Provably Efficient Neural Estimation of Structural Equation Model: An Adversarial Approach

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Abstract

Structural equation models (SEMs) are widely used in sciences, ranging from economics to psychology, to uncover causal relationships underlying a complex system under consideration and estimate structural parameters of interest. We study estimation in a class of generalized SEMs where the object of interest is defined as the solution to a linear operator equation. We formulate the linear operator equation as a min-max game, where both players are parameterized by neural networks (NNs), and learn the parameters of these neural networks using the stochastic gradient descent. We consider both 2-layer and multi-layer NNs with ReLU activation functions and prove global convergence in an overparametrized regime, where the number of neurons is diverging. The results are established using techniques from online learning and local linearization of NNs, and improve in several aspects the current state-of-the-art. For the first time we provide a tractable estimation procedure for SEMs based on NNs with provable convergence and without the need for sample splitting.

1 Introduction

Structural equation models (SEMs) are widely used in economics [45], psychology [7], and causal inference [26]. In the most general form [36], an SEM defines a joint distribution over $p$ observed random variables $\{X_j\}_{j=1}^p$ as $X_j = f_j(X_{\text{pa}_D(j)}, \varepsilon_j), j = 1, \ldots, p$, where $\{f_j\}$ are unknown functions of interest, $\{\varepsilon_j\}$ are mutually independent noise variables, $D$ is the underlying directed acyclic graph (DAG), and $\text{pa}_D(j)$ denotes the set of parents of $X_j$ in $D$. The joint distribution of $\{X_j\}$ is Markov with respect to the graph $D$.

In most cases, estimation of SEMs are based on the conditional moment restrictions implied by the model. For example, some observational data can be thought of as coming from the equilibrium of a dynamic system. Examples include dynamic models where an agent interacts with the environment, such as in reinforcement learning [13], consumption-based asset pricing models [15], and rational expectation models [20]. In these models, the equilibrium behavior of the agent is characterized by conditional moment equations. A second example is instrument variable (IV) regression, where conditional moment equations also play a fundamental role. IV regression is used to estimate causal effects of input $X$ on output $Y$ in the presence of confounding noise $\varepsilon$ [33]. Finally, in time-series and panel data models, observed variables exhibit temporal or cross-sectional dependence that can also be depicted by conditioning [41].

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For these reasons, we study estimation of structural parameters based on the conditional moment restrictions implied by the model. We propose the generalized structural equation model, which takes the form of a linear operator equation

$$Af = b,$$  

(1)

where $A : \mathcal{H} \to \mathcal{E}$ is a conditional expectation operator, which in most settings is only accessible by sampling, $\mathcal{H}$ and $\mathcal{E}$ are separable Hilbert spaces of square integrable functions with respect to some random variables, $f \in \mathcal{H}$ is the structural function of interest, and $b \in \mathcal{E}$ is known or can be estimated. Section 1.1 [1] provides a number of important examples from causal inference and econometrics that fit into the framework (1).

Our contribution is threefold. First, we propose a new min-max game formulation for estimating $f$ in (1), where we parameterize both players by neural networks (NN). We derive a stochastic gradient descent algorithm to learn the parameters of both NNs. In contrast to several recent works that rely on RKHS theory [12, 31, 39], our method enjoys expressiveness thanks to the representation power of NNs. Moreover, our algorithm does not need sample splitting, which is a common issue in some recent works [21, 27]. Second, we analyze convergence rates of the proposed algorithm in the setting of 2-layer and deep NNs using techniques from online learning and neural network linearization. We show the algorithm finds a globally optimal solution as the number of iterations and the width of NNs go to infinity. In comparison, recent works in incorporating NNs into SEM [21, 27, 6] lack convergence results. Furthermore, we derive a consistency result under suitable smoothness assumptions on the unknown function $f$. Finally, we demonstrate that our model enjoys wide application in econometric and causal inference literature through concrete examples, including non-parametric instrumental variable (IV) regression, supply and demand equilibrium model, and dynamic panel data model.

1.1 Examples of generalized SEM

We describe three examples of generalized SEM: IV regression, simultaneous equations models, and dynamic panel data model. In Appendix A we introduce two more examples: proxy variables of unmeasured confounders in causal inference [29] and Euler equations in consumption-based asset pricing model [15]. Other examples that fit into the generalized SEM framework, but are not detailed in the paper, include nonlinear rational expectation models [20], policy evaluation in reinforcement learning, inverse reinforcement learning [35], optimal control in linearly-solvable MDP [12], and hitting time of stationary process [12].

Example 1 (Instrumental Variable Regression [33, 21, 23]). In many applied problems endogeneity in regressors arises from omitted variables, measurement error, and simultaneity [35]. IV regression provides a general solution to the problem of endogenous explanatory variables. Without loss of generality, consider the model of the form

$$Y = g_0(X) + \varepsilon, \quad \mathbb{E}[\varepsilon | Z] = 0,$$  

(2)

where $g_0$ is the unknown function of interest, $Y$ is the response, $X$ is a vector of explanatory variables, $Z$ is a vector of instrumental variables, and $\varepsilon$ is the noise term. To see how the model fits our framework, define the operator $A : L^2(X) \to L^2(Z)$, $(Ag)(z) = \mathbb{E}[g(X) | Z = z]$. Let $b(z) = \mathbb{E}[Y | Z = z] \in L^2(Z)$. The structural equation (2) can be written as $Ag = b$.

Example 2 (Simultaneous Equations Models). Dynamic models of agent’s optimization problems or of interactions among agents often exhibit simultaneity. Consider a demand and supply model as a prototypical example [28]. Let $Q$ and $P$ denote the quantity sold and price of a product, respectively. Then

$$Q = D(P, I) + U_1, \quad P = S(Q, W) + U_2,$$

$$\mathbb{E}[U_1 | I, W] = 0, \quad \mathbb{E}[U_2 | I, W] = 0,$$  

(3)

where $D$ and $S$ are functions of interest, $I$ denotes consumers’ income, $W$ denotes producers’ input prices, $U_1$ denotes an unobservable demand shock, and $U_2$ denotes an unobservable supply shock. Each observation of $\{P, Q, I, W\}$ is a solution to the equation (3). In Appendix A we cast it into the form (1). The knowledge of $D$ is essential in predicting the effect of financial policy. For example, let $\tau$ be a percentage tax paid by the purchaser. Then the resulting equilibrium quantity is the solution $\hat{Q}$ to the equation $\hat{Q} = D((1 + \tau)(S(\hat{Q}, I) + U_1), W) + U_2$. 

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We call $p$ (GMM) [19] are two important tools in structural estimation. Nonparametric methods such as kernel inner product is defined by $x$ functions, respectively. Denote by $X$ distribution of $A$ a $b$ $A$ $φ$ $1.3$ Notations adaptation of these results. linear function when they are trained using gradient type methods. The present paper is built on an out that NNs exhibit an implicit local linearization which allows us to interpret the former as a related to recent advances in overparametrized NNs [3, 2, 17, 24, 26, 47, 34]. These works point similar philosophy, by reducing the analysis of neural gradient update to regret analysis of convex saddle-point problem derivation and non-linearity of NNs, these methods suffer from computational issues. Kernel IV [39] and Dual IV [31] apply reproducing kernel Hilbert space (RKHS) theory to Farrell et al. [16] discusses the use of NN in semi-parametric estimation but not computational density estimators [33, 10] and spline regression [14, 9] have been applied to IV regression. However, $t$ time in the dataset is a common approach to identifying causal effects [1]. Panel data are comprised that includes time-varying regressors and allows us to investigate the long-run relationship between economic factors [41].

### 1.2 Related work

**Neural networks in structural equation models.** IV regression and generalized method of moments (GMM) [19] are two important tools in structural estimation. Nonparametric methods such as kernel density estimators [33] and spline regression [14, 9] have been applied to IV regression. However, these methods suffer from the curse of dimensionality and the lack of guidance on the choice of kernels and splines. Existing work on structural estimation using NNs, best to our knowledge, includes Deep IV [21], Deep GMM [6] and Adversarial GMM [27]. However, due to the artifacts in saddle-point problem derivation and non-linearity of NNs, these methods suffer from computational cost [21], the need of sample splitting [27, 21] or lack of convergence results [6, 27]. The work of Farrell et al. [16] discusses the use of NN in semi-parametric estimation but not computational issues. Kernel IV [39] and Dual IV [31] apply reproducing kernel Hilbert space (RKHS) theory to IV regression. Dual IV is closely related to the work of Dai et al. [12], where the authors discuss problems of the form $\min_f \mathbb{E}_{x,y}[f(y, \mathbb{E}_z[f(x, z)])]$ and reformulate it as a min-max problem using duality, interchangeability principle, and dual continuity. In Appendix [5] we show that our minimax formulation of IV has a natural connection to GMM compared to Dual IV.

**Neural tangent kernel and overparametrized NN.** Recent work on neural tangent kernel (NTK) [24] shows that in the limit when the number of neurons goes to infinity, the nonlinear NN function can be represented by a linear function specified by the NTK. Consequently, the optimization problem parametrized by NNs reduces to a convex problem, and can be tackled by tools in classical convex optimization. Examples following this idea include [8, 43, 46]. In fact, the present paper follows a similar philosophy, by reducing the analysis of neural gradient update to regret analysis of convex online learning, in the presence of bias and noise in the gradient. Finally, the present work is also related to recent advances in overparametrized NNs [3, 2, 17, 24, 26, 47, 34]. These works point out that NNs exhibit an implicit local linearization which allows us to interpret the former as a linear function when they are trained using gradient type methods. The present paper is built on an adaptation of these results.

### 1.3 Notations

We call $(f^*, u^*) \in \mathcal{F} \times \mathcal{U}$ a saddle point of a function $\phi : \mathcal{F} \times \mathcal{U} \rightarrow \mathbb{R}$ if for all $f \in \mathcal{F}, u \in \mathcal{U}, \phi(f^*, u) \leq \phi(f^*, u) \leq \phi(f, u^*)$. The indicator function $\mathbb{I}\{\cdot\}$ is defined as $\mathbb{I}\{A\} = 1$ if the event $A$ is true; otherwise $\mathbb{I}\{A\} = 0$. Let $[n] = \{1, 2, \ldots, n\}$. For two sequences $\{a_n\}, \{b_n\}$, the notation $a_n \sim b_n$ if $a_n = O(b_n)$ and $b_n = O(a_n)$. The notation $O$ ignores logarithmic factors. For a matrix $A$, let $\|A\|_F$ be the Frobenius norm.

For a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, let $X : \Omega \rightarrow \mathbb{R}^p$ be a $p$-dimension random vector. The probability distribution of $X$ is characterized by its joint cumulative distribution function $F$. Partition $X$ into $X = [X_1^T, X_2^T]^T$ where $X_1 \in \mathbb{R}^{p_1}, X_2 \in \mathbb{R}^{p_2}$, and let $F_{X_1}, F_{X_2}$ be the marginal distribution functions, respectively. Denote by $L^2_F(\mathbb{R}^{p_1}, F_{X_1}) = \{f_1 : \mathbb{R}^{p_1} \rightarrow \mathbb{R} : \mathbb{E}_{X_1}[f_1(X_1)^2] < \infty\}$ the Hilbert space of real-valued square integrable functions of $X_1$ and similarly define $L^2_F(\mathbb{R}^{p_2}, F_{X_2})$. For ease of presentation we denote $L^2_F(\mathbb{R}^{p_1}, F_{X_1})$ by $L^2(X_1)$ when the context is clear. For $f, g \in L^2_F$, the inner product is defined by $\langle f, g \rangle_{L^2(X)} = \mathbb{E}_X[f(X)g(X)]$. For a linear operator $A : \mathcal{H} \rightarrow \mathcal{E}$ denote by $\mathcal{N}(A) = \{f \in \mathcal{H} : Af = 0\}$ its null space. Denote by $A^*$ the adjoint of a bounded linear operator.
We remark that as long as \( \alpha \neq 0 \), we want to estimate the solution to \( f \). Moreover, the function \( b \) can be known or estimable from the data, i.e., \( b \) can be of the form \( \sum_1^2 \alpha f \) or both \( \alpha \) and \( b \) have to be estimated \( \hat{b} \). In the linear integral equation literature, when \( A \) is compact, \( f \) belongs to the class of Fredholm equations of type I. An inverse problem perspective on conditional moment problems is provided in \( \cite{7} \).

A compact operator with infinite dimensional range cannot have a continuous inverse \( \cite{7} \), which raises concerns about stability of operator equation \( \cite{1} \). A classical way to overcome the problem of instability is to look for a Tikhonov regularized solution, which is uniquely defined \( \cite{3} \). For all \( \alpha \) the orthogonal complement of \( B \) is known. Let \( B_A \) denote by \( B_A \), for some positive number \( \alpha \) we define the Tikhonov regularized problem

\[
\hat{f}^\alpha = \arg\min_{f \in \mathcal{H}} \frac{1}{2} \| A f - b \|_\mathcal{E}^2 + \frac{\alpha}{2} \| f \|_\mathcal{H}^2. \tag{5}
\]

2.2 Saddle-point formulation

From an optimization perspective, problem \( \cite{8} \) is difficult to solve in that the conditional expectation operator is nested inside the square loss. Moreover, it is impossible to estimate the conditional expectation in some cases since we have only limited samples coming from the conditional distribution \( p(X_1 \mid X_2) \). Our saddle-point formulation circumvents such problems by using the probabilistic property of conditional expectation. The proposed method also offers some new insights into the saddle-point formulation of IV regression \( \cite{31, 6} \), which shows our derivation is closely related to GMM. This is discussed in Appendix \( \cite{14} \).

Now we derive a min-max game formulation for \( \cite{8} \). Assume \( b \) is known. Let \( R : \mathcal{H} \rightarrow \mathbb{R}^+ \) be some suitable norm on \( \mathcal{H} \) that captures smoothness of the function \( f \). We consider the constrained form of minimization problem \( \cite{8} \): \( \min_{f \in \mathcal{H}} \frac{1}{2} R(f) \) subject to \( A f = b \). For some positive number \( \alpha > 0 \), we define the Lagrangian with penalty on the multiplier \( u \in \mathcal{E} \) :

\[
\tilde{L}(f, u) = \frac{1}{2} R(f) + \langle A f - b, u \rangle_\mathcal{E} - \frac{\alpha}{2} \| u \|_\mathcal{E}^2.
\]

Without loss of generality, we move the penalty level \( \alpha \) to \( R(f) \). Finally, using a property of conditional expectation that \( \langle A f, u \rangle_\mathcal{E} = \mathbb{E}_{X_2} \left[ \mathbb{E}[f(X_1) \mid X_2] \right] = \mathbb{E}[f(X_1)u(X_2)] \) and choosing \( R(f) = \| f \|_\mathcal{E}^2 \), we arrive at our saddle-point problem

\[
\min_{f \in \mathcal{L}(X_1)} \max_{u \in \mathcal{L}(X_2)} \mathbb{E} \left[ (f(X_1) - b(X_2)) u(X_2) + \frac{\alpha}{2} f(X_1)^2 - \frac{1}{2} u(X_2)^2 \right]. \tag{6}
\]

We remark that as long as \( R(f) \) can be estimated from samples, our subsequent algorithm and analysis work with some adaptations. Note that the above derivation is also suitable for equations of the form \((I - K)f = b\), where \( K \) is a conditional expectation operator (e.g., Example \( \cite{4} \) in Appendix \( \cite{A} \)). Moreover, the function \( b \) can be either known or estimable from the data, i.e., \( b \) can be of the form \( b(X_2) = \mathbb{E}[b(X_1, X_2) \mid X_2] \) where \( b \) is known.

\footnote{See Appendix \( \cite{14} \) for a discussion of when a conditional expectation operator is compact.}
3 Neural Network Parametrization

The recent surge of research on the representation power of NNs [24, 3, 2, 20, 4, 3] motivates us to use NNs as approximators in (6). Consider the 2-layer NN with parameters \( B \) and \( m \) (to be defined in (9)). As the width of the NN, \( m \), goes to infinity, the class NNs approximates a subset of the reproducing kernel Hilbert space induced by the kernel \( K(x, y) = \mathbb{E}_{\alpha \sim \mathcal{N}(0, \frac{1}{2} L_a)} \left[ \mathbb{I} \{ a^\top x > 0 \} \mathbb{I} \{ a^\top y > 0 \} x^\top y \right] \). Such a subset is a ball with radius \( B \) in the corresponding RKHS norm. This function class is sufficiently rich, if the width \( m \) and the radius \( B \) are sufficiently large [4].

However, due to non-linearity of NNs, to devise an algorithm for the NN-parametrized problem (6) with theoretical guarantee is no easy task. In this section, we describe the NN parametrization scheme and the algorithm. As a main contribution of the paper, we then provide formal statements of results on convergence rate and estimation consistency.

To keep the notation simple, we assume \( X_1 \) and \( X_2 \) are of the same dimension \( p \). We parametrize the function spaces \( L^2(X_1) \) and \( L^2(X_2) \) in (6) by a space of NNs, \( \mathcal{F}_{\text{NN}} \), defined in (9) and (10) below. With this parameterization, we write the primal problem in (5) as

\[
\min_{f \in \mathcal{F}_{\text{NN}}} L(f) := \frac{1}{2} \| Af - b \|^2_2 + \frac{\alpha}{2} \| f \|^2_H,
\]

and the min-max problem in (6) becomes

\[
\min_{f \in \mathcal{F}_{\text{NN}}} \max_{u \in \mathcal{F}_{\text{NN}}} \phi(f, u) := \mathbb{E} \left[ (f(X_1) - b(X_2)) u(X_2) + \frac{\alpha}{2} f(X_1)^2 - \frac{1}{2} u(X_2)^2 \right].
\]

Problem (8) involves simultaneous optimization over two NNs. Notice that for each fixed \( f \) in the outer minimization, the maximum of the inner maximization over \( E \) is attained at \( u(\cdot) = \mathbb{E}[f(X_1)] \). This can be seen by noting \( \max_{u \in E} \langle Af - b, u \rangle_E - \frac{1}{2} \| u \|^2_E = \frac{1}{2} \| Af - b \|^2_2 \). If for all \( f \in \mathcal{F}_{\text{NN}} \) such maximum is attained in \( \mathcal{F}_{\text{NN}} \), then every primal solution \( f^a \in \mathcal{F}_{\text{NN}} \) in the saddle point of (8), (\( f^a, u^a \)), is also an optimal solution to the problem (7).

Next we introduce the function classes of NNs and the initialization schemes.

3.1 Neural Network Parametrization

2-layer NNs. Consider the space of 2-layer NNs with ReLU activations and initialization \( \Xi_0 = [W(0), b_1, \ldots, b_r] \)

\[
\mathcal{F}_{B, m}(\Xi_0) = \left\{ x \mapsto \frac{1}{\sqrt{m}} \sum_{r=1}^m b_r \sigma(W_r \top x) : W \in S_B \right\}, \tag{9}
\]

where \( \sigma(z) = \mathbb{I} \{ z > 0 \} \cdot z \) is the ReLU activation, \( b_1, \ldots, b_r \) are scalars, and

\[ S_B = \{ W \in \mathbb{R}^{md} : \| W - W(0) \|_2 \leq B \} \]

is the \( B \)-sphere centered at the initial point \( W(0) \in \mathbb{R}^{md} \). Here we denote succinctly by \( W \) the weights of a 2-layer NN stacked into a long vector of dimension \( md \), and use \( W_r \in \mathbb{R}^m \) to access the weights connecting to the \( r \)-th neuron, i.e., \( W = [W_1 \top, \ldots, W_m \top] \top \). Each function in \( \mathcal{F}_{B, m} \) is differentiable with respect to \( W \), 1-Lipschitz, and bounded by \( B \). We state the following distributional assumption on initialization.

Assumption A.1 (NN initialization, 2-layer, [24]). Consider the 2-layer NN function space (9). All initial weights and parameters, collected as \( \Xi_0 = [W(0), b_1, \ldots, b_m] \), are independent, and generated as \( b_r \sim \text{Uniform} \{-1, 1\} \) and \( W(0) \sim \mathcal{N}(0, \frac{1}{2} I_d) \). During training we fix \( \{ b_r \}_{r=1}^m \) and update \( W \).

Multi-layer NNs. The class of \( H \)-layer NN, \( \mathcal{F}_{B, H, m} \) with initialization \( \Xi_{H, 0} = \{ A, \{ W(h)(0) \}_{h=1}^H \} \) is defined as

\[
\mathcal{F}_{B, H, m}(\Xi_{H, 0}) = \left\{ x \mapsto b^\top x^{(H)} \right. \text{ where } x^{(h)} = \frac{1}{\sqrt{m}} \cdot \sigma(W^{(h)} x^{(h-1)}), h \in [H], \left. x^{(0)} = Ax : W \in S_{B, H} \right\}. \tag{10}
\]
where \( W = (\text{vec}(W^{(1)})^T, \ldots, \text{vec}(W^{(H)})^T)^T \in \mathbb{R}^{Hm^2} \) is the collection of weights \( W^{(h)} \in \mathbb{R}^{m^2} \) from all middle layers, \( x^{(h)} \) is the output from the \( h \)-th layer, \( A \in \mathbb{R}^{m \times d}, b \in \mathbb{R}^m \), the function \( \sigma \) is applied element-wise, and

\[
S_{B,H} = \{ W \in \mathbb{R}^{Hm^2} : \| W^{(h)} - W^{(h)}(0) \|_F \leq B \text{ for any } h \in [H] \}.
\]

We use the following initialization scheme.

**Assumption A.2 (NN initialization, multi-layer, \([3,17]\)).** Consider the space of multi-layer NNs defined in \((10)\). Each entry of \( A \) and \( \{ W^{(h)}(0) \}_{h=1}^H \) is independently initialized by \( N(0,2) \), and entries of \( b \) are independently initialized by \( N(0,1) \). Assume \( m = \Omega(d^{3/2}B^{-1}H^{-3/2} \log^{3/2}(m^{1/2}B^{-1})) \) and \( B = \mathcal{O}(m^{1/2}H^{-6} \log^{-3} m) \). All initial parameters, \( \Xi_{H,0} = \{ A, \{ W^{(h)}(0) \}_{h=1}^H, b \} \), are independent. During training we keep \( A, b \) fixed and update \( W \).

### 3.2 Algorithm

Denote the weights of NNs \( f \) and \( u \) in \((8)\) by \( \theta \) and \( \omega \), respectively. Now \( \theta \) and \( \omega \) play the role of \( W \) in \((9)\) (or in \((10)\)) since during training only the weights \( W \) in \((9)\) (or in \((10)\)) are updated. For brevity we denote \( f_0 = f(\theta; X_1) \) and \( u_0 = u(\omega; X_2) \). With a slight abuse of notation, we use \( \phi(\theta, \omega) \) and \( \phi(f_0, u_0) \) (defined in \((8)\)) interchangeably since we always denote the NN weights of \( f \) by \( \theta \) and that of \( u \) by \( \omega \). Let \( F(\theta; \omega; X_1, X_2) = u_0 f_0 - u_0 b - \frac{1}{2} u_0^2 + \frac{\gamma}{2} f_0^2 \). The saddle-point problem \((8)\) is now rewritten as

\[
\min_{\theta \in S_B} \max_{\omega \in S_B} \phi(\theta, \omega) = \mathbb{E}[F(\theta, \omega; X_1, X_2)].
\]

**Algorithm 1** is the proposed stochastic primal-dual algorithm for solving the game \((8)\). Given initial weights \( \theta_1 \) and \( \omega_1 \), stepsize \( \eta \), and i.i.d. samples \( \{ X_1,t, X_2,t \} \), for \( t = 1, \ldots, T - 1 \),

\[
\begin{align*}
\theta_{t+1} &= \Pi_{S_B} \left( \theta_t - \eta \nabla_{\theta} F(\theta_t, \omega_t; X_1,t, X_2,t) \right), \\
\omega_{t+1} &= \Pi_{S_B} \left( \omega_t + \eta \nabla_{\omega} F(\theta_t, \omega_t; X_1,t, X_2,t) \right).
\end{align*}
\]

**Algorithm 1**

Here \( \Pi_{S_B} \) is the projection operator. The search spaces in \((11)\) and the projection operator should be replaced by \( S_{B,m} \) and \( \Pi_{S_{B,m}} \), respectively, when multi-layer NNs are used. If \( b \) takes the form \( b(X_2) = \mathbb{E}[b(X_1, X_2) | X_2] \) our algorithm proceeds by replacing \( b \) in \( F \) with \( \tilde{b} \).

### 4 Main results

Due to nonlinearity of NNs, \( \phi \) is not convex-concave in \((\theta, \omega)\), which makes the analysis of **Algorithm 1** difficult. However, as will be shown in **Theorem 4.1** under certain assumptions **Algorithm 1** enjoys global convergence as \( T \) and \( m \) go to infinity. For a candidate solution \( f \), we consider the suboptimality \( E(f) \) as a measure of quality of solution, i.e.,

\[
E(f) = L(f) - L^*,
\]

where \( L^* = \min_{f \in F_{B,m}} L(f) \) is the minimum value of \( L \) over the space of NNs. We define similar quantities when multi-layer NNs are used. Next we describe regularity assumptions on the data distribution.

**Assumption A.3 (Regularity of data distribution).** Assume that there exists \( c > 0 \), such that for any unit vector \( v \in \mathbb{R}^p \) and any \( \zeta > 0 \), \( \mathbb{P}(|v^T X_1| \leq \zeta) \leq c \zeta, \mathbb{P}(|v^T X_2| \leq \zeta) \leq c \zeta \). Without loss of generality assume \( \max(\|X_1\|_2, \|X_2\|_2) \leq 1 \) almost surely. Assume \( b(X_2) \) is bounded almost surely.

**Assumption A.4.** With high probability with respect to NN initialization, for any \( f \in F_{B,m} \) (or \( F_{B,H,m} \)) \( u(\cdot) = \mathbb{E}[f(X_1) | X_2 = \cdot] - b(\cdot) \) belongs to the class \( F_{B,m} \) defined in \((5)\) (or \( F_{B,H,m} \) defined in \((10)\), in the multi-layer NN case).

In **Assumption A.3** boundedness of the random variable \( b(X_2) \) is satisfied in common applications. **Assumption A.4** ensures the connection between the min-max problem \((8)\) and the primal problem \((7)\). We are ready to state the global convergence results for **Algorithm 1**. The proof is presented in Appendix D.7.
Theorem 4.1 (Global convergence of Algorithm 1). Consider the iterates generated by Algorithm 1 with stepsize $\eta$. Let $\alpha = \max\{\alpha, 1\}$. We denote by $E_{\text{init}}[\cdot]$ the expectation w.r.t. NN initialization. For a given number of training steps $T > 0$, define $\bar{f}_T(\cdot) = \frac{1}{T} \sum_{t=1}^T f(\theta_t, \cdot)$.

1. (2-layer NNs) Under Assumption A.1, A.3 and A.4 with probability over $\mathcal{A}$, with probability over $1 - 2\delta$ with respect to the sampling process,

$$
E_{\text{init}}[E(\bar{f}_T)] = \mathcal{O}\left(\alpha \eta B + \frac{B}{T\eta} + \frac{\alpha B^{3/2} \log^{1/2}(1/\delta)}{T^{1/2}} + \frac{\alpha B^{5/2}}{m^{1/4}}\right).
$$

2. (Multi-layer NNs) Under Assumption A.2 and A.4 with probability over $1 - \delta = \omega(\Omega(\log^2 m))$ with respect to the sampling process and initialization,

$$
E(\bar{f}_T) = \mathcal{O}\left(P_1 \eta a \log m + \frac{P_2}{T\eta} + \frac{P_3 a \log m \log^{1/2}(1/\delta)}{T^{1/2}} + \frac{P_4 a \log^{3/2} m}{m^{1/6}}\right),
$$

where $P_1 = H^4 B^{5/3}$, $P_2 = H^1 B$, $P_3 = H^5 B^2$, $P_4 = H^6 B^3$, and $c$ is an absolute constant.

Each of the error rates in Theorem 4.1 consists of two parts: the optimization error and the linear approximation error; see Section 5.2 for a detailed derivation. For the two-layer case, if the total training step $T$ is known in advance, the optimal stepsize choice is $\eta \sim T^{-1/2}$, and the resulting error rate is $\mathcal{O}(T^{-1/2} + m^{-1/4})$. The $\mathcal{O}(T^{-1/2})$ term is comparable to the rate in [32] where stochastic mirror descent method is used in stochastic saddle-point problems. Importantly, the error bound converges to zero as $T, m \to \infty$. For the multi-layer case, optimizing $\eta$ yields the error rate $\mathcal{O}(T^{-1/2} + m^{-1/6})$; the linear approximation error has increased due to the highly non-linear nature of multi-layer NNs.

### 4.1 Consistency

If we assume smoothness of the solution to the operator equation $Af = b$ defined in (1) and compactness of the operator $A$, we are able to control the rate of regularization bias. For a compact operator $A$, let $\{\lambda_j, \phi_j, \psi_j\}_{j=1}^\infty$ be its singular system [25], i.e., $\{\phi_j\}$ and $\{\psi_j\}$ are orthonormal sequences in $\mathcal{H}, \mathcal{E}$, respectively, $\lambda_j \geq 0$, and satisfy $A\phi_j = \lambda_j \psi_j, A^* \psi_j = \lambda_j \phi_j$, where $A^*$ is the adjoint operator of $A$. For any $\beta > 0$, define the $\beta$-regularity space [9]

$$
\Phi_\beta = \left\{ f \in \mathcal{N}(A) \subseteq \mathcal{H} \text{ such that } \sum_{j=1}^\infty \frac{|f, \phi_j|^2}{\lambda_j^{2/\beta}} < \infty \right\} \subseteq \mathcal{H}.
$$

Equipped with the definition of $\beta$-regularity space, we are now ready to state the consistency result for 2-layer NN. The proof is presented in Appendix D.8

Theorem 4.2 (Consistency, 2-layer NN). Consider the iterates generated by Algorithm 7 with stepsize $\eta \sim (\alpha T)^{-1/2}$, where $\alpha = \max\{\alpha, 1\}$. Assume the operator $A$ defined in (1) is injective and compact, and that the solution to (1) lies in the regularity space $\Phi_\beta$ defined in (14) for some $\beta > 0$. Assume A.1, A.3 and A.4. If the primal problems (5) and (7) yield the same solution $f^*$, then with probability at least $1 - \delta$ over the sampling process, the average of the NNs, $\bar{f}_T = \frac{1}{T} \sum_{t=1}^T f(\theta_t)$, satisfies

$$
E_{\text{init}}[\|f_T - f\|^2_{\mathcal{H}}] = \mathcal{O}\left(\alpha \min\{\beta, 2\} + \frac{1}{\alpha^{\sqrt{\beta}}} \frac{1}{T^{1/2}} + \frac{1}{\alpha^\beta} \left(\frac{T^{1/2}}{T^{1/2}} + \frac{1}{m^{1/4}}\right)\right),
$$

where $C$ is a constant independent of $\beta, \alpha, T$ and $m$.

If $0 < \beta \leq 2$ and $0 < \alpha \leq 1$, the optimal choice of $\alpha$ is $\alpha \sim (T^{-1/2} + m^{-1/4})^{1/(\beta+1)}$, assuming $T$ and $m$ are large enough, and the estimation error (15) is of order $\mathcal{O}(T^{-1/2} + m^{-1/4})^{1/(\beta+1)}$. To the best of our knowledge, this is the first estimation error rate of structural equation models using NNs. We remark [16] also provides bounds on the estimation error of an NN-based estimator in the setting of semi-parametric inference, but they do not discuss computational issues.

### 5 Proof sketch

In this section, we introduce results in approximating the NNs functions with the linearized functions. The control of approximation error is the building block of our subsequent analysis.
5.1 Local linearization of NNs

The key observation is that as the width of NN increases, NN exhibits similar behavior to its linearized version [2]. For an NN \( f \in \mathcal{F}_{B,m} \) (or \( \mathcal{F}_{B,H,m} \), with slight notation overload), we denote its linearized version at \( W(0) \) by

\[
\hat{f}(x, W) = f(x, W(0)) + \langle \nabla_W f(x, W(0)), W - W(0) \rangle.
\]

The following lemma offers a precise characterization of linearization error for 2-layer NNs; the proof is presented in Section D.1 in Appendix D. Essentially, it shows that for 2-layer NNs the expected approximation error of the function \( f(\cdot, W) \) by \( \hat{f}(\cdot, W) \) decays at the rate \( O(m^{-1/2}) \), for any \( W \in S_B \). In other words, as the width of NN goes to infinity, the NN function behaves like a linear function. Similar results on approximation error for multi-layer NNs hold; see Appendix B.

**Lemma 5.1** (Error of local linearization, 2-layer). Consider the 2-layer neural networks in (9). Assume that there exists \( c > 0 \), for any unit vector \( v \in \mathbb{R}^d \) and any constant \( \zeta > 0 \), such that \( \mathbb{P}_X(|v^T X| \leq \zeta) \leq c\zeta \). Under Assumption A.1 we have for all \( W \in S_B \) and all \( x \),

\[
\begin{align*}
\mathbb{E}_{\text{init},X}[|f(X, W) - \hat{f}(X, W)|^2] & = O(B^3 m^{-1/2}), \quad \text{and} \\
\mathbb{E}_{\text{init},X}[|\nabla_W f(X, W) - \nabla_W \hat{f}(X, W)|^2] & = O(Bm^{-1/2}).
\end{align*}
\]

5.2 Convergence analysis

In this section, we discuss techniques used to bound the minimization via the analysis of the regret, in the case of 2-layer NNs. The same reasoning applies to the maximizing player \( \omega \) and extension to multi-layer NN is obvious. The following lemma relates regret and primal error. The proof is presented in Section D.3 in Appendix D.

**Lemma 5.2** (A bound on primal error). Consider a sequence of candidates \( \{(f_t, u_t)\}_{t=1}^T \) for the minimax problem (5) that satisfy the following regret bounds

\[
\frac{1}{T} \sum_{t=1}^T \phi(f_t, u_t) \leq \min_f \frac{1}{T} \sum_{t=1}^T \phi(f, u_t) + \epsilon_f, \quad \frac{1}{T} \sum_{t=1}^T \phi(f_t, u_t) \geq \max_u \frac{1}{T} \sum_{t=1}^T \phi(f_t, u) - \epsilon_u.
\]

Denote \( \bar{f}_T = \frac{1}{T} \sum_{t=1}^T f_t \). If Assumption A.4 holds, then \( E(\bar{f}_T) - L^* \leq \epsilon_f + \epsilon_u \).

The above lemma suggests we separate our analysis for the two players. For example, to analyze \( \epsilon_f \) we can think of the sequence \( \{u_t\} \) as fixed and find an upper bound of the quantity \( \frac{1}{T} \sum_{t=1}^T \phi(f_t, u_t) - \frac{1}{T} \sum_{t=1}^T \phi(f, u_t) \). We will demonstrate our proof idea via the analysis of \( \epsilon_f \); it can easily extend to \( \epsilon_u \).

We focus on the analysis of the minimizer \( \theta \) and therefore we denote \( \phi_t(\cdot) = \phi(\cdot, \omega_t) \) (defined in (8)). Also let \( \tilde{\phi}_t(\theta) = \mathbb{E}_X[\tilde{w}_t \tilde{f}_t - \hat{u}_t b - \frac{1}{2} \tilde{z}_t^2 + \frac{1}{2} \tilde{g}_t^2] \), obtained by replacing \( f \) and \( u \) in \( \phi_t(\cdot) \) with their linearized counterparts defined in (16). The most important property of the linearized surrogate \( \tilde{\phi}_t(\theta) \) is that it is convex in \( \theta \). To estimate the rate of \( \epsilon_f \), we start with the decomposition of regret. For any \( \theta \in S_B \), define the regret \( \text{Reg}(\theta) = \frac{1}{T} \sum_{t=1}^T \phi_t(\theta_t) - \frac{1}{T} \sum_{t=1}^T \tilde{\phi}_t(\theta_t) \). Then we have the decomposition

\[
\text{Reg}(\theta) = \frac{1}{T} \sum_{t=1}^T \phi_t(\theta_t) - \frac{1}{T} \sum_{t=1}^T \tilde{\phi}_t(\theta_t) + \frac{1}{T} \sum_{t=1}^T \hat{\phi}_t(\theta_t) - \frac{1}{T} \sum_{t=1}^T \hat{\phi}_t(\theta_t) + \frac{1}{T} \sum_{t=1}^T \hat{\phi}_t(\theta_t) - \frac{1}{T} \sum_{t=1}^T \phi_t(\theta_t).
\]

(21)

We bound each term separately. To control the terms (18) and (20) we use the linearization of NN, which shows that the linearized NN and the original one behave similarly in terms of output and gradient as the width of NN \( m \) grows (cf. Lemma 5.1 and Lemma B.1). The term (19) is bounded using techniques in convex online learning. The idea is to treat the algorithm designed for solving min-max game associated with \( \phi \) as a biased primal-dual gradient methods for the one with \( \hat{\phi} \). We illustrate our techniques in further details in Appendix C.
6 Conclusions

We have derived saddle-point formulation for a class of generalized SEMs and parametrized the players with NNs. We show that the gradient-based primal-dual update enjoys global convergence in the overparametrized regimes \( m \to \infty \), for both 2-layer NNs and multi-layer NNs. Our results shed new light on the theoretical understanding of structural estimation with neural networks.

Broader Impact

In recent years, the impact of machine learning (ML) on economics is already well underway [5][11], and our work serves as a complement to this line of research. On the one hand, machine learning methods such as random forest, support vector machines and neural networks provide great flexibility in modeling, while traditional tools in structural estimation that are well versed in the econometrics community are still primitive, despite recent advances [27][21][6][16]. On the other hand, to facilitate ML-base decision making, one must be aware of the distinction between prediction and causal inference. Our method provides an NN-based solution to estimation of generalized SEMs, which encompass a wide range of econometric and causal inference models. However, we remark that in order to apply the method to policy and decision problems, one must pay equal attention to other aspects of the model, such as interpretability, robustness of the estimates, fairness and nondiscrimination, assumptions required for model identification, and the testability of those assumptions. Unthoughtful application of ML methods in an attempt to draw causal conclusions must be avoided for both ML researchers and economists.

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APPENDICES TO PROVABLY EFFICIENT NEURAL ESTIMATION OF STRUCTURAL EQUATION MODEL: AN ADVERSARIAL APPROACH

A Examples of generalized structural equation models

In Section 2 we introduce our model in its full generality. Here we specialize it in concrete examples from the causal inference literature and econometrics.

We remark that the convergence result detailed in Theorem 4.1 applies to all examples while consistency result (Theorem 4.2) applies only to Example 1 because compactness of the conditional expectation operator is required in Theorem 4.2.

Example 1 revisited (Instrumental Variable Regression. [33, 21, 23]). In applied econometrics, endogeneity in regressors usually arises from omitted variables, measurement error, and simultaneity [45]. The method of instrumental variables (IV) provides a general solution to the problem of an endogenous explanatory variable. Without loss of generality, consider the model of the form

\[ Y = g_0(X) + \varepsilon, \quad \mathbb{E}[\varepsilon | Z] = 0, \]

(2 revisited)

where \( g_0 \) is the unknown function of interest, \( Y \) is an observable scalar random variable, \( X \) is a vector of explanatory variables, \( Z \) is a vector of instrument variables, and \( \varepsilon \) is the noise term. For the special case \( X = Z \), the estimation of \( g_0 \) reduces to simple nonparametric regression, since \( \mathbb{E}[Y | X = x] = g_0(x) \), and can be solved via spline regression or kernel regression [44]. When \( X \) is endogenous, which is usually the case in observational data, traditional prediction-based methods fail to estimate \( g_0 \) consistently. In this case, \( g_0(x) \neq \mathbb{E}[Y | X = x] \), and prediction and counterfactual prediction become different problems.

To see how the model fits our framework, define the operator \( A : L^2(X) \rightarrow L^2(Z) \), \( Ag = \mathbb{E}[g(X) | Z] \). Let \( b = \mathbb{E}[Y | Z] \in L^2(Z) \). The structural equation (2) can be written as \( Ag = b \). The minimax problem with penalty level \( \alpha (\alpha > 0) \) takes the form

\[ \min_{f \in L^2(X)} \max_{u \in L^2(Z)} \mathbb{E}[f(X)u(Z) - Y : u(Z) - \frac{1}{2}u^2(Z) + \frac{\alpha}{2}f^2(X)], \]

(22)

where the expectation is taken over all random variables.

The IV framework enjoys a long history, especially in economics [18]. It provides a means to answer counterfactual questions like what is the efficacy of a given drug in a given population? What fraction of crimes could have been prevented by a given policy? However, the presence of confounders makes these questions difficult. If \( X \) is endogenous, which is usually the case in observational data, then \( g_0(x) \neq \mathbb{E}[Y | X = x] \), and prediction and counterfactual prediction become different problems. When valid IVs are identified, we have a hope to answer these counterfactual questions.

Counterfactual prediction targets the quantity \( \mathbb{E}[Y | \text{do}(X = x)] \) defined by the causal graph (see Figure 1), where the \( \text{do}(\cdot) \) operator indicates that we have intervened to set the value of variable \( X \) to \( x \) while keeping the distribution of \( \varepsilon \) fixed [56]. To facilitate counterfactual prediction, we need to impose stronger conditions on the model [31, 21]: (i) relevance: \( \mathbb{P}(X | Z = z) \) is not constant in \( z \); (ii) exclusion: \( Y \perp Z | X, \varepsilon \); and (iii) unconfounded instrument: \( \varepsilon \perp Z \). Figure 1 encodes such assumptions succinctly.

![Causal Diagram of IV](image)

Figure 1: A causal diagram of IV. Three observable variables \( X, Y, Z \) (denoted by filled circles) and one unobservable confounding variable \( \varepsilon \). There is no direct effect of the instrument \( Z \) on the outcome \( Y \) except through \( X \).

Example 2 revisited (Simultaneous Equations Models). Dynamic models of agent’s optimization problems or of interactions among agents often exhibit simultaneity. Demand and supply model is
such an example. Let $Q$ and $P$ denote the quantity sold and price of a product. Consider the demand and supply model adapted from [28].

$$Q = D(P, I) + U_1,$$
$$P = S(Q, W) + U_2,$$
$$\mathbb{E}[U_1 \mid I, W] = 0, \ \mathbb{E}[U_2 \mid I, W] = 0. \quad (3) \text{ revisited}$$

Here $D$ and $S$ are functions of interest, $I$ denotes consumers’ income, $W$ denotes producers’ input prices, $U_1$ denotes an unobservable demand shock, and $U_2$ denotes an unobservable supply shock. Equation (3) is generally the results of equilibrium. Due to simultaneity, there is no hope to recover demand function $D$ by simple nonparametric regression of $Q$ on $P$ and $I$; nor can we recover supply function $S$ by regressing $P$ on $Q$ and $W$. The knowledge of $D$ is essential in predicting the effect of financial policy. For example, let $\tau$ be a percentage tax paid by the purchaser. Then the resulting equilibrium quantity is the solution $\hat{Q}$ to the equation

$$\hat{Q} = D((1 + \tau)(S(\hat{Q}, I) + U_1), W) + U_2.$$

To cast the model (3) to a minimax problem, define the operators

$$A_1 : L^2(P, I) \to L^2(I, W), \ A_1 D = \mathbb{E}[D(P, I) \mid I, W],$$
$$A_2 : L^2(Q, W) \to L^2(I, W), \ A_2 S = \mathbb{E}[S(Q, W) \mid I, W].$$

The resulting minimax problem is

$$\min_{D \in L^2(P, I)} \max_{u_1, u_2 \in L^2(I, W)} \left\{ \mathbb{E}[u_1(I, W) : (D(P, I) - Q) + u_2(I, W) : (S(Q, W) - P)] \right\}.$$

Note in this case the operators $A_1$ and $A_2$ are not compact [9] due to common elements. The min-max derivation remains valid but the stability of the solution is left for future work.

The causal reading of the simultaneous equations models is an open question since an important assumption often made in causal discovery is that the causal mechanism is acyclic, i.e., that no feedback loops are present in the system [30]. There are efforts in bridging this gap; see, for example, [31].

**Example 3, revisited (Dynamic Panel Data Model, [41])**. Panel data is a common form of econometric data; it contains observations of multiple units measured over multiple time periods. We consider the dynamic model of the following form that includes time-varying regressors, allowing us to investigate the long-run relationship between economic factors [41].

\[
Y_{it} = m(Y_{i,t-1}, X_{it}) + \alpha_i + \varepsilon_{it},
\]
\[
\mathbb{E}[\varepsilon_{it} \mid Y_{i,t-1}, X_{it}] = 0, \quad i = 1, \ldots, N, \quad t = 1, \ldots, T,
\]

where $X_{it}$ is a $p \times 1$ vector of regressors, $m$ is the unknown function of interest, $\alpha_i$’s are the unobserved individual-specific fixed effects, potentially correlated with $X_{it}$, and $\varepsilon_{it}$’s are idiosyncratic errors. $X_{it} := (X_{1t}^\top, \ldots, X_{1t}^\top)^\top$ and $Y_{i,t-1} := (Y_{i,t-1}, \ldots, Y_{i,t})^\top$ are the history of individual $i$ up to time $t$. We assume that $(Y_{it}, X_{it}, \varepsilon_{it})$ are i.i.d. along the individual dimension $i$ but may not be strictly stationary along the time dimension $t$. Clearly, for a large $t$ the conditional set $\{Y_{i,t-1}, X_{it}\}$ contains a large number of valid instruments. We do not pursue a search for an efficient choice of IVs in the paper.

To see how it relates to model [1], we consider the first-differenced model

\[
\Delta Y_{it} = m(U_{i,t-1}) - m(U_{i,t-2}) + \Delta \varepsilon_{it},
\]
\[
\mathbb{E}[\Delta \varepsilon_{it} \mid U_{i,t-2}] = 0, \quad i = 1, \ldots, N, \quad t = 3, \ldots, T, \quad (23)
\]

where $\Delta Y_{it} := Y_{it} - Y_{i,t-1}, U_{i,t-2} := [Y_{i,t-2}, X_{i,t-1}^\top]^\top$ and $\Delta \varepsilon_{it} := \varepsilon_{it} - \varepsilon_{i,t-1}$. The conditional expectation (24) is obtained by applying law of iterated expectation to (4) conditional on $U_{i,t-2}$. Model (23) cannot be solved via traditional nonparametric regression because $\Delta \varepsilon_{it}$ is generally correlated with $Y_{i,t-1}$ on the RHS of (23).

Now we cast the model (24) into a minimax problem. For ease of exposition we assume strict stationarity on the sequence $\{U_{it}\}$, which implies that the marginal distribution of $U_{i,t-1}$ and
We remark that \( g \) (CCAPM) is such an example. Here we consider a simplified setting of \([15]\) where at time \( t \) the goal is to estimate the function \( g \). The key difference between type I and type II Fredholm equations lies in stability of the solution. If \( I - K : \mathcal{H} \to \mathcal{H} \) is injective, then it is surjective, the inverse operator \((I - K)^{-1}\) is continuous and therefore the solution to type II equation is stable \([25]\).

We remark that 1 is the greatest eigenvalue of \( A \) because \((D', E')\) and \((D, E)\) are identically distributed. Therefore we assume the multiplicity of 1 is one in order to identify \( m \) up to a constant. The resulting min-max problem is

\[
\min_{m \in L^2(D', E')} \max_{u \in L^2(E, D)} \mathbb{E}[u(E, D) \cdot (F - m(D', E') + m(D, E)) - \frac{1}{2} u(E, D)^2].
\]

In the absence of the lagged term \( Y_{i,t-1} \) on the RHS of \((4)\), the model \((4)\) reduces to the nonparametric panel data model \((27)\).

If the lag term does not appear, we recover the measurement error model studied in \([9]\). Example 4 (Euler Equation and Utility, \([15]\)). In economic models, the behavior of an optimizing agent can be characterized by Euler equations \([20]\). Consumption-based capital asset pricing model (CCAPM) is such an example. Here we consider a simplified setting of \([15]\) where at time \( t \) an agent receives income \( W_t \) and purchases or sells certain units of an asset at price \( P_t \). For simplicity we assume there is only one asset on the market. Let \( U \) be the time-invariant utility function, and \( b \in (0,1) \) be the discount factor. \( U \) and \( b \) are parameters of interests known to the agent but unknown to the researchers. The stream of consumption \( \{C_t\} \) is the solution to the optimization problem

\[
\max_{\{C_t, Q_t\}_{t=0}^{\infty}} \mathbb{E} \left[ \sum_{t=0}^{\infty} \beta^t U(C_t) \right] \quad \text{s.t.} \quad C_t + P_t Q_t = P_t Q_{t-1} + W_t, \quad (26)
\]

where \( Q_t \) is the quantity of the asset owned by the agent at time \( t \). RHS of the constraint \((26)\) is the total value owned by the agent before the exchange at time \( t \), while the LHS represents the total value after the exchange. The agent manipulates his consumption, \( C_t \), and the quantity of the asset he holds, \( Q_t \), to maximize his expected long-run discounted utility.

Define \( R_t = P_{t+1}/P_t \). Using the method of Lagrange multiplier, one can obtain the optimality condition of \((25)\)

\[
\mathbb{E} \left[ R_{t+1} \beta \frac{U'(C_{t+1})}{U'(C_t)} - 1 \mid I_t \right] = 0, \quad (27)
\]

where \( I_t \) represents the information available at time \( t \). A derivation can be found in \([15]\). Let \( g = U' \) be the marginal utility function. Conditioning on \( C_t \) in \((27)\), we obtain

\[
\mathbb{E}[\beta R_{t+1} g(C_{t+1}) \mid C_t] = g(C_t). \quad (28)
\]

The goal to estimate the function \( g \) given \( \{C_t, R_{t+1}, C_{t+1}\} \). To see how our min-max derivation applies, define the operator \( A : L^2(C_t) \to L^2(C_t) \), \((Ag)(c) = \mathbb{E}[g(C_{t+1}) R_{t+1} \mid C_t = c]\). We assume \( A \) is well-defined. Then \((27)\) can be succinctly written as

\[
\beta Ag = g.
\]

We remark that \( g \) is identified up to an arbitrary sign and scale normalization; \([15]\) provides a detailed discussion on identification. Assuming \( \beta \) is known, the resulting min-max problem is

\[
\min_{g \in L^2(C_{t+1})} \max_{u \in L^2(C_t)} \mathbb{E}[\beta g(C_{t+1}) R_{t+1} u(C_t) - g(C_t) u(C_t) - \frac{1}{2} u^2(C_t)].
\]

One caveat is that \( g = 0 \) is a trivial solution to \((28)\) and therefore during the training of NNs we should avoid such a solution. The empirical performance of Algorithm 1 in this example is left for future work.
Example 5 (Proxy Variables of an Unmeasured Confounder, [29]). Consider the causal DAG in Figure 2 in the sense of Pearl [36]. Here X and Y denote the treatment and the outcome, respectively. The confounder U is unobserved, while its proxies Z and W are observed. Assume U, W, Z are continuous and in the discussion we assume X and Y are fixed at (x, y). The conditional independence encoded in Figure 2 is W ⊥⊥ (Z, X) | U and Z ⊥⊥ Y | (U, X). Using the do-operator of Pearl [36], the causal effect of X on Y is

\[ p(y|\text{do}(x)) = \int p(y|x, u)p(u)du, \]

where \( p(\cdot) \) stands for probability mass functions of a discrete variable or the probability density function for a continuous variable. However, U is unobserved so we cannot directly calculate the causal effect.

The work of Miao et al. [29] provides an identification strategy for the causal effect of X on Y with the help of the confounder proxies Z and W. Consider the solution \( h(w, x, y) \) to the following integral solution: for all (x, y) and for all z,

\[ p(y|z, x) = \int_{-\infty}^{+\infty} h(w, x, y)p(w|z, x)dw, \]  

(29)

which is a Fredholm integral equation of the first kind.

Lemma A.1 (Theorem 1 of [29]). Assume the causal DAG in Figure 2 and that a solution to (29) exists. Assume the following completeness condition: \( E[g(U)|Z, X] = 0 \) almost surely if and only if \( g(u) = 0 \) almost surely. Then \( p(y|\text{do}(x)) = \int_{-\infty}^{+\infty} h(w, x, y)p(w)dw. \)

The result suggests that one can identify the causal effect by first solving for \( h \) in (29) and then applying Lemma A.1 since \( p(y|z, x), p(w|z, x) \) and \( p(w) \) can be estimated from the data. To see how (29) fits into our framework, we note that Equation (29) implies \( E[\mathbb{1}\{Y = y\} | Z, X] = E[h(W, X, y) | Z, X] \) for all y, and thus similar min-max problem derivation goes through. However, in [29] the identification strategy is limited to the case where X and Y are categorical, and it would be interesting to see how our method performs in the setting of continuous treatment and continuous outcome.

![Causal graph of confounder proxies](image)

Figure 2: A causal graph of confounder proxies. Adapted from Figure 1(f) of [29].

B Linear approximation error of multi-layer NNs

Without assumptions on the distribution of data (Assumption A.3), we have slightly worse upper bounds on the error of linearization for multi-layer NNs.

Lemma B.1 (Error of local linearization, multi-layer, [2] [17]). Consider the multi-layer neural networks described in (10). Under Assumption A.2, with probability at least \( 1 - \exp(-\Omega(\log^2 m)) \) with respect to the random initialization, for any \( W \in S_{B, H} \) and all x such that \( ||x|| = 1 \),

1. \( |\hat{f}(x, W)| = O(BH^{1/2}\log m), \)
2. \( \|\nabla_W f(x, W)\| = O(H), \)
3. \( |f(x, W) - \hat{f}(x, W)| = O(B^{4/3}m^{-1/6}H^{3}\log^{1/2} m), \) and
4. \( \|\nabla_W f(x, W) - \nabla_W \hat{f}(x, W)\| = O(B^{1/3}m^{-1/6}H^{5/2}\log^{1/2} m). \)

Proof. See Section D.2 in Appendix D. \( \square \)
C  Bounds on the terms (18), (19) and (20)

C.1  Bounds on the terms (18), (19)

First, we establish the closeness between the original function $\phi$ and the one consisting of linearized NNs, $\hat{\phi}$. The following lemma shows that $\hat{\phi}$ is a good surrogate for $\phi$ in the sense that the approximation error is of order $O(aB^{5/2}m^{-1/4})$, which vanishes as $m \to \infty$.

Denote $F(\theta, \omega; X_1, X_2) = u_\omega f_\theta - u_\omega b - \frac{1}{2} u_\omega^2 + \frac{a}{2} f_\theta^2$. Note $\mathbb{E}_X [F(\theta, \omega; X_1, X_2)] = \phi(\theta, \omega)$.

Similarly we define $\hat{F}(\theta, \omega; X_1, X_2) = \hat{u}_\omega f_\theta - \hat{u}_\omega b - \frac{1}{2} \hat{u}_\omega^2 + \frac{a}{2} \hat{f}_\theta^2$.

Lemma C.1 (Closeness between $\hat{\phi}$ and $\phi$). Let $a = \max\{1, \alpha\}$. For any $\theta, \omega \in S_B$, we have

$$\mathbb{E}_{\text{init}} \left[ |\hat{\phi}(\theta, \omega) - \phi(\theta, \omega)| \right] = O(aB^{5/2}m^{-1/4}).$$

Proof. See Section D.4 in Appendix D. The proof relies on the decay rates of approximation error, as detailed in Lemma 5.1.

Lemma C.1 suggests it suffices to set

$$\epsilon_f = O(aB^{5/2}m^{-1/4}) + \max_{\theta} \left( \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}(\theta_t) - \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}(\theta) \right).$$

(30)

We now turn to bound the term (19) using techniques adapted from convex online learning analysis.

C.2  A bound on the term (19)

We emphasize we apply online learning analysis (Lemma C.2) to the regret associated with $\hat{\phi}_t$’s but using updates designed for $\phi_t$’s.

Lemma C.2 (Online convex learning with noisy and biased gradient). Given a sequence of convex functions on a convex space $\Theta, f_1, f_2, \cdots : \Theta \to \mathbb{R}$, consider the projected gradient descent updates

$$\theta_{t+1} = \Pi_{\Theta} \left( \theta_t - \eta (\zeta_t + \xi_t) \right),$$

(31)

where $\mathbb{E} [\zeta_t | \theta_t] = \nabla f_t (\theta_t)$, $\Pi_{\Theta}(\theta) \in \arg \max_{\theta' \in \Theta} |\theta - \theta'|$ is the projection map to $\Theta$. Assume $\sup_t \|\zeta_t + \xi_t\| < K$ a.s. and $\sup_\theta \|\theta\| < M$. Then with probability at least $1 - \delta$,

$$\frac{1}{T} \sum_{t=1}^{T} f_1(\theta_t) - \frac{1}{T} \sum_{t=1}^{T} f_1(\theta) \leq \frac{\eta K}{2} + \frac{M}{T\eta} + 8K \sqrt{\frac{M \ln(1/\delta)}{T}} + 2\sqrt{2M} \sum_{t=1}^{T} \|\xi_t\|$$

(32)

for all $\theta \in \Theta$.

Proof. See Section D.5 in Appendix D.

In order to apply Lemma C.2 to analyze the regret generated by the sequence $\{\hat{\phi}_t\}$ with actual updates being $\nabla \hat{\phi}_t(\theta_{1:t}, X_{1:t}, X_{2:t})$ instead of $\nabla \hat{\phi}_t(\theta_t)$, we need to verify two conditions: (i) bounded update steps, i.e., $\|\nabla \hat{\phi}_t(\theta_{1:t}, X_{1:t}, X_{2:t})\|$ is bounded for all $t$, and (ii) bounded parameter space.

To achieve global convergence, we also require that bias in updates, $\|\nabla \hat{\phi}_t(\theta_{1:t}, X_{1:t}, X_{2:t}) - \nabla \hat{\phi}_t(\theta_t)\|$, which corresponds to the $\|\xi_t\|$ term in (32), converges to zero as $m \to \infty$. In our analysis we assume $\nabla \hat{\phi}_t(\theta_{1:t}, X_{1:t}, X_{2:t})$ is an unbiased estimate of $\nabla \hat{\phi}_t(\theta_t)$. The following lemma summarizes the results we need to apply Lemma C.2 and obtain a bound on the term (19).

Lemma C.3 (Bounded gradient and vanishing bias). Consider the updates in algorithm (Algorithm 1). For all $\omega, \theta$, the following holds.

1. $\|\nabla \hat{\phi}_t(\theta_{1:t}, X_{1:t}, X_{2:t})\| = O(aB)$ for all $x, y$, and

2. $\mathbb{E}_{\text{init}, X} \left[ \|\nabla \hat{\phi}_t(\theta_{1:t}, X_{1:t}, X_{2:t}) - \nabla \hat{\phi}_t(\theta_{1:t}, X_{1:t}, X_{2:t})\| \right] = O(aB^{3/2}m^{-1/4})$. 

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Proof. See Section D.6 in Appendix D.

Equipped with Lemma C.1 and Lemma C.2 we are now ready to obtain a bound on the regret $\epsilon_f$ defined in (17). Set $M = B$, $K = aB$. $\|\epsilon_f\| = O(aB^{3/2}m^{-1/4})$ in the RHS of (32), continue (30), and we obtain with probability at least $1 - \delta$ with respect to sampling process,

$$
\mathbb{E}_{\text{init}}[\epsilon_f] = \mathcal{O}(aB^{5/2}m^{-1/4}) + \mathcal{O}\left(\frac{anB}{2} + \frac{B}{T\eta} + \frac{aB^{3/2}\log^{1/2}(1/\delta)}{T^{1/2}} + \frac{aB^4}{m^{1/4}}\right).
$$

It can be shown $\epsilon_u$ is of the same order, thus completing the proof of claim 1 in Theorem 4.1.

D. Proof of theorems

A remark on notations. Throughout the proof we ignore dependence on $\theta, \omega, X_1, X_2$ and the NN initial parameters $\Xi_0$ or $\Xi_{H,0}$ defined in (3) and (10), respectively. For readers’ convenience, we now restate the dependence of all the functions on their parameters. Recall the NN $f_{\theta}(X_1) = f(\theta; X_1)$ is an NN with weights $\theta$ and input $X_1$ and similarly for $u_\omega(X_2) = u(\omega; X_2)$. Note $f_{\theta}$ and $u_\omega$ depend on the initialization implicitly through the range of NN weights (which is centered around the initial weight) and the output layer weights (and the input layer weight, too, in the case of multi-layer NNs). Recall

$$
\phi = \phi(\theta, \omega) = \phi(f_{\theta}, u_\omega) := \mathbb{E}\left[(f(\theta; X_1) - b(X_2))u(\omega; X_2) + \frac{1}{2}f(\theta; X_1)^2 - \frac{1}{2}u(\omega; X_2)^2\right],
$$

and

$$
F = F(\theta, \omega; X_1, X_2) = (f(\theta; X_1) - b(x_2))u(\omega; X_2) + \frac{1}{2}f(\theta; X_1)^2 - \frac{1}{2}u(\omega; X_2)^2,
$$

and they satisfy $\phi(\theta, \omega) = \mathbb{E}_{X_1,X_2}[F(\theta, \omega; X_1, X_2)]$. Note $\phi$ is convex-concave in $(f, u)$ but not in $(\theta, \omega)$. Recall the linearized counterparts of $f$ and $u$, defined in (16), are $\hat{f}_\theta = \hat{f}(\theta(0); X_1) = \langle \nabla_\theta f(\theta(0), X_1), \theta - \theta(0) \rangle$ and similarly for $\hat{u}_\omega$. Now we replace NNs $f_{\theta}$ and $u_\omega$ by their hat-versions in the definition of $\phi$ and $F$ and obtain $\hat{\phi} = \hat{\phi}(\theta, \omega, \Xi_0)$, and $\hat{F} = \hat{F}(\theta, \omega, \Xi_0; X_1, X_2)$. In the proof we only discuss the case where $b = b(X_2)$ is known. The proof goes thorough for the more general case $b(X_2) = \mathbb{E}[b(X_1, X_2) | X_2]$ with little modifications.

D.1 Proof of Lemma 5.1

Proof. The proof follows closely Lemma 5.1 and Lemma 5.2 in [8]. Recall that the weights of a 2-layer NN is represented by $W \in \mathbb{R}^{md}$ where $d$ is the input dimension and $m$ is the number of neurons. $W_r \in \mathbb{R}^d$ represents the weights connecting inputs and the $r$-th neuron. $W = [W_1, \ldots, W_r]^T$.

We start with

$$
||\nabla_W f(x; W)||_2^2 \leq \frac{1}{m} \sum_{r=1}^m \mathbb{I} \{W_r^T x > 0\} ||x||_2^2 \leq 1
$$

for all $W \in S_B$, all $x$. So claim 2 follows. Claim 1 is indeed true because $f(x, W)$ is 1-Lipschitz wrt $W$ and that $||W - W(0)||_2 \leq B$ for all $W \in S_B$. To show claim 3 we first analyze the expression $|f(x, W) - \hat{f}(x, W)|$,

$$
|f(x, W) - \hat{f}(x, W)|
$$

$$
\leq \frac{1}{m} \sum_{r=1}^m \mathbb{I} \{W_r^T x > 0\} \cdot b_r W_r^T x
$$

$$
\leq \frac{1}{m} \sum_{r=1}^m \mathbb{I} \{W_r^T x > 0\} \cdot \mathbb{I} \{W_r(0)^T x > 0\} \cdot (||W_r(0)^T x|| + ||W_r - W_r(0)||_2)
$$

$$
\leq \frac{1}{m} \sum_{r=1}^m \mathbb{I} \{W_r(0)^T x \leq ||W_r - W_r(0)||_2\} \cdot (||W_r(0)^T x|| + ||W_r - W_r(0)||_2)
$$

$$
\leq \frac{2}{m} \sum_{r=1}^m \mathbb{I} \{W_r(0)^T x \leq ||W_r - W_r(0)||_2\} \cdot ||W_r - W_r(0)||_2.
$$

(33)
Here the first inequality follows from $\|x\|_2 = 1$. The second inequality follows from the following reasoning.

\[ \mathbb{1} \{ W_r^T x > 0 \} \neq \mathbb{1} \{ W_r(0)^T x > 0 \} \]

\[ \implies |W_r(0)^T x| \leq |W_r^T x - W_r(0)^T x| \leq \|W_r - W_r(0)\|_2. \]

The third inequality follows from $\mathbb{1} \{|x| \leq y\} |x| \leq \mathbb{1} \{|x| \leq y\} y$ for all $x, y > 0$.

Next we take squares of both sides of (35), invoke Cauchy-Schwartz inequality, and the fact that $\|W - W(0)\|_2 \leq B$. 

\[
|f(x, W) - \hat{f}(x, W)|^2 \leq \frac{4B^2}{m} \sum_{r=1}^{m} \mathbb{1} \{ |W_r(0)^T x| \leq \|W_r - W_r(0)\|_2 \}. \tag{34}
\]

To control the expectation of the RHS of (34), we introduce the following lemma.

**Lemma D.1.** There exists a constant $c_1 > 0$, such that for any random vector $W$ such that $\|W - W(0)\|_2 \leq B$, it holds that

\[
E_{\text{init}, x} \left[ \frac{1}{m} \sum_{r=1}^{m} \mathbb{1} \{ |W_r(0)^T x| \leq \|W_r - W_r(0)\|_2 \} \right] \leq c_1 B \cdot m^{-1/2}.
\]

Taking expectation on both sides of (34) we get

\[
E_{\text{init}, x} \left[ |f(x, W) - \hat{f}(x, W)|^2 \right] \leq 4c_1 B^3 \cdot m^{-1/2},
\]

establishing claim 3. Claim 4 also follows from Lemma D.1 as follows.

\[
\|\nabla_W f(x, W) - \nabla_W \hat{f}(x, W)\|^2
\]

\[ = \frac{1}{m} \sum_{r=1}^{m} \left( \left\{ W_r^T x > 0 \right\} - \left\{ W_r(0)^T x > 0 \right\} \right)^2 \cdot \|x\|^2 \]

\[ \leq \frac{1}{m} \sum_{r=1}^{m} \left\{ W_r(0)^T x \right\} \leq \|W_r - W_r(0)\|_2. \]

**Proof of Lemma D.1**

**Proof.** The proof follows Lemma H.1 of [3] and is stated for completeness. By the assumption that there exists $c_0 > 0$, for any unit vector $v \in \mathbb{R}^d$ and any constant $\zeta > 0$, such that $\mathbb{P}_X(|v^T X| \leq \zeta) \leq c_\zeta$, we have

\[
E_{\text{init}, x} \left[ \frac{1}{m} \sum_{r=1}^{m} \mathbb{1} \{ |W_r(0)^T x| \leq \|W_r - W_r(0)\|_2 \} \right]
\]

\[ \leq E_{\text{init}} \left[ \frac{1}{m} \sum_{r=1}^{m} c_0 \cdot \frac{\|W_r - W_r(0)\|_2}{\|W_r(0)\|_2} \right]. \tag{35}
\]

Note the expectation in (35) does not involve the data distribution. Next we apply Hölder’s inequality.

\[
E_{\text{init}, x} \left[ \frac{1}{m} \sum_{r=1}^{m} \mathbb{1} \{ |W_r(0)^T x| \leq \|W_r - W_r(0)\|_2 \} \right]
\]

\[ \leq \frac{c_0}{m} \cdot \mathbb{E}_{\text{init}} \left[ \left( \sum_{r=1}^{m} \frac{\|W_r - W_r(0)\|_2^2}{\|W_r(0)\|_2^2} \right)^{1/2} \cdot \left( \sum_{r=1}^{m} \frac{1}{\|W_r(0)\|_2^2} \right)^{1/2} \right]
\]

\[ \leq c_0 B m^{-1} \cdot \mathbb{E}_{\text{init}} \left[ \sum_{r=1}^{m} \frac{1}{\|W_r(0)\|_2^2} \right]^{1/2}
\]

\[ \leq c_0 B m^{-1} \cdot \sqrt{m} \cdot \mathbb{E}_{W \sim N(0, I_d/d)} \left[ 1/\|w\|_2^2 \right]^{1/2}. \]

Setting $c_1 = c_0 \cdot \mathbb{E}_{W \sim N(0, I_d/d)} \left[ 1/\|w\|_2^2 \right]^{1/2}$ finishes the proof. \qed
D.2 Proof of Lemma F.1

Proof. See [3,17] for a detailed proof. Also see Appendix F in [8]. In detail, claim 1 follows from equation F.10 of [8]. Claim 2 and claim 4 follow from Lemma F.1 of [8]. Claim 3 follows from Lemma F.2 of [8].

D.3 Proof of Lemma F.2

Proof. Recall \( \phi(f, u) \) is convex in \( f \) and concave in \( u \), and that \( L(f) \) is convex in \( f \). The final output \( \bar{f}_T \) is the average of the sequence \( \{f_t\}_{t=1}^T \) and so is \( \bar{u}_T \). Recall \( \epsilon_f, \epsilon_u \) satisfy

\[
\frac{1}{T} \sum_{t=1}^{T} \phi(f_t, u_t) \leq \min_f \frac{1}{T} \sum_{t=1}^{T} \phi(f, u_t) + \epsilon_f,
\]

\[
\frac{1}{T} \sum_{t=1}^{T} \phi(f_t, u_t) \geq \max_u \frac{1}{T} \sum_{t=1}^{T} \phi(f_t, u) - \epsilon_u.
\]

Note both \( f \) and \( u \) range over the space of NNs. We start with the equivalent expression for \( L \) defined in [7]. Note \( L(f) = \max_u \phi(f, u) \) with \( \phi \) defined in [8]. We have

\[
L(\bar{f}_T) - L^* \leq \max_u \phi(\bar{f}_T, u) - \min_u \phi(f, \bar{u}_T) \leq \max_u \left[ \frac{1}{T} \sum_{t=1}^{T} \phi(f_t, u_t) - \min_f \frac{1}{T} \sum_{t=1}^{T} \phi(f_t, u_t) \right]
\]

\[
\leq \epsilon_f + \epsilon_u.
\]

In fact, we easily have \( \frac{1}{T} \sum_{t=1}^{T} L(f_t) - L^* \leq \epsilon_f + \epsilon_u \).

D.4 Proof of Lemma C.1

Proof. Recall \( X = [X_1^+, X_2^+]^\top, \phi(\theta, \omega) = \mathbb{E}_X[F(\theta, \omega; X_1, X_2)] = \mathbb{E}_{XY}[uf - ub - (1/2)u^2 + (\alpha/2)f^2] \).

Denote \( \hat{F}(\theta, \omega) = \hat{u}\hat{f} - \hat{u}b - (1/2)\hat{u}^2 + (\alpha/2)\hat{f}^2 \), where the hat-version are the linearized NN. We start by noting

\[
\mathbb{E}_{\text{init}}[|\hat{\phi}(\theta, \omega) - \phi(\theta, \omega)|] = \mathbb{E}_{\text{init},X}[|\hat{F} - F|] \leq \mathbb{E}_{\text{init},X}[|\hat{u}\hat{f} - \hat{u}b|] + (1/2)\mathbb{E}_{\text{init},X}[|u^2 - \hat{u}^2|] + (\alpha/2)|\mathbb{E}_{\text{init},X}[f^2 - \hat{f}^2]|.
\]

Now bound the terms

\[
\mathbb{E}_{\text{init},X}[|\hat{u}\hat{f} - uf|], \quad \mathbb{E}_{\text{init},X}[|\hat{u} - u|b], \quad \mathbb{E}_{\text{init},X}[|u^2 - \hat{u}^2|], \quad \mathbb{E}_{\text{init},X}[|f^2 - \hat{f}^2|].
\]
For the term (36), we have
\[
E_{\text{init},XY} \left[ \| \hat{u} f - uf \| \right] \\
\leq E_{\text{init},XY} \left[ \| \hat{u} (\hat{f} - f) \| \right] + E_{\text{init},X} \left[ \| \hat{u} - u \| f \right] \\
\leq \sqrt{E_{\text{init},XY} \left[ \hat{u}^2 \right] E_{\text{init},X} \left[ \| \hat{f} - f \|^2 \right]} + \sqrt{E_{\text{init},XY}\left[ f^2 \right] E_{\text{init},X} \left[ \| \hat{u} - u \|^2 \right]}
\]
(Cauchy-Schwarz inequality)
\[
= \sqrt{O(B^2 \cdot B^3 m^{-1/2})} + \sqrt{O(B^3 m^{-1/2}) \cdot O(B^2)}
\]
= \( O(B^{5/2} m^{-1/4}) \).

We can apply similar techniques and obtain the following bounds on (37) and (39),
\[
E_{\text{init},X} \left[ \| \hat{u} - u \| b \right] = O(B^{3/2} m^{-1/2}),
\]
\[
E_{\text{init},X} \left[ \| \hat{u}^2 - u^2 \| \right] = O(B^{5/2} m^{-1/4}).
\]

Putting all pieces together we get
\[
E_{\text{init}} \left[ \| \hat{\phi} (\theta, \omega) - \phi (\theta, \omega) \| \right] = O((1 + \alpha) B^{5/2} m^{-1/4}).
\]

\[\]

\subsection*{D.5 Proof of Lemma \ref{lem:regret}}

\textbf{Proof}. We need the following lemma that controls regret in the context of online learning with exact gradient, and then we extend it to our noisy and biased gradient scenario.

\textbf{Lemma D.2 (Regret analysis in online learning. \cite{40})}. Let \( f_1, f_2, \ldots : \Theta \to \mathbb{R} \) be convex functions, where \( \Theta \) is convex. Consider the mirror descent updates,
\[
\zeta_{t+1} = \nabla h^* (\nabla h (\theta_t) - \eta \nabla f_t (\theta_t)),
\]
\[
\theta_{t+1} = \arg \min_{\theta \in \Theta} D_h (\theta, \zeta_{t+1}),
\]
where \( h \) is 1-strongly convex with respect to the norm \( \| \cdot \|, D_h (x, y) = h(x) - h(y) - \nabla h(y)^T (x - y) \) is the Bregman divergence, \( h^* \) is the convex conjugate of \( h \), and \( \| \cdot \|_u \) is the dual norm of \( \| \cdot \| \). Suppose that \( \sup_{t} \| \nabla f_t (\theta_t) \|_u < K \) and \( \sup_{\theta \in \Theta} h(\theta) < M \). Then for all \( \theta \in \Theta \),
\[
\frac{1}{T} \sum_{t=1}^{T} f_t (\theta_t) - \frac{1}{T} \sum_{t=1}^{T} f_t (\theta) \leq \frac{\eta K}{2} + \frac{M}{T \eta}.
\]

We refer readers to \cite{40} for a proof of Lemma D.2. Now we take \( h(x) = \frac{1}{2} \| x \| \), and \( \| x \| \) is the Euclidean norm.

Note that in our case the actual update is \( \zeta_t + \xi_t \), where \( \zeta_t \) is an unbiased estimate of the gradient \( \nabla f_t (\theta_t) \), and \( \xi_t \) is a noise term. We construct linear surrogate functions \( \tilde{f}_t (\theta) = f_t (\theta_t) + (\zeta_t + \xi_t)^T (\theta - \theta_t) \) and notice that \( \zeta_t + \xi_t \) is indeed the gradient of the surrogate at \( \theta_t \), i.e.,
\[
\nabla \tilde{f}_t (\theta_t) = \zeta_t + \xi_t.
\]
Now we apply Lemma D.2 to the sequence \( \{ \tilde{f}_t \} \) and obtain
\[
\frac{1}{T} \sum_{t=1}^{T} \tilde{f}_t (\theta_t) - \frac{1}{T} \sum_{t=1}^{T} \tilde{f}_t (\theta) \leq \frac{\eta B}{2} + \frac{M}{T \eta},
\]
which implies
\[
\frac{1}{T} \sum_{t=1}^{T} f_t (\theta_t) - \frac{1}{T} \sum_{t=1}^{T} f_t (\theta) \\
\leq \frac{\eta B}{2} + \frac{M}{T \eta} + \frac{1}{T} \sum_{t=1}^{T} \tilde{f}_t (\theta_t) - \frac{1}{T} \sum_{t=1}^{T} f_t (\theta) \\
\leq \frac{\eta B}{2} + \frac{M}{T \eta} + \frac{1}{T} \sum_{t=1}^{T} (\zeta_t - \nabla f_t (\theta_t))^T (\theta - \theta_t) + \frac{1}{T} \sum_{t=1}^{T} \xi_t^T (\theta - \theta_t).
\]
Theorem 4.1. The bound (40) implies that in terms of choosing the final output it suffices to just pick 

Now we bound the term \( \sum_{t=1}^{T} (\zeta_t - \nabla f_t (\theta_t)) (\theta - \theta_t) \). We note the boundedness of the quantities

\[
(\zeta_t - \nabla f_t (\theta_t))^T (\theta - \theta_t) \leq \| \zeta_t - \nabla f_t (\theta_t) \| 2\sqrt{2M} \leq 4B\sqrt{2M}.
\]

To control the sum of bounded random variables, we invoke Hoeffding-Azuma inequality, and obtain

\[
P \left\{ \frac{1}{T} \sum_{t=1}^{T} (\zeta_t - \nabla f_t (\theta_t))^T (\theta - \theta_t) \geq 8B \sqrt{\frac{M \log (1/\delta)}{T}} \right\} \leq \delta.
\]

Finally we have \( \zeta_t^T (\theta - \theta_t) \leq \| \zeta_t \| 2\sqrt{2M} \). Putting all the pieces together completes the proof. \( \square \)

D.6 Proof of Lemma 5.1

Proof. The gradients of \( F \) with respect to \( \omega, \theta \) are

\[
\nabla_\theta F = (u_\omega + \alpha f_\theta) \nabla \theta f, \\
\nabla_\omega F = (f_\theta - b - u_\omega) \nabla \omega u.
\]

First we show for all \( x_1, x_2, \omega \) and \( \theta \), we have that \( \nabla \theta F \) is bounded. It is easy to see by Lemma 5.1

\[
\| \nabla_\theta F \|_2 = O((1 + \alpha) B).
\]

Next we show that for all \( \theta, \omega \), \( \mathbb{E}_{\text{init}, X} \left[ \| \nabla_{\theta} F - \nabla_{\theta} \bar{F} \| \right] \) goes to zero as \( m \to \infty \).

\[
\mathbb{E}_{\text{init}, X} \left[ \| \nabla_{\theta} F - \nabla_{\theta} \bar{F} \| \right] \\
\leq \sqrt{\mathbb{E}_{\text{init}, X} \left[ \| \nabla_{\theta} F \|^2 \right] \mathbb{E}_{\text{init}, X} \left[ (u - \hat{u})^2 \right] } \\
+ \sqrt{\mathbb{E}_{\text{init}, X} \left[ \| \nabla_{\theta} \bar{F} - \nabla_{\theta} f \|^2 \right] \mathbb{E}_{\text{init}, X} \left[ \hat{u}^2 \right] } \\
+ \alpha \sqrt{\mathbb{E}_{\text{init}, X} \left[ \| \nabla_{\theta} \bar{F} \|^2 \right] \mathbb{E}_{\text{init}, X} \left[ (f - \hat{f})^2 \right] } \\
+ \alpha \sqrt{\mathbb{E}_{\text{init}, X} \left[ \| \nabla_{\theta} f \|^2 \right] \mathbb{E}_{\text{init}, X} \left[ \hat{f}^2 \right] } \\
= O((1 + \alpha) B^{3/2} m^{-1/4})
\]

\( \square \)

D.7 Proof of Theorem 4.1

Remark. In fact, the two bounds in Theorem 4.1 are also valid bounds on \( \mathbb{E}_{\text{init}} \left[ \frac{1}{T} \sum_{t=1}^{T} E(f_t) \right] \) and \( \frac{1}{T} \sum_{t=1}^{T} E(f_t) \), respectively. For example, in the 2-layer NN case, it also holds that

\[
\mathbb{E}_{\text{init}} \left[ \frac{1}{T} \sum_{t=1}^{T} E(f_t) \right] = O \left( \frac{b}{T} + \frac{B3/2 \log (1/\delta)}{T^{1/2}} + \frac{aB5/2}{m^{1/4}} \right), \tag{40}
\]

During training we obtain a sequence of NN weights \( \theta_1, \theta_2, \ldots, \theta_T \) and the corresponding NNs \( f_1, f_2, \ldots, f_T \). The difference lies in that in \( \text{40} \) we bound the average of the suboptimality of the NNs \( f_1, f_2, \ldots, f_T \) rather than the suboptimality of the averaged NN \( \bar{f}_T = \frac{1}{T} \sum_{t=1}^{T} f_t \), as is done in Theorem 4.1. The bound \( \text{40} \) implies that in terms of choosing the final output it suffices to just pick one NN from the sequence of NNs \( f_1, f_2, \ldots, f_T \).

Proof of Theorem 4.1 two-layer NN

Proof. Based on the analysis in Appendix C, all we need to do is to estimate the rate of the following quantities

1. \( \mathbb{E}_{\text{init}} \left[ | \hat{\phi} (\theta) - \phi (\theta) | \right] = O((1 + \alpha) B^{5/2} m^{-1/4}) \),

\[ \]
2. sup |\theta| = O(B), |\nabla_\theta F| = O((1 + \alpha)B),
3. sup |\omega| = O(B), |\nabla_\omega F| = O(B),
4. E_{\text{init}, X} [||\nabla_\theta F - \nabla_\theta \hat{F}||] = O((1 + \alpha)B^{3/2}m^{-1/4}), and
5. E_{\text{init}, X} [||\nabla_\omega F - \nabla_\omega \hat{F}||] = O(B^{3/2}m^{-1/4}).

The missing pieces are

- \|\nabla_\theta F\| is bounded, and
- E_{\text{init}, X} [||\nabla_\omega F - \nabla_\omega \hat{F}||] = O(B^{3/2}m^{-1/4}).

First we bound the term \|\nabla_\omega F\|. It is easy to see

\[ \|\nabla_\omega F\| = O(B). \]

Then we show E_{\text{init}, X} [||\nabla_\omega F - \nabla_\omega \hat{F}||] = O(B^{3/2}m^{-1/4})

\[
E_{\text{init}, X} [||\nabla_\omega F - \nabla_\omega \hat{F}||] \\
\leq \sqrt{E_{\text{init}, X} [||f - b - u||^2] E_{\text{init}, X} [||\nabla_\omega \hat{u} - \nabla_\omega u||^2]} \\
+ \sqrt{E_{\text{init}, X} [||(f - \hat{f}) + (u - \hat{u})||^2] E_{\text{init}, X} [||\nabla_\omega \hat{u}||^2]} \\
= O(B^{3/2}m^{-1/4}) \tag{Cauchy-Schwarz inequality}
\]

Proof of Theorem 4.1, multi-layer NN

Proof. We mimic the same proof technique as the two-layer case. We need to verify with probability at least 1 − exp(Ω(log^2 m)) over the NN initialization,

1. |\hat{\phi}(\theta, \omega) - \phi(\theta, \omega)| = O((1 + \alpha)B^{8/3}H^6m^{-1/6} log^{3/2} m), for all \theta, \omega \in S_{B,H},
2. sup |\theta|_2 = H^{1/2}B, ||\nabla_\theta F|| = O((1 + \alpha)B^{4/3}H^4 \log m) for all \theta, \omega \in S_{B,H} and x_1, x_2,
3. sup |\omega|_2 = H^{1/2}B, ||\nabla_\omega F|| = O(B^{3/2}H^4 \log m), for all \theta, \omega \in S_{B,H} and x_1, x_2,
4. E_X [||\nabla_\theta F - \nabla_\theta \hat{F}||] = O(B^{4/3}H^4m^{-1/6} log^{3/2} m), for all \theta, \omega \in S_{B,H}, and
5. E_X [||\nabla_\omega F - \nabla_\omega \hat{F}||] = O((1 + \alpha)B^{4/3}H^4m^{-1/6} log^{3/2} m) for all \theta, \omega \in S_{B,H}.

To show claim 1, we need to find high probability bounds of the terms

- |\hat{u} - u|,
- |(\hat{u} - u)b|,
- |\hat{u}^2 - u^2|,
- |\hat{f}^2 - f^2|.

(41) (42) (43) (44)
For the term (41),
\[|\hat{\alpha} \hat{f} - u f| \]
\[\leq |\hat{\alpha}(\hat{f} - f)| + |(\hat{\alpha} - u) f|\]
\[\leq \sqrt{\hat{\alpha}^2 |\hat{f} - f|^2 + |f|^2 |\hat{\alpha} - u|^2} \quad \text{(Cauchy-Schwarz inequality)}\]
\[= \sqrt{\mathcal{O}(B^2 H^3 \log^2 m \cdot B^{8/3} H^6 m^{-1/3} \log m)} \]
\[+ \sqrt{\mathcal{O}(B^{8/3} H^6 m^{-1/3} \log m) \cdot \mathcal{O}(B^2 H^3)} \quad \text{(45)}\]
\[= \mathcal{O}(B^{7/3} H^{9/2} m^{-1/6} \log^{3/2} m),\]
where equality (45) is valid with probability at least \(1 - \exp(\Omega(\log^2 m))\). Similarly we have the following high probability bounds.
\[|(\hat{\alpha} - u)b| = \mathcal{O}(B^{4/3} m^{-1/6} H^3 \log^{1/2} m),\]
\[|\hat{\alpha}^2 - u^2| = \mathcal{O}(B^{8/3} m^{-1/6} H^6 \log^{3/2} m).\]

Putting all the pieces together completes the proof of claim 1.

For claim 2, \(\|W - W(0)\|_2 \leq \sqrt{H} B\) implies \(\|\theta\|_2 \leq H^{1/2} B\). For \(\|\nabla_\theta F\|_2\),
\[
\|\nabla_\theta F\|_2 = \|u + \alpha f\| \nabla_\theta F\|_2 \]
\[= \mathcal{O}((1 + \alpha)B^{4/3} H^4 \log m).\]

This completes proof of claim 2. Claim 3 follows similarly. For claim 4,
\[
\|\nabla_\omega F - \nabla_\omega \hat{F}\|_2 \]
\[= \|(f - b - u) \nabla_\omega u - (\hat{f} - b - \hat{\alpha}) \nabla_\omega \hat{u}\|_2 \]
\[\leq \sqrt{|\hat{f} - b - \hat{\alpha}|^2 \|\nabla_\omega \hat{u} - \nabla_\omega u\|^2} \]
\[+ \sqrt{|(f - \hat{f}) + (u - \hat{\alpha})|^2 \|\nabla_\omega u\|^2} \]
\[= \mathcal{O}(B^{4/3} H^4 m^{-1/6} \log^{3/2} m)\]

where the last equality holds with high probability. Recall the decomposition (21),
\[
\frac{1}{T} \sum_{t=1}^{T} \phi_t(\theta_t) - \frac{1}{T} \sum_{t=1}^{T} \phi_t(\theta) \quad \text{(21 revisited)}
\]
\[= \frac{1}{T} \sum_{t=1}^{T} \phi_t(\theta_t) - \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta_t) + \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta_t) - \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta) + \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta) - \frac{1}{T} \sum_{t=1}^{T} \phi_t(\theta).\]

Define the events
\[E_1 = \left\{ \frac{1}{T} \sum_{t=1}^{T} \phi_t(\theta_t) - \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta_t) + \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta_t) - \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta) + \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta) - \frac{1}{T} \sum_{t=1}^{T} \phi_t(\theta) \right\} \]
\[= \mathcal{O}((1 + \alpha)B^{8/3} H^6 m^{-1/6} \log^{3/2} m)\]

and
\[E_2 = \left\{ \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta_t) - \frac{1}{T} \sum_{t=1}^{T} \hat{\phi}_t(\theta) \right\} \]
\[= \mathcal{O}(P_1 \eta a \log m + \frac{P_2}{T \eta} + \frac{a P_1 \log m \log^{1/2}(1/\delta)}{T^{1/2}} + \frac{P_3 a \log^{3/2} m}{m^{1/6}})\]
where \( P_1 = H^1 B^{4/3}, P_2 = H^1 B^2 \) and \( P_3 = H^2 B^2 \), defined in Theorem 4.1. By claim 1 we have \( \mathbb{P}(E_1) \geq 1 - \exp(\Omega(\log^2 m)) \). By claim 2, claim 5 and Lemma C.2 we have \( \mathbb{P}(E_2) \geq 1 - \delta - \exp(\Omega(\log^2 m)) \). Then \( \mathbb{P}(E_1 \cap E_2) \geq 1 - c\delta - c\exp(\Omega(\log^2 m)) \) for some absolute constant \( c \). The same analysis applies for \( \omega \) and therefore we complete the proof. □

D.8 Proof of Theorem 4.2

The proof relies on the following lemma that controls the regularization bias by imposing smoothness assumption on the truth.

Lemma D.3 (Hilbert scale and regularization bias). Assume the operator \( A \) in (1) is injective and compact. Let \( f^* = \arg\min_{f \in \mathcal{H}} \frac{1}{2} \| Af - b \|_E^2 + \frac{\alpha}{2} \| f \|_H^2 \) for some \( \alpha > 0 \). If the solution \( f \) to (1) lies in the regularity space \( \Phi_\beta \) defined in (14) for some \( \beta > 0 \), then

\[
\| f - f^* \|_H^2 = O(\alpha^\min(\beta, 2)).
\]

Proof. See Section 3.3 of [9]. □

Compactness of a conditional expectation operator is a mild condition; see Appendix E for a discussion.

We remark that four quantities are involved in this proof: the truth \( f \) that uniquely solves \( Af = b \), the Tikhonov regularized solution \( f^\alpha \) defined in (5), the Tikhonov regularized solution approximated by the class of NNs (see Equation (7)), denoted \( f_{NN}^\alpha \), and the average of the iterates generated by Algorithm 1. Lemma D.3 provides a bound on the gap between \( f \) and \( f^\alpha \); Theorem 4.1 controls \( f_{NN}^\alpha - f_{NN} \). Theorem 4.2 assumes that \( f_{NN}^\alpha = f^\alpha \).

We start with the decomposition of \( \| f_{NN} - f \|_H^2 = \| f_{NN} - f \|_H^2 + \| f - f^\alpha \|_H^2 + \| f^\alpha - f \|_H^2 \).

Here the first term on the RHS represents optimization error and the second term is regularization bias. Lemma D.3 provides a bound on the second term. Now we bound the first term.

Recall the definition of Tikhonov regularized functional for a compact linear operator \( A \)

\[
L(f) = L_\alpha(f) = \frac{1}{2} \| Af - b \|_E^2 + \frac{\alpha}{2} \| f \|_H^2.
\]

Denote by \( f^\alpha \) the unique minimizer of \( L \) over \( \mathcal{H} \). This is always well-defined for a compact linear operator \( A \). We want to show the strong convexity of \( L_\alpha \), i.e.,

\[
\frac{\alpha}{2} \| f_{NN} - f^\alpha \|_H^2 \leq L_\alpha(f_{NN}) - L_\alpha(f^\alpha).
\] (46)

If (46) is true, under the conditions of Theorem 4.1 (2-layer NN case), we have with probability at least \( 1 - \delta \) over the sampling process,

\[
\mathbb{E}_{init}[\| f_{NN} - f^\alpha \|_H^2] \leq \frac{2}{\alpha} \mathbb{E}_{init}[L_\alpha(f_{NN}) - L_\alpha(f^\alpha)]
\]

\[
= \frac{2}{\alpha} \mathbb{E}_{init} \left( \frac{a B^3}{T^{1/2}} \log^{1/2}(1/\delta) + \frac{a B^{5/2}}{m^{1/4}} \right).
\] (48)

Setting \( \eta = (aT)^{-1/2} \) where \( a = \max\{\alpha, 1\} \), and combining results from Lemma D.3 and (48) we complete the proof.

Now we show (46). For all \( x \in \mathcal{H}, x + h \in \mathcal{H}, \)

\[
2L_\alpha(x + h) = \| A(x + h) - b \|_E^2 + \alpha \| x + h \|_H^2
\]

\[
= \| Ax - b \|_E^2 + \| Ah \|_H^2 + \langle Ax - b, Ah \rangle_H + \alpha \| x \|_H^2 + \alpha \| h \|_H^2 + 2\alpha \langle x, h \rangle_H
\]

\[
= 2L_\alpha(x) + 2\alpha \langle x, h \rangle_H + \alpha \| x \|_H^2 + \alpha \| h \|_H^2
\]

\[
= 2L_\alpha(x) + 2\alpha \langle x, h \rangle_H + \alpha \| x \|_H^2 + \alpha \| h \|_H^2
\]

Moreover, the regularized solution \( f^\alpha \) is given by the unique solution to the equation \( \alpha f^\alpha + A^* Af^\alpha = A^* b \) and depends continuously on \( b \) [25]. Setting \( x = f^\alpha, h = f - f^\alpha \) and applying \( \alpha f^\alpha + A^* Af^\alpha = A^* b \) complete the proof of (46).
E  Compactness of conditional expectation operators

Let \( X = [X_1^T, X_2^T]^T \) be a random vector with distribution \( F_X \) and let \( F_{X_1}, F_{X_2} \) be the marginal distributions of \( X_1 \) and \( X_2 \), respectively. Assume there is no common elements in \( X_1 \) and \( X_2 \). Define Hilbert spaces \( \mathcal{H} = L^2(X_1) \) and \( \mathcal{E} = L^2(X_2) \). Let \( A \) be the conditional expectation operator:

\[
A : \mathcal{H} \to \mathcal{E}
\]

\[
f(\cdot) \to \mathbb{E}[f(X_1) \mid X_2 = \cdot].
\]

If there is no common elements in \( X_1 \) and \( X_2 \), compactness of an conditional expectation operator is in fact a mild condition \([2]\). If p.d.f.s of \( X, X_1 \) and \( X_2 \) exist, denoted \( f_X, f_{X_1}, \) and \( f_{X_2} \), then \( A \) can be represented as an integral operator with kernel

\[
k(x_1, x_2) = \frac{f_{X_1, X_2}(x_1, x_2)}{f_{X_1}(x_1)f_{X_2}(x_2)},
\]

and \((Af)(x_2) = \int k(x_1, x_2)f(x_1)dx_2\). In this case, a sufficient condition for compactness of \( A \) is

\[
\int \left( \int f_{X_2}(x_2)dx_2 \right)^2 f_{X_1}(x_1)f_{X_2}(x_2)dx_1dx_2 < \infty.
\]

We now discuss well-posedness of \((1)\). The operator equation \((1)\) is called well-posed (in Hadamard’s sense) if (i) \((existence)\) a solution \( f \) exists, (ii) \((uniqueness)\) the solution \( f \) is unique, and (iii) \((stability)\) the solution \( f \) is continuous as a function of \( b \). More precisely, if \( A : \mathcal{H} \to \mathcal{E} \) is bijective and the inverse operator \( A^{-1} \) is continuous, then equation \((1)\) is well-posed \([25]\). Injectivity is usually a property of the data distribution and is tantamount to assuming identifiability of the structural function.

F  A comment on Dual IV

In this section, we review the work of Dual IV \([31]\) and point out the differences between their work and ours. Dual IV considers nonparametric IV estimation using min-max game formulation and bears similarities with this work. However, we remark that our framework \((1)\) includes a wide range of models, including IV regression, and that the use of NNs and detailed analysis on the convergence of the training algorithm also distinguish our work from Dual IV. The goal of this section is to show the resulting min-max problem for IV regression in this paper has a natural connection with GMM.

Recall that IV regression considers the following conditional moment equation

\[
\mathbb{E}[Y - g(X) \mid Z] = 0. \tag{2 \text{ revisited}}
\]

Let \( \mathcal{G} \) be an arbitrary class of continuous functions which we assume contains the truth that fulfills the integral equation. Dual IV proposes to solve

\[
\min_{g \in \mathcal{G}} R(g) := \mathbb{E}_{YZ} \left[ (Y - \mathbb{E}[g(X) \mid Z])^2 \right],
\]

while this paper solves

\[
\min_{g \in \mathcal{G}} L(g) = \|Af - b\|_2^2 = \mathbb{E}_{Z} \left[ (\mathbb{E}[Y \mid Z] - \mathbb{E}[g(X) \mid Z])^2 \right],
\]

an unregularized version of Example \([1]\). The operator \( A \) and \( b \in \mathcal{E} \) are defined in Example \([1]\).

To introduce the maximizer, Dual IV \([31]\) resorts to the interchangeability principle.

**Lemma F.1** (Interchangeable principle). Let \((\Omega, \mathcal{F}, \mathbb{P})\) be a probability space, \( f : \mathbb{R}^n \times \Omega \to \mathbb{R} \cup \{+\infty\} \), and \( \mathcal{L}_2 = L_2(\Omega, \mathcal{F}, \mathbb{P}) \) be the class of square integrable functions. Let \( X \) be the set of mappings \( \chi : \Omega \to \mathbb{R}^n \) such that \( f_X \in \mathcal{L}_2 \), where \( f_X(\cdot) := f(\chi(\cdot), \cdot) \). Assume \( F(\omega) := \sup_{x \in X} f(x, \omega) \in \mathcal{L}_2 \) and that \( f \) is upper semi-continuous\footnote{Random upper semi-continuous, to be precise.} Then the following holds.

\[
\mathbb{E}\left[ \sup_{x \in X} f(x, \omega) \right] = \sup_{\chi \in \mathcal{X}} \mathbb{E}[f(\chi(\omega), \omega)].
\]
Proof. See Proposition 2.1 in \[38\]. See also Proposition 1 in \[12\] for a proof for the case where \(f : \mathbb{R} \times \Omega \rightarrow \mathbb{R}\).

With the interchangeability principle, (54) can be rewritten as
\[
\min_{g \in L^2(X)} \max_{u \in U} \Psi(g, u) := E_{XYZ}[(g(X) - Y)u(Y, Z)] - \frac{1}{2}E_{YZ}[u(Y, Z)^2].
\]
By comparison, an unregularized version of the min-max problem derived in this paper (22) is
\[
\min_{g \in L^2(X)} \max_{u \in U} E_{XYZ}[(g(X) - Y)u(Z)] - \frac{1}{2}u^2(Z). \tag{55}
\]
The absence of the variable \(Y\) in the maximizer \(u\) in (55) facilitates a natural connection between (55) and GMM.

To achieve such interpretation, we first introduce a GMM estimator for (2). The conditional moment restriction (2) implies that for a set of functions \(f_1, f_2, \ldots, f_m\) of \(Z\), we have \(E[(Y - g(X))f_j(Z)] = 0\). Define by \(\psi(f, g) := E_{XYZ}[(Y - g(X))f(Z)]\) the moment violation function, and the GMM estimator
\[
g_{\text{GMM}} \in \arg \min_{g \in U} \frac{1}{2} \sum_{j=1}^{m} \psi(f_j, g)^2.
\]
Collect the moment violations by a vector \(\psi_v(g) := (\psi(f_1, g), \ldots, \psi(f_m, g))^T \in \mathbb{R}^m\). To achieve efficiency the moments are usually weighted. Let \(\Lambda\) be a \(m \times m\) symmetric matrix. We define the quadratic norm \(\|\phi\|_{\Lambda}^2 = \phi^T \Lambda \phi\) given a vector \(\phi\).

Now we are ready to state the connection between GMM and (55). Define the space of maximizer \(U = \text{span} \{f_1, \ldots, f_m\}\). We focus on the inner maximization of (55). Define
\[
J(g) := \max_{u \in U} E_{XYZ}[(g(X) - Y)u(Z)] - \frac{1}{2}u^2(Z).
\]
Note that maximizer is now constrained in \(U\). Mimicking Theorem 5 in \[31\], we can show \(J(g)\) is in fact a weighted sum of the moment violations \(\{\psi(f_j, g)\}\).

Lemma F.2. Let \(f_1, f_2, \ldots, f_m\) be a set of real-valued functions of \(Z\). Define the weight matrix \(\Lambda := E[Z f(Z)^T]\) where \(f := (f_1(Z), \ldots, f_m(Z))^T\). Then \(J(g) = \frac{1}{2} \|\psi_v(g)\|_{\Lambda}^2\).

Proof. The proof is identical to Appendix C of \[31\] except for replacing \(f(Y, Z)\) with \(f(Z)\). The proof relies on simple algebra manipulation and is presented for completeness. For any \(u \in U, u = \sum_{j=1}^{m} \alpha_j f_j\) for some \(\alpha = (\alpha_1, \ldots, \alpha_m)^T \in \mathbb{R}^m\).

\[
J(g) = \max_{\alpha \in \mathbb{R}^m} E_{XYZ} \left[ (g(X) - Y) \left( \sum_{j=1}^{m} \alpha_j f_j(Z) \right) \right] - \frac{1}{2}E_Z \left[ \left( \sum_{j=1}^{m} \alpha_j f_j(Z) \right)^2 \right]
\]
\[
= \max_{\alpha \in \mathbb{R}^m} \sum_{i=1}^{m} \alpha_i E_{XYZ} \left[ (g(X) - Y) f_j(Z) \right] - \frac{1}{2}E_Z \left[ \left( \sum_{j=1}^{m} \alpha_j f_j(Z) \right)^2 \right]
\]
\[
= \max_{\alpha \in \mathbb{R}^m} \alpha^T \psi_v - \frac{1}{2} \alpha^T \Lambda \alpha
\]
\[
= \frac{1}{2} \psi_v^T \Lambda^{-1} \psi_v.
\]

Lemma F.2 shows that if the maximizer is constrained to be in the span of a set of pre-defined test functions \(\{f_j\}\), the minimization in (55) in fact produces a weighed GMM estimator. In contrast, the GMM interpretation provided in Section 3.5 of \[31\] requires the definition of a so-called augmented IV \(W := (Y, Z)\). It is unnatural to view the response variable \(Y\) as a component of the IV.