq 1$. As $\Omega$ is bounded and $\partial^2 u_\theta, \gamma_\theta \in C(\Omega)$, there exists $M > 0$ such that $L(\theta)$ has $M$-Lipschitz continuous gradient $\nabla_\theta L(\theta)$, since $L(\theta)$ is composed of integrals of $\partial^2 u_\theta$ and $\gamma_\theta$ over $\Omega$.

Recall that the projected stochastic gradient descent step [15], started from initial $\theta_1$, generates the sequence $\{\theta_j\}$ as follows:

$$\theta_{j+1} = \Pi(\theta_j - \tau G_j) = \arg\min_{\theta \in \Theta} \left( G_j^\top \theta + \frac{1}{2\tau} |\theta - \theta_j|^2 \right)$$

(27)

where $G_j$ denotes the stochastic gradient of $L(\theta)$ at $\theta_j$ using $N_r$ ($N_b$ resp.) sample collocation points in $\Omega$ (on $\partial \Omega$ resp.) with $N_r, N_b = O(N)$. We let $g_j := \nabla_\theta L(\theta_j)$ denote the true (but unknown) gradient of $L$ at $\theta_j$, and define a companion sequence $\{\tilde{\theta}_j\}$ using $g_j$ as

$$\tilde{\theta}_{j+1} = \Pi(\theta_j - \tau g_j) = \arg\min_{\theta \in \Theta} \left( g_j^\top \theta + \frac{1}{2\tau} |\theta - \theta_j|^2 \right).$$

(28)

Note that $\{\tilde{\theta}_j\}$ is not computed in practice (computation of $\tilde{\theta}_j$ is not possible as $g_j$ is unknown), but only defined for convergence analysis here. Also note that $\Theta$ and $\Omega$ are bounded, and hence all integrals of $\partial^2 u_\theta$ and $\gamma_\theta$ are bounded, we know $G_j$ is an unbiased estimate of $g_j$ with bounded variance, denoted by $\sigma^2 > 0$, according to Lemma [4]. Moreover, Lemma [3] implies that there exists $E > 0$ dependent on $B, \Omega, A,$ and $B$ only (as the bound of $\|A[u_\theta, \gamma_\theta]\|_{op}^2$ and $\|B[u_\theta, \gamma_\theta]\|_{L^2(\partial \Omega)}^2$ due to the boundedness of $\Theta$ and $\Omega$) the integral such that $E[|G_j - g_j|^2] \leq \sigma^2 \leq E/N$ as $N_r, N_b = O(N)$.

Now we are ready to verify the convergence of the projected SGD iterations [27]. First, the $M$-Lipschitz continuity of $\nabla_\theta L$ implies that

$$L(\theta_{j+1}) \leq L(\theta_j) + g_j^\top e_j + \frac{M}{2} |e_j|^2,$$

(29)

where we denote $e_j := \theta_{j+1} - \theta_j$ for all $j$. Also due to the $M$-Lipschitz continuity of $\nabla_\theta L$, we have

$$-L(\tilde{\theta}_{j+1}) \leq -L(\theta_j) - g_j^\top \tilde{e}_j + \frac{M}{2} |\tilde{e}_j|^2,$$

(30)

where we denote $\tilde{e}_j := \tilde{\theta}_{j+1} - \theta_j$. Note that $G(\theta_j) = \tau^{-1}[\theta_j - \Pi(\theta_j - \tau g_j)] = \tau^{-1}(\theta_j - \tilde{\theta}_{j+1}) = -\tau^{-1}\tilde{e}_j$, whose magnitude is what we want to bound eventually. Furthermore, due to the optimality of $\tilde{\theta}_{j+1}$ in (27) (which is convex in $\theta$), we know that

$$0 \leq \left(G_j + \frac{\theta_{j+1} - \theta_j}{\tau}\right)^\top (\tilde{\theta}_{j+1} - \theta_{j+1}) = \left(G_j + \frac{\tilde{e}_j}{\tau}\right)^\top (\tilde{e}_j - e_j).$$

(31)

Adding (29), (30), and (31) yields

$$L(\theta_{j+1}) - L(\tilde{\theta}_{j+1}) \leq (g_j - G_j)^\top (e_j - \tilde{e}_j) + \frac{e_j^\top (\tilde{e}_j - e_j)}{\tau} + \frac{M}{2} |e_j|^2 + \frac{M}{2} |\tilde{e}_j|^2.$$
Adding (32) and (33) yields
\[
L(\bar{\theta}_{j+1}) - L(\theta_j) \leq -\left(\frac{1}{\tau} - \frac{M}{2}\right)|\bar{e}_j|^2.
\] (33)

Adding (32) and (33) yields
\[
L(\theta_{j+1}) - L(\theta_j) \leq (g_j - G_j)^\top (e_j - \bar{e}_j) + \frac{e_j^\top (\bar{e}_j - e_j)}{\tau} + \frac{M}{2}|e_j|^2 - \left(\frac{1}{\tau} - M\right)|\bar{e}_j|^2.
\] (34)

Now due to Cauchy-Schwarz inequality, the definitions of \(\theta_{j+1}\) and \(\bar{\theta}_{j+1}\) in (27) and (28), and that the projection \(\Pi\) onto the convex set \(\Theta\) is a non-expansive operator (i.e., \(|\Pi(\theta) - \Pi(\hat{\theta})| \leq |\theta - \hat{\theta}|\) for any \(\theta, \hat{\theta}\)), we can show that
\[
(g_j - G_j)^\top (e_j - \bar{e}_j) = (g_j - G_j)^\top (\theta_{j+1} - \bar{\theta}_{j+1}) = (g_j - G_j)^\top (\Pi(\theta_j - \tau G_j) - \Pi(\theta_j - \tau g_j))
\leq |g_j - G_j|\ |\Pi(\theta_j - \tau G_j) - \Pi(\theta_j - \tau g_j)| \leq \tau |g_j - G_j|^2.
\] (35)

Moreover, we have that
\[
e_j^\top (\bar{e}_j - e_j) = \frac{1}{2\tau} \left(|\bar{e}_j|^2 - |e_j|^2 - |e_j - \bar{e}_j|^2\right).
\] (36)

Substituting (35) and (36) into (34), we obtain
\[
L(\theta_{j+1}) - L(\theta_j) \leq \tau |g_j - G_j|^2 - \left(\frac{1}{2\tau} - M\right)|\bar{e}_j|^2 - \left(\frac{1}{2\tau} - \frac{M}{2}\right)|e_j|^2 - \frac{1}{2\tau}|e_j - \bar{e}_j|^2.
\] (37)

Taking expectation on both sides of (37) and discarding the last negative term, we obtain
\[
\left(\frac{1}{2} - \tau M\right)\tau E[|G(\theta_j)|^2] = \left(\frac{1}{2\tau} - M\right)E[|\bar{e}_j|^2] \leq L_j - L_{j+1} + \tau \sigma^2 - \left(\frac{1}{2\tau} - \frac{M}{2}\right)E[|e_j|^2]
\] (38)

where we used the fact \(E[|G_j - g_j|^2] \leq \sigma^2\) and the notation \(L_j := E[L(\theta_j)]\). Now taking sum \(\sum_j\) of (38) for \(j = 1, \ldots, J\), dividing both sides by \((\frac{1}{2} - \tau M)\tau J\), and setting \(\tau = \frac{1}{16}\) (hence \(\frac{1}{2} - \tau M = \frac{1}{4}\) and \(\frac{1}{2\tau} - \frac{M}{2} = \frac{7M}{2} > 0\)), we know that
\[
\min_{1 \leq j \leq J} E[|G(\theta_j)|^2] \leq \frac{1}{J} \sum_{j=1}^{J} E[|G(\theta_j)|^2] \leq \frac{16M(L_1 - L_{j+1})}{J} + 4\sigma^2 \leq \frac{16M(L_1 - L^*)}{J} + \frac{4E}{N} \leq \varepsilon
\] (39)

by choosing per-iteration sample complexity \(N\) and iteration number \(J\) as \(N = J = [16M(L_1 - L^*) + 4E]^{-1} = O(\varepsilon^{-1})\) where \(L^* := \min_{\theta \in \Theta} L(\theta) \geq 0\) (and hence \(L_{j+1} = E[L(\theta_{j+1})] \geq J^*\)). This completes the proof. 

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