Dual IV: A Single Stage Instrumental Variable Regression

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Abstract

We present a novel single-stage procedure for instrumental variable (IV) regression called DualIV which simplifies traditional two-stage regression via a dual formulation. We show that the common two-stage procedure can alternatively be solved via generalized least squares. Our formulation circumvents the first-stage regression which can be a bottleneck in modern two-stage procedures for IV regression. We also show that our framework is closely related to the generalized method of moments (GMM) with specific assumptions. This highlights the fundamental connection between GMM and two-stage procedures in IV literature. Using the proposed framework, we develop a simple kernel-based algorithm with consistency guarantees. Lastly, we give empirical results illustrating the advantages of our method over the existing two-stage algorithms.

1 INTRODUCTION

Learning meaningful causal relationships under the influence of unobserved confounders remains one of the most challenging problems in econometrics, health care and social sciences [4, 25]. In this work, we look into how one could uncover the (potentially non-linear) causal relation between a treatment variable $X$ and an outcome variable $Y$ under the presence of an unobserved confounder $H$ that affects both $X$ and $Y$. In economics, studies on the return from schooling, which measure the causal effect of education on labor market earnings [10], is a typical example of such a problem. For an individual, $X$ represents the level of education and $Y$ represents how much he/she earns.

However, one’s level of education and income is likely confounded by his/her socioeconomic status or other unobserved factors $H$ [4, Ch. 4]. Thus, we cannot distinguish the true causal effect of $X$ on $Y$ from the effect that comes from $H$.

Conducting randomized control trials (RCT), the gold standard in determining causal effects in the presence of confounding, is often infeasible in most econometric studies. An alternative approach is to use instrumental variables (IVs) to correct for confounding in observational studies. Informally, instrumental variable(s) $Z$ are defined as variables that are associated with treatment $X$, affect the outcome $Y$ only through $X$ and do not share common causes with $Y$; see Assumption 1 for formal definitions. For instance, the season of birth was used as an instrument variable in [2] to estimate the impact of compulsory schooling on earnings. Identifying valid instrumental variable(s) for specific problems is a common task in econometrics [4].

Although IV analysis is widely used, the statistical methods employed for estimating causal effect are fairly rudimentary. Most applications of instrumental variables make use of a two-stage procedure [4, 48, 40, 21]. For instance, the classic two-stage least squares (2SLS) algorithm relies on the assumption that the relationship between $X$ and $Y$ are linear [32]. 2SLS first estimates the conditional mean $\mu(z) := \mathbb{E}_{X|Z=z}[X]$ via linear regression and then regresses $Y$ on the estimate of $\mu(z)$ to obtain an estimate of the causal effect. Since $\mu$, estimated using instrumental variable(s) $Z$, is by construction independent from the hidden confounders, the estimate obtained from regressing $Y$ on $\mu$ should be free from hidden confounding. In the non-linear setting, however, the difficulty of first-stage regression may result in a poor second-stage estimate [4, Ch. 4.6].

To avoid this problem, we propose a single-stage procedure—called DualIV—to directly estimate the structural causal function. Unlike previous works which extend 2SLS by employing non-linear models in place of their linear counterparts [21, 40], we solve the
The rest of this paper is organised as follows. Section 2 introduces the IV regression problem, reviews related work and identifies current limitations. Our new formulation is then presented in Section 3, followed by the estimation method based on a reproducing kernel Hilbert space (RKHS) in Section 4. Then, Section 5 reports empirical comparisons between DualIV and existing two-stage algorithms. Finally, we discuss the limitations of our work and suggest future directions in Section 6.

2 PRELIMINARIES

2.1 Instrumental Variable Regression

We denote an outcome variable by $Y$, an endogenous treatment variable by $X$, and an instrumental variable by $Z$ which take values in $\mathcal{X}$, $\mathcal{Y}$, and $\mathcal{Z}$, respectively. In this work, we assume $\mathcal{Y} \in \mathbb{R}$, and $\mathcal{X}$ and $\mathcal{Z}$ to be Polish spaces. Throughout this paper, we assume that $Y$ is bounded, i.e., $\|Y\|_\mathcal{Y} < \infty$ almost surely. Moreover, we have unobserved confounder(s) $H$ that affects both $X$ and $Y$. The underlying causal mechanism can be described by the causal graph in Figure 1 equipped with the following structural causal model (SCM):

$$Y = f^*(X) + \epsilon$$  \hspace{1cm} (1)

where $f^*$ is an unknown, potentially non-linear continuous function and $\epsilon$ denotes the additive noise which depends on the hidden confounder(s) $H$ and $\mathbb{E}[\epsilon] = 0$. If $\mathbb{E}[\epsilon|X] = 0$, we can identify the causal function $f^*$ and can estimate it consistently from observational data. Essentially, this allows us to identify $\mathbb{E}[Y|do(X = x)]$ from observations where $do(X = x)$ represents an intervention on $X$ by setting it to the value $x$ [31]. However, due to the presence of $W$, the error $\epsilon$ correlates with $X$, i.e., $\mathbb{E}[\epsilon|X] \neq 0$.

Following [30, 21, 40], we define the counterfactual prediction function as

$$f(x) := \mathbb{E}[Y|X = x] = f^*(x) + \mathbb{E}[\epsilon],$$  \hspace{1cm} (2)

which implies that the distribution of $\epsilon$ is invariant to changes in treatment $X$. While this condition is always satisfied in a randomized experiment, we are interested in estimating $f(x)$ from observational data, i.e., treatment assignment may not be random. As a result, $\mathbb{E}[Y|x] = f^*(x) + \mathbb{E}[\epsilon|x] \neq f(x)$ and we cannot use $f(x)$ to make a prediction about the outcome of an intervention on $X$.

To deal with hidden confounders, we assume that we have access to instrumental variable(s) $Z$ which satisfies the following assumptions:

**Assumption 1.** (i) **Relevance:** $\mathbb{P}(X|Z) \neq$ constant in $Z$. (ii) **Exclusion:** $Z$ affects $Y$ only through $X$, i.e., $Y \perp \!\!\!\!\perp Z|X, \epsilon$. (iii) **Unconfounded Instrument(s):** $Z$ is independent of the error, i.e., $\epsilon \perp \!\!\!\!\perp Z$.

Under Assumption 1, taking an expectation of (1) w.r.t. $Y$ conditioned on $Z$ yields the integral equation

$$\mathbb{E}[Y|Z = z] = \int f(x) \, d\mathbb{P}(X|Z = z).$$  \hspace{1cm} (3)

From the functional analysis perspective, we can view (3) as a Fredholm integral equation of the first kind. Solving (3) directly for $f$ is an ill-posed problem as it involves inverting linear compact operators [26, 29, 30]. This is the common perspective adopted by recent works in nonparametric IV regression [22, 30, 21, 40].

To understand the role of instrumental variable $Z$, let us consider two special cases. When $Z = X$, $X$ is perfectly correlated with $Z$ which implies that the treatment $X$ is uncorrelated with the hidden confounder by Assumption 1(iii). In other words, we recover the strong ignorability assumption [35, 36] required for causal inference with no hidden confounding. When $Z$ is independent of $X$, the instrument is not useful and the structural function $f$ cannot be identified from the data. Therefore, the interesting cases lie between these two extremes, especially when $X$ and $Z$ are weakly correlated, see, e.g., [9, 44][4, pp. 205–216].

2.2 Related Work

Early applications of IV in econometrics often rely on the assumption that the relationships between $Z$ and $X$ as well as between $X$ and $Y$ are linear [5, 4]. In the case where there is a single endogeneous variable $x$ and instrument $z$, under the linear structural model $y = \beta x + \epsilon$ and $x = \alpha z + \eta$, the structural parameter $\beta$ can be estimated consistently by the instru-
mental variable (IV) estimator \( \hat{\beta}^{IV} := (Z^\top X)^{-1}Z^\top y \) where \( Z, X, y \) are data matrices [5]. Interestingly, we can also obtain \( \hat{\beta}^{IV} \) by a two-stage procedure: regress \( x \) on \( z \) using ordinary least square (OLS) to calculate the predicted value \( \hat{x} \) and used that as an explanatory variable in the structural equation to estimate \( \beta \) using OLS. When there are multiple instruments, the two-stage least squares (2SLS) estimator is obtained by using all the instruments simultaneously in the first-stage regression. The explicit form of the 2SLS estimator is \( \hat{\beta}^{2SLS} = (X^\top P_Z X)^{-1}X^\top P_Z y \) where \( P_Z = Z(Z^\top Z)^{-1}Z^\top \) is known as the projection matrix. Wooldridge [40, Theorem 5.3] asserts that the 2SLS estimator is the most efficient IV estimator. See, e.g., [49, 4] for a detailed exposition.

Recently, several nonparametric extensions of 2SLS have been proposed to overcome the linearity assumption. The first line of work replaces linear regression by a linear projection onto a set of known basis functions [30, 8, 22, 12]. In [11], the authors provide a uniform convergence rate of this approach. However, there exists no principled way of choosing the appropriate set of basis functions for these methods. The second line of work replaces the first-stage regression by a conditional density estimate of \( \mathbb{P}(X|Z) \) using kernel density estimators [19, 15]. Despite their greater flexibility, approaches based on conditional density estimation suffer from the curse of dimensionality [46, Ch. 1]. Recent extensions of 2SLS from the machine learning perspective include DeepIV [21] and KernelIV [40]. Specifically, [21] proposes to solve (3) by first estimating \( \mathbb{P}(X|Z) \) with a mixture of deep generative models on which \( g(x) \) is learned with another deep neural network. Instead of neural networks, [40] proposes to model the first-stage regression using the conditional mean embedding of \( \mathbb{P}(X|Z) \) [41, 43, 28] which is then used in the second-step kernel ridge regression. In other words, the first-stage estimation in [40] becomes a vector-valued regression problem.

Limited information maximum likelihood (LIML) [18, 1] and generalized method of moments (GMM) [20, 27, 7] are two closely related approaches. The former maximizes the log likelihood and can be understood as a linear combination of the OLS and 2SLS estimates, whereas the latter operates by satisfying moment conditions (see Section 3.5 for more details). We refer the readers to [4] for a review of these two approaches.

### The Curse of Two-Stage Methods

Two-stage procedures have two fundamental issues. First, such procedures could violate Vapnik’s principle: “... when solving a problem of interest, do not solve a more general problem as an intermediate step” [47]. Specifically, estimating the conditional density function [21] or the conditional mean embedding [40] via regression in the first stage can be harder than estimating the parameter of interest \( f^* \) in the second stage. Econometrists even call the first stage a “forbidden regression” [4, Ch. 4.6]. On top of that, in counterfactual inference we only observe a single sample from each \( \mathbb{P}(X|Z = z) \), which further increases the difficulty of the task. Second, although two-stage procedures are asymptotically consistent, the first-stage estimate induces a finite-sample bias in the second-stage estimate [4, Sec. 4.6.4]. This bias can be alleviated through sample splitting [3] which is also used in [21, 40]. Thus, two-stage procedures are less sample efficient and could yield biased estimates when run on the smaller datasets common in econometrics, medicine, and social sciences.

### 3 DUAL INSTRUMENTAL VARIABLE REGRESSION

In what follows, we reformulate the integral equation (3) as an empirical risk minimization (ERM) problem before presenting the DualIV formulation.

#### 3.1 Primal Formulation

Let \( \ell : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}_+ \) be a proper, convex, and lower semi-continuous loss function for any value in its first argument. Let \( \mathcal{G} \) be an arbitrary class of continuous functions which we assume contains \( g \) that fulfills the integral equation (3). Then, we can formulate (3) as

\[
\min_{g \in \mathcal{G}} R(g) := \mathbb{E}_{(Y,Z)} \left[ \ell(Y, \mathbb{E}_{X|Z}[g(X)]) \right].
\]

(4)

To understand how it is related to (3), let us consider the squared loss \( \ell(y, y') = (y - y')^2 \) and define \( h(z) := \mathbb{E}_{X|Z}[g(X)] \). Then, the minimum of (4) is given by the minimum mean square error (MMSE) estimator \( h^*(z) := \mathbb{E}[Y|z] \), which is the LHS of (3). If there exists no \( g \in \mathcal{G} \) for which \( h^*(z) = \mathbb{E}[Y|z] \), we use \( h^*(z) \) as the best MMSE approximation of \( \mathbb{E}[Y|z] \). In this work, we focus only on the squared loss.

The biggest challenge in estimating \( g \) from (4) is the noncontinuity of \( g \) in \( h(z) \). If \( g \) is noncontinuous in \( h(z) \), \( g \) is not assured to be consistently estimated even if \( h(z) \) is [30]. We further discuss the issue of identifiability in Section 3.3.

To circumvent the first-stage regression, we look to two-stage problems in stochastic programming [39, 14] which resembles (4). In [14], the problem of learning from conditional distributions was formulated in a...
similar fashion to (4). The authors note that machine learning tasks such as learning with invariant representations and policy evaluation in reinforcement learning fall within this class of problems. Moreover, [24] proposes the deconditional mean embedding (DME) which solves the integral equation (3) by performing a closed-form “inversion” of the conditional mean embedding of \( P(X|Z) \) (see [28, 42] for a review). In contrast, we solve the integral equation (3) by resorting to the dual formulation of (4).

3.2 Dual Formulation

To derive the dual problem of (4), we require two results, namely interchangeability and Fenchel duality, which we review below; see, e.g., [14, Lemma 1], [33, Ch. 14], and [39, Ch. 7] for more details.

**Theorem 1** (Interchangeability). Let \( \omega \) be a random variable on \( \Omega \) and for any \( \omega \in \Omega \) the function \( f(\cdot, \omega) : \mathbb{R} \to (-\infty, \infty) \) is proper and upper semi-continuous concave function. Then,

\[
E_{\omega} \left[ \max_{u \in \mathbb{R}} f(u, \omega) \right] = \max_{(u, \cdot) \in \mathcal{U}(\Omega)} E_{\omega}[f(u(\omega), \omega)],
\]

where \( \mathcal{U}(\Omega) := \{(u, \cdot) : \Omega \to \mathbb{R} \} \) is the entire space of functions defined on the support \( \Omega \).

**Definition 2** (Fenchel duality). Let \( \ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}_+ \) be a proper, convex, and lower semi-continuous loss function for any value in its first argument and \( \ell^*_y := \ell^*(y, \cdot) \) a convex conjugate of \( \ell_y := \ell(y, \cdot) \) which is also proper, convex, and lower semi-continuous w.r.t. the second argument. Then, \( \ell_y(v) = \max_u \{ uv - \ell_y^*(u) \} \). It is known that the maximum achieves if \( v \in \partial \ell^*(u) \), or equivalently \( u \in \partial \ell(v) \).

Using the Fenchel duality and the interchangeability principle, we can rewrite the expected loss \( R(g) \) as

\[
R(g) = E_{YZ} \left[ \max_{u \in \mathbb{R}} \left\{ E_{X|Z}[g(X)]u - \ell_Y^*(u) \right\} \right] = \max_{g \in \mathcal{G}} E_{YZ} \left[ E_{X|Z}[g(X)]u(Y, Z) - \ell_Y^*(u(Y, Z)) \right] = \max_{g \in \mathcal{G}} E_{XYZ} \left[ g(X)u(Y, Z) - E_{YZ}[\ell_Y^*(u(Y, Z))] \right],
\]

where \( \mathcal{U} \) is the space of continuous functions over \( \mathcal{Y} \times \mathcal{Z} \). Finally, we can reformulate (4) as

\[
\min_{g \in \mathcal{G}} \max_{u \in \mathcal{U}} \left[ E_{XYZ}[g(X)u(Y, Z)] - E_{YZ}[\ell_Y^*(u(Y, Z))] \right]. \tag{6}
\]

Following [14], we refer to \( u \in \mathcal{U} \) as the dual function. Note that it depends on the outcome \( Y \) and the instrumental variable \( Z \), but not the treatment \( X \).

The advantages of (6) over (3) and (4) are clear. First, there is no need to estimate \( E_{X|Z}[g(X)] \) or \( P(X|Z) \) explicitly. Second, the function \( g \) appears linearly in (6) which therefore makes it convex in \( g \). Since \( \ell_y^* \) is also convex due to the convexity of \( \ell_y \), (6) is concave in the dual function \( u \). Hence, (6) is a convex-concave saddle-point problem in \( g \in \mathcal{G} \) and \( u \in \mathcal{U} \) [14].

For the squared loss \( \ell(y, y') = (y - y')^2 \), \( \ell_y^*(w) = w^2 + \frac{1}{2}w^2 \) (see Appendix A for the derivation) and the saddle-point formulation (6) becomes

\[
\min_{g \in \mathcal{G}} \max_{u \in \mathcal{U}} \left[ E_{XYZ}[g(X) - Y]u(Y, Z) - \frac{1}{2}E_{YZ}[u(Y, Z)^2] \right]. \tag{7}
\]

We focus on this formulation throughout. Figure 2 illustrates the loss surface associated with (7).

3.3 Theoretical Guarantee

Here, we provide the conditions for which the true structural function \( f^* \) is identified by the optimum of the saddle-point problem (7). We lay out the assumptions needed for the optimal dual function \( u^* \) to be unique and continuous, show that the saddle-point formulation (7) is equivalent to the empirical risk minimization problem (4) under the squared loss and prove that the solution of the (7) given \( u^* \) is indeed \( f^* \).

**Assumption 2.** (i) \( P(X|Z) \) is continuous in \( Z \) for any values of \( X \). (ii) The selected function class \( \mathcal{G} \) in (4) contains \( f^* \).

We follow Dai et al. [14] and define the optimal dual function for any pair of \( (y, z) \) in \( \mathcal{Y} \times \mathcal{Z} \) as \( u^* \in \arg \max_{u \in \mathcal{U}} \left\{ E_{X|Z}[g(X) - y]u - (1/2)u^2 \right\} \). Since this is an unconstrained quadratic program w.r.t. \( u \), the optimal dual function \( u^* \) takes the form \( E_{X|Z}[g(X)] - y \). Given Assumption 2 and the loss function \( \ell \) is convex and continuously differentiable, it follows from [14, Proposition 1] that \( u^* \) is unique and continuous.

Next we shows that if \( (g^*, u^*) \) is the saddle-point of (7), then \( g^* \) minimizes the original objective (4).

**Proposition 3.** Let \( \ell(y, y') = \frac{1}{2}(y - y')^2 \). Then, for any fixed \( g \), we have \( R(g) = \max_u \Psi(g, u) \).
Proof. This follows from plugging $u^* = \mathbb{E}_{XY|z}[g(X)] - y$ into the dual loss $\Psi(g, u)$ in (7). See Appendix B for the detailed proof.

Theorem 4. Let $\ell(y, y') = \frac{1}{2}(y - y')^2$ and assume that Assumption 2 holds. Then, $(f^*, u^*)$ is the saddle-point of a minimax problem $\min_{g \in \mathcal{G}} \max_{u \in \mathcal{U}} \Psi(g, u)$.

Proof. The above result follows directly from Proposition 3 and the convexity of the loss $\ell(y, y')$.

By virtue of Theorem 4, we can identify the true structural function $f^*$ under relatively weak assumptions. In contrast, past works usually require strong assumptions such as the completeness condition [30, 40] which specifies that the first-stage conditional expectation $\mathbb{E}_{X|z}[g(X)]$ is injective, or $h(z) = \mathbb{E}_{X|z}[g(X)]$ is a smooth function of $z$ [40, 11, 12]. Since there is no first-stage regression in our framework, we only require $P(X|Z)$ is continuous in $Z$ for any value of $X$. The requirement that (4) is correctly specified, i.e., $f^* \in \mathcal{G}$, is standard across the literature; see, e.g., Newey and Powell [30], Horowitz [22], Singh et al. [40].

3.4 Interpreting the Dual Function

The dual function $u(y, z)$ plays an important part in our framework. To interpret its role, we consider the minimization and maximization problems in (7) separately to ensure clarity. For any $g \in \mathcal{G}$, the maximization problem w.r.t. $u$ is

$$\max_{u \in \mathcal{U}} \left\{ \mathbb{E}_{XYZ}[\eta(X, Y)u(Y, Z)] - \frac{1}{2}\|u\|^2_{L^2(P_{YZ})} \right\}, \quad (8)$$

where $\eta(x, y) := g(x) - y$ is the residual associated with $g$. The first term in (8) can be viewed as a (negative) loss function and the second term as a regularizer. Intuitively, we obtain a solution $u^* \in \mathcal{U}$ that is least statistically orthogonal to the residual associated with the function $g$. Given $u^*$, the outer minimization problem in (7) is

$$\min_{g \in \mathcal{G}} \mathbb{E}_{XYZ} \left[ (g(X) - Y)u^*(Y, Z) \right]. \quad (9)$$

That is, (9) finds the $g \in \mathcal{G}$ that yields the most orthogonal residual to $u^*$ from the inner maximization problem (8). Note that our procedure differs fundamentally from the two-stage procedures as (8) and (9) are interdependent.

From the causal perspective, the residuals $\eta$ contains the variation that cannot be explained by the current estimate of $g$ due to hidden confounding. We then select the specific $u$ that maximally reweights $\eta$ according to how inconsistent they are w.r.t. the unconfounded joint distribution of $Y$ and $Z$. With this new $u$, we update $g$ in the direction which minimizes the inconsistency between $\eta$ and $u$, i.e., the direction independent of hidden confounding. Hence, at the equilibrium, $\eta$ would contain noise independent of $Y$ and $Z$ that can be only attributed to confounding.

The form of optimal dual function $u^*$ from Section 3.3 provides us with an alternative interpretation. $u^* = \mathbb{E}_{X|z}[g(X)] - y$ acts as a surrogate function measuring the discrepancy between $\eta$ and $\mathbb{E}_{X|z}[g(X)]$ for any pair of $(y, z) \in Y \times Z$ [14]. Since $\mathbb{E}_{X|z}[g(X)]$ allows for $X$ and $Z$ to have a non-linear relationship, $u$ can be non-linear even when the true structural function $f^*$ is linear. This flexibility enables $u$ to accommodate a larger class of functions that maps $Z$ to $X$. Figure 3 illustrates this given the following generative process:

$$Y = X\beta + e + \epsilon, \quad X = (1 - \rho)Z_1 + pe + \eta \quad (10)$$

where $e \sim \mathcal{N}(0, 2), Z_1 \sim \mathcal{N}(0, 2), \epsilon \sim \mathcal{N}(0, 0.1)$, and $\eta \sim \mathcal{N}(0, 0.1)$. The parameter $\rho$ controls the strength of the instrument w.r.t. hidden confounder $e$. Here, we set $n = 300, \beta = 0.7, \hat{\beta} = 0.4$, and $\rho = 0.2$ where $\hat{\beta}$ is an estimate of $\beta$. Under this model, we have $u^*(y, z) \approx \hat{\beta}(1 - \rho)z - y$.

3.5 Generalized Method of Moments (GMM)

The GMM approach for nonparametric IV regression [20, 27, 7] relies on the orthogonality condition $E[e|Z] = 0$. Specifically, let $f_1, f_2, \ldots, f_m$ be real-valued functions used to specify the $m$ moment conditions. Then, we have $E[\eta(g) f_j(Z)] = 0$ for $j = 1, \ldots, m$ where $\eta(g)$ denotes the residual of $g$. Let $\psi(f, g) := \mathbb{E}_{XYZ}[(Y - g(X)) f(Z)]$ be a real-valued function that defines the moment condition w.r.t. $f$. Then, the GMM estimate of $g$ is

$$g_{GMM} \in \arg\min_{g \in \mathcal{G}} \frac{1}{2} \sum_{j=1}^{m} \psi(f_j, g)^2. \quad (11)$$

If we let $\psi := (\psi(f_1, g), \ldots, \psi(f_m, g))^\top \in \mathbb{R}^m$, (11) becomes $g_{GMM} \in \arg\min_{g \in \mathcal{G}} \frac{1}{2}\|\psi\|^2$. In practice, we seek to optimize an empirical version of (11) by replacing $\psi(f, g)$ with its empirical counterpart $\psi_n(f, g) :=$
Theorem 5. Let $f_1, f_2, \ldots, f_m$ be real-valued functions on $\mathcal{Y} \times Z$, $\psi(f, g) := E XYZ[(Y - g(x))]$, and $J(g) := \max g \in U E XYZ[(g(X) - Y)u(Y, Z)] - \frac{1}{2} E YZ[u(Y, Z)^2]$. Assume that $\mathcal{U} = \text{span}\{f_1, \ldots, f_m\}$. Then, $J(g) = \frac{1}{2}||\psi||^2_{\mathcal{U}}$, where $\Lambda := E XYZ[f \otimes f]$ with $f := (f_1(Y, Z), \ldots, f_m(Y, Z))^T$.

Theorem 5 links our formulation—which is the dual problem—to the GMM estimate as well as its recent nonparametric extensions [24, 7]. For example, if we let $u(y, z) = u(z)$, i.e., the dual function depends only on the instrumental variable $Z$, then (7) takes the form of vanilla GMM. In particular, the resulting formulation resembles that in Lewis and Syrgkanis [24, Eq. 3]. On the other hand, this result also highlights their fundamental differences as $f$ depends on both $Y$ and $Z$. We leave a thorough analysis for future work.

4 ESTIMATION

In this section, we develop algorithms for learning $g$. To simplify notation, we call $W := (Y, Z)$ an augmented instrumental variable which is a random variable taking value in $W := \mathcal{Y} \times Z$.

Let $\mathcal{G}$ and $\mathcal{U}$ be reproducing kernel Hilbert spaces (RKHSs) associated with positive definite kernels $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ and $l : \mathcal{W} \times \mathcal{W} \rightarrow \mathbb{R}$, respectively. Let $\phi : x \mapsto k(x, \cdot)$, $\varphi : w \mapsto l(w, \cdot)$ be the canonical feature maps of $k$ and $l$, respectively [37]. We assume throughout that both $\mathcal{G}$ and $\mathcal{U}$ are universal such that they are both dense in the space of bounded continuous functions (see, e.g., [45, Ch. 4]). Furthermore, let $\text{HS}(G, U)$ be a Hilbert space of Hilbert-Schmidt operators mapping from $\mathcal{G}$ to $\mathcal{U}$ with an inner product (\cdot, \cdot)\text{HS}$ (see, e.g., [24, Sec. 2.3]). Then, for any $g \in \mathcal{G}$ and $u \in \mathcal{U}$, we can rewrite the objective in (7) as a functional

\[
\Psi(g, u) = E_X W[(g(X)u(W)] - E_Y Z[Yu(Y, Z)] - \frac{1}{2} E_W [u(W)^2] \\
= E_X W[(g, \varphi(X))\varphi(u, \varphi(W))u] - E_Y Z[Yu(u, \varphi(Y, Z))u] - \frac{1}{2} E_W [u, \varphi(W)^2] \\
= E_X W[(g \otimes u, \varphi(X) \otimes \varphi(W))\text{HS}] - \langle u, E_Y Z[Y \varphi(Y, Z)]\rangle_U \\
= \frac{1}{2} E_W [(u \otimes u, \varphi(W) \otimes \varphi(W))\text{HS}] \\
= \langle c_{XW}, g \otimes u \rangle_{\text{HS}} - \langle u, b \rangle_U - \frac{1}{2} \langle c_W, u \otimes u \rangle_{\text{HS}} \\
= \langle g, c_{XW}u \rangle_{\mathcal{G}} - \langle u, b \rangle_U - \frac{1}{2} \langle c_W, c_Wu \rangle_U \\
= \langle c_{WX}g - b, u \rangle_{\mathcal{U}} - \frac{1}{2} \langle c_W, c_Wu \rangle_U \\
(12)
\]

where $b := E_Y Z[Y \varphi(Y, Z)] \in \mathcal{U}$, $C_W := E_W [\varphi(W) \otimes \varphi(W)] \in \mathcal{U} \otimes \mathcal{U}$ is a covariance operator, and $C_{XW} := E_X W[\varphi(X) \otimes \varphi(W)] \in \mathcal{G} \otimes \mathcal{U}$ is a cross-covariance operator [6, 16].

Since (12) is quadratic in $u$, we have $c_{XW}u^* = c_{WX}g - b$. Assuming that $c_W^{-1}$ exists and substituting $u^*$ back into (12) yields

\[
g^* = \arg \min_{g \in \mathcal{G}} \frac{1}{2} \langle c_{WX}g - b, c_W^{-1}(c_{WX}g - b) \rangle_U \\
= (c_{XW}c_W^{-1}c_{WX})^{-1}c_{WX}c_W^{-1}b. \hspace{1cm} (13)
\]

In other words, we can view (13) as a generalized least squares solution in Hilbert space. Since $c_{XW}^{-1}$ and $(c_{XW}c_W^{-1}c_{WX})^{-1}$ do not exist in general, we replace them with regularized versions $(c_{XW} + \lambda_1 I)^{-1}$ and $(c_{XW}c_W^{-1}c_{WX} + \lambda_2 I)^{-1}$ where $I$ is an identity operator and $\lambda_1, \lambda_2 > 0$ are regularization parameters.

Given a set of i.i.d. samples $\{(x_i, y_i, z_i)\}_{i=1}^n$ from $\mathcal{P}(X, Y, Z)$, we define $\Phi := \{\phi(x_1), \ldots, \phi(x_n)\}$, $\Upsilon := \{\varphi(y_1, z_1), \ldots, \varphi(y_n, z_n)\}$, and $\mathcal{Y} := \{y_1, \ldots, y_n\}$. Then, we can estimate $b$, $c_W$, and $c_{XW}$ with their empirical counterparts $\hat{b} := \frac{1}{n} \sum_{i=1}^n y_i \varphi(y_i, z_i) =: n^{-1} \mathcal{Y} \varphi$, $\hat{c}_{XW} := \frac{1}{n} \sum_{i=1}^n \phi(x_i) \varphi(y_i, z_i) = n^{-1} \Phi \Upsilon$ and $\hat{c}_W := n^{-1} \sum_{i=1}^n \varphi(y_i, z_i) \varphi(y_i, z_i) = n^{-1} \Upsilon \Upsilon^T$.

We denote the empirical version of (12) by $\hat{\Psi}(g, u)$ and the estimate of $g^*$ in (13) by $\hat{g}$.

Next, we show that the representer theorem [38] for $\hat{\Psi}(g, u)$ holds for both $g$ and $u$ (see Appendix D).

Lemma 6. For any $g \in \mathcal{G}$ and $u \in \mathcal{U}$, there exist $g_\alpha = \sum_{i=1}^n \beta_i k(x_i, \cdot)$ and $u_\alpha = \sum_{i=1}^n \alpha_i l(w_i, \cdot)$ for some $\alpha, \beta \in \mathbb{R}^n$ such that $\hat{\Psi}(g, u) = \hat{\Psi}(g_\alpha, u_\alpha)$.

By virtue of Lemma 6, the solution to (13) can be expressed as $g(x) = \sum_{i=1}^n \beta_i k(x_i, x)$ where the coefficients $\beta$ are given by the following proposition. The proof can be found in Appendix E.

Proposition 7. Given a set of i.i.d. samples $\{(x_i, y_i, z_i)\}_{i=1}^n$ from $\mathcal{P}(X, Y, Z)$, let $\mathbf{K} := \Phi^\top \Phi$ and $\mathbf{L} := \Upsilon^\top \Upsilon$ be the Gram matrices such that $K_{ij} = k(x_i, x_j)$ and $L_{ij} = l(w_i, w_j)$ where $w_i := (y_i, z_i)$. Then, $\hat{g} = \Phi \beta$ where

$\beta = (\mathbf{MK} + n \lambda_2 \mathbf{K})^{-1} \mathbf{My} \hspace{1cm} (14)$

with $\mathbf{M} := \mathbf{K}(\mathbf{L} + n \lambda_1 \mathbf{I})^{-1} \mathbf{L}$. 

Dual IV: A Single Stage Instrumental Variable Regression
Algorithm 1 DualIV

Input: Data \( \{(x_i, y_i, z_i)\}_{i=1}^n \), kernels \( k, l \).
1: Let \( K_{ij} = k(x_i, x_j) \) and \( L_{ij} = l((y_i, z_i), (y_j, z_j)) \).
2: \((\lambda_1, \lambda_2) \leftarrow \text{SelectParams}(K, L)\).
3: \( M \leftarrow K(L + n \lambda_1 I)^{-1}L \).
4: \( \beta \leftarrow (MK + n \lambda_2 K)^{-1}My \).
Output: A function \( g(x) = \sum_{i=1}^n \beta_i k(x_i, x) \).

Compared to previous work which involved conditional density estimation [19, 15, 21] and vector-valued regression [40] as first-stage regression, estimating the dual function \( u \), a real-valued function, is arguably easier. This is especially so when \( X \) and \( Z \) are high-dimensional.

Parameter Selection. We provide a simple method to empirically determine the values of \((\lambda_1, \lambda_2)\). First, we estimate \( \hat{g} \) via Proposition 7 on \( \{(x_i, y_i, z_i)\}_{i=1}^n \). Next, we evaluate \( \hat{g} \) using the out-of-sample loss evaluated on an independent set of \( m \) points \( \{(\tilde{x}_i, \tilde{y}_i, \tilde{z}_i)\}_{i=1}^m \), i.e.,

\[
\hat{R}(\hat{g}) = \frac{1}{m} \sum_{i=1}^m (\hat{g}(X) - \tilde{y}_i)^2 \approx \frac{1}{m} \sum_{i=1}^m \hat{u}(\tilde{y}_i, \tilde{z}_i)^2,
\]

where the last equality follows from the interpretation of \( u \) provided in Section 3.4 (see Figure 3). Note that \( \hat{u} = (\hat{C}_W + \lambda_1 I)^{-1}(\hat{C}_{WX} \hat{g} - \hat{b}) = Y(L + n \lambda_1 I)^{-1}(K\beta - y) = Y\alpha \) where \( \alpha := (L + n \lambda_1 I)^{-1}(K\beta - y) \) and \( K, L \in \mathbb{R}^{n \times n} \) are Gram matrices evaluated on \( (x_i, y_i, z_i) \). Hence, \( \hat{R}(\hat{g}) \approx \alpha^\top L1/m \) where \( L_{ij} = l((y_i, z_i), (y_j, z_j)) \). In our experiments, we fix \( \lambda_1 \) that appears in \( \hat{u} \) to \( 10^{-8} \) and only optimize the \((\lambda_1, \lambda_2)\) that appear in \( \beta \). Our procedure differs from the two-stage causal validation procedure used in [21, 40]. Algorithm 1 summarizes the DualIV algorithm.

Consistency. Previously, we described the proposed regularized empirical estimator for the IV regression problem. Here, we discuss the asymptotic properties of the estimator. We show that the proposed estimator is asymptotically consistent given \( C_W^{-1} \) and \( C_{WX}C_W^{-1}C_{WX} \) exist. This assumption is similar to the one made in Fukumizu et al. [17]. In practice however, it is relatively easy to come up with a case where \( C_W^{-1} \) and \( C_{WX}C_W^{-1}C_{WX} \) does not exist [41, 17, 28]. But for now, we leave this as future work. For the sake of simplicity, we also assume that the operator norm of the inverse covariance functions are bounded from below. Under the above assumptions, we show that the solution \( g^* \) of the saddle-point problem (12) can be expressed as \( g^* = (C_{WX}C_W^{-1}C_{WX})^{-1}C_{WX}C_W^{-1}b \).

Theorem 8. Assume that \( C_W^{-1} \) and \( C_{WX}C_W^{-1}C_{WX} \) exist and the operator norm of the inverse are bounded, then for sufficiently slow decay of regularization parameters \( \lambda_1, \lambda_2 \), \( \hat{g} \) is a consistent estimator of \( g^* \) in RKHS norm i.e. \( \|\hat{g} - g^*\|_2 \to 0 \) as \( n \to \infty \).

Proof. See Appendix F.

5 EXPERIMENTS

To demonstrate the effectiveness of DualIV empirically, we compare it with the following two-stage algorithms. (i) 2SLS [5]: the vanilla two-stage least squares. (ii) DeepIV [21]: We used the original implementation provided by the authors. (iii) KernelIV [40]: We use the MATLAB implementation provided to us by the authors of Singh et al. [40].

Simulations. We consider the demand design used in [21, 40]: \( Y = f(X) + \epsilon, \mathbb{E}[\epsilon|Z] = 0 \) where \( Y \) is outcome, \( X = (P, T, S) \) are inputs, and \( Z = (C, T, S) \) are instruments. Specifically, \( Y \) is sales, \( P \) is price (endogeneous), \( C \) is a supply cost shifter (instrument), and \( (T, S) \) are time of year and customer sentiment (exogeneous variables). We want to learn the demand function \( f(p, t, s) = 100 + (10 + p)u(t) - 2p \) where \( u(t) = 2(t - 5)^4/600 + \exp(-4(t - 5)^2) + t/10 - 2 \). The data are sampled as \( S \sim \text{Unif}[1, \ldots, 7], T \sim \text{Unif}[0, 10], (C, V) \sim \mathcal{N}(0, I_2), \epsilon \sim \mathcal{N}(\rho V, 1 - \rho^2), P = 25 + (C + 3)\psi(T) + V \). The parameter \( \rho \in [0.9, 0.75, 0.5, 0.25, 0.1] \) controls the extent to which price \( P \) is confounded by supply-side market forces. In our notation, \( X = (P, T, S), Z = (C, T, S), \) and \( W = (Y, Z) = (Y, C, T, S) \). Figure 4 illustrates the demand function.

![Figure 4: The demand function.](https://github.com/jhartford/DeepIV)
Dual IV: A Single Stage Instrumental Variable Regression

\[ c_j \] where \( V_{jc} \) is a symmetric bandwidth matrix and \( k_p, k_t, k_s \) are all Gaussian kernels. The values of all bandwidth parameters are determined by the median heuristic. To learn \( (\lambda_1^*, \lambda_2^*) \), we adopt the validation procedure described in Section 4. We split the dataset in half. The first half is used to fit the model \( \hat{g} \), whereas the second half is used to evaluate the out-of-sample risk \( \hat{R}(\hat{g}) \). Once \( (\lambda_1^*, \lambda_2^*) \) is determined, we refit \( \hat{g} \) on the entire dataset. For each algorithm and sample size, we repeat the simulation 20 times and calculate the MSE w.r.t. the true function \( f \).

Results. Figure 5 and 6 depict the MSE of 2SLS, DeepIV, KernelIV, and DualIV with \( \rho \in \{0.9, 0.75, 0.5, 0.25, 0.1\} \) and \( n \in \{50, 100, 1000\} \). As the variance of 2SLS is relatively high, we disentangle the MSE of 2SLS and show them in separate figures to ease visualization. First, it is clear that 2SLS does not perform well in this setting because the linearity assumption is violated. Second, both DualIV and KIV consistently outperform DeepIV which also confirms the results reported in [40]. Lastly, DualIV consistently achieves the smallest average MSE throughout compared to 2SLS, DeepIV, and KIV which are all two-stage algorithms.

6 DISCUSSION

This paper proposes a general framework for IV regression called DualIV. Unlike previous work, DualIV does not require the first-stage regression which is the critical bottleneck of modern two-stage procedures. Under certain assumptions, DualIV is closely related to the generalized method of moments (GMM). This provides additional insights into the connection between two-stage procedures and GMM-based methods in the IV literature. We demonstrate the validity of our framework with a kernel-based algorithm which not only is easy to use, but also works well in practice. Our experiments show the advantages of our algorithm over existing two-stage algorithms.

Instead of first-stage regression, our framework requires the dual function \( u \) to be estimated. However, as mentioned earlier, estimating \( u \) is arguably easier than first-stage regression, especially when the instruments and treatments are high-dimensional. Potential directions for future work are: a minimax convergence analysis of the proposed estimator could provide additional insight into the benefits of our framework over the two-stage procedures, parameterizing the dual function with more flexible and scalable models such as deep neural networks, and use stochastic gradient descent-based methods to solve the convex-concave saddle-point problem (12) to scale [14]. Lastly, we believe our framework can be applied more broadly to other two-stage estimation problems in causal inference such as double machine learning [13].

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A Conjugate of Squared Loss

Let \( \ell_y(v) := \frac{1}{2} (y - v)^2 \) be a proper, convex, and lower semi-continuous function for all \( y \in \mathbb{R} \). It follows from the definition of Fenchel conjugate (see, e.g., [33, Ch. 14], and [39, Ch. 7]) that for any \( y \in \mathbb{R} \),

\[
\ell^*_y(u) := \sup \{ uv - \ell_y(v) : v \in \mathbb{R} \} = \sup \left\{ uv - \frac{1}{2} (y - v)^2 : v \in \mathbb{R} \right\}. \tag{15}
\]

Hence, \( \ell^*_y(u) \) is also a proper, concave, and upper semi-continuous function. Taking a derivative of \( uv - \frac{1}{2} (y - v)^2 \) w.r.t. \( v \) and setting it to zero yield a critical point \( v^* = u + y \) for any \( u, y \in \mathbb{R} \). Since \( uv - \frac{1}{2} (y - v)^2 \) is a concave function in \( v \), we can substituting \( v^* \) back into (15) to obtain

\[
\ell^*_y(u) = u(u + y) - \frac{1}{2} (y - (u + y))^2 = u^2 + uy - \frac{1}{2} u^2 = uy + \frac{1}{2} u^2.
\]

B Proof of Proposition 3

Proposition 3. Let \( \ell(y, y') = \frac{1}{2} (y - y')^2 \). Then, for any fixed \( g \), we have \( R(g) = \max_u \Psi(g, u) \).

Proof. Taking \( \ell \) in (4) to be \( \frac{1}{2} (y - y')^2 \), plugging \( u^*(y, z) = E_{X|z}[g(X)] - y \) into (7) yields

\[
\Psi(g, u^*) = E_{XYZ}[(g(X) - Y)u^*(Y, Z)] - \frac{1}{2} E_{YZ}[u^*(Y, Z)^2]
\]

Then, for any \( g \in G \), we have \( g_{\beta, \alpha} = \sum_{i=1}^{n} \beta_i k(x_i, \cdot) \) and \( u_{\alpha} = \sum_{i=1}^{n} \alpha_i l(w_i, \cdot) \) for some \( \alpha, \beta, u \in \mathbb{R}^n \) such that \( \Psi(g, u) = \Psi(g_{\beta, \alpha}, u_{\alpha}) \).

Proof. Let \( \mathcal{U} := span(f_1, \ldots, f_m) \). That is, for any \( u \in \mathcal{U} \), \( u = \sum_{j=1}^{m} \alpha_j f_j \) for some \( (\alpha_1, \ldots, \alpha_m)^\top \in \mathbb{R}^m \).

\[
J(g) = \max_{\alpha \in \mathbb{R}^m} E_{XYZ} \left[ (g(X) - Y) \left( \sum_{j=1}^{m} \alpha_j f_j(Y, Z) \right) \right] - \frac{1}{2} E_{YZ} \left[ \left( \sum_{j=1}^{m} \alpha_j f_j(Y, Z) \right)^2 \right]
\]

Then, for any \( g \in G \), we have \( \Psi(g, u) = \Psi(g_{\beta, \alpha}, u_{\alpha}) \).

This concludes the proof.

D Proof of Lemma 6

Lemma 6. For any \( g \in G \) and \( u \in \mathcal{U} \), there exist \( g_{\beta, \alpha} = \sum_{i=1}^{n} \beta_i k(x_i, \cdot) \) and \( u_{\alpha} = \sum_{i=1}^{n} \alpha_i l(w_i, \cdot) \) for some \( \alpha, \beta, u \in \mathbb{R}^n \) such that \( \Psi(g, u) = \Psi(g_{\beta, \alpha}, u_{\alpha}) \).

Proof. Given a fixed sample of size \( n \) \( (x_1, y_1), \ldots, (x_n, y_n, z_0) \), any RKHSs \( G \) and \( U \) can be decomposed as \( G = G_{\beta} \oplus G_\perp \) and \( U = U = U_{\alpha} \oplus U_\perp \) where \( G_{\beta} \) and \( U_{\alpha} \) are subspaces consisting of functions of the following forms

\[
g_{\beta, \alpha} = \sum_{i=1}^{n} \beta_i k(x_i, \cdot), \quad u_{\alpha} = \sum_{i=1}^{n} \alpha_i l(w_i, \cdot),
\]

for some \( \beta, u \in \mathbb{R}^n \). The orthogonal subspaces \( G_\perp \) and \( U_\perp \) consist of elements which are orthogonal to \( G_{\beta} \) and \( U_{\alpha} \), respectively, i.e., for any \( g_{\beta} \in G_{\beta}, u_\perp \in G_{\perp}, u_{\alpha} \in U_{\alpha}, u_\perp \in U_{\perp} \), we have \( \langle g_{\beta}, u_\perp \rangle = 0, \quad \langle u_{\alpha}, u_\perp \rangle = 0 \).

Any elements \( g \in G \) and \( u \in U \) can be expressed as \( g = g_{\beta} + g_\perp \) and \( u = u_{\alpha} + u_\perp \) where \( g_{\beta} \in G_{\beta}, g_{\perp} \in G_\perp, u_{\alpha} \in U_{\alpha}, u_\perp \in U_{\perp} \).
Next, recall that
\[ \tilde{\Psi}(g, u) = \langle g, \tilde{C}_{XW}u \rangle_{\mathcal{G}} - \langle u, b \rangle_{\mathcal{U}} - \frac{1}{2} \langle u, \tilde{C}_{W}u \rangle_{\mathcal{U}} \]
where \( \tilde{C}_{XW} = n^{-1} \Phi \Sigma^{\top}, \tilde{C}_{W} = n^{-1} \Sigma \Sigma^{\top}, b = n^{-1} \Sigma \gamma, \Phi = \{k(x_1, \cdot), \ldots, k(x_n, \cdot)\}, \Sigma = \{l(w_1, \cdot), \ldots, l(w_n, \cdot)\}, \) and \( \gamma = [y_1, \ldots, y_n]^\top. \) For some \( u \in \mathcal{U}, \) let \( c(u) := \langle u, b \rangle_{\mathcal{U}} - \frac{1}{2} \langle u, \tilde{C}_{W}u \rangle_{\mathcal{U}}. \) Then, we have
\[
\tilde{\Psi}(g, u) = \langle g, \tilde{C}_{XW}u \rangle_{\mathcal{G}} - c(u)
= \left( \sum_{i=1}^{n} \alpha_i^l l(w_i, \cdot), u_{\alpha} + u_{\perp} \right)_{\mathcal{U}}
= \left( u_{\alpha} + u_{\perp}, \sum_{i=1}^{n} \alpha_i^l l(w_i, \cdot) \right)_{\mathcal{U}}
= \left( u_{\alpha}, \sum_{i=1}^{n} \alpha_i^l l(w_i, \cdot) \right)_{\mathcal{U}}
= \left( u_{\alpha}, \sum_{i=1}^{n} \alpha_i^l l(w_i, \cdot) \right)_{\mathcal{U}}
= \frac{1}{2} \left( u_{\alpha}, \tilde{C}_{W}u_{\alpha} \right)_{\mathcal{U}}.
\]
The first equality follows from \( \langle g, \tilde{C}_{XW}u \rangle_{\mathcal{G}} = \langle \tilde{C}_{XW}g, u \rangle_{\mathcal{U}} \) as \( \tilde{C}_{XW} \) is an adjoint operator of \( \tilde{C}_{XW}. \) Since the choice of \( g \) is arbitrary, the maximizer of \( \tilde{\Psi}(g, u) \) w.r.t. \( u \) also lies in the subspace \( \mathcal{U}_{\alpha}. \)

Consequently, we have that \( \tilde{\Psi}(g, u) = \tilde{\Psi}(g_{\beta}, u_{\alpha}) \) for some \( \beta \in \mathbb{R}^n \) and \( \alpha \in \mathbb{R}^n. \) This completes the proof.

\[ \square \]

**E Proof of Proposition 7**

**Proposition 7.** Given a set of i.i.d. samples \( \{(x_i, y_i, z_i)\}_{i=1}^{n} \) from \( \mathcal{P}(X, Y, Z), \) let \( K := \Phi \Sigma \) and \( L := \Sigma \Sigma \) be the Gram matrices such that \( K_{ij} = k(x_i, x_j) \) and \( L_{ij} = l(w_i, w_j) \) where \( w_i := (y_i, z_i). \) Then, \( \hat{g} = \Phi \beta \) where
\[
\beta = (MK + n\lambda_2 K)^{-1}My,
\]
with \( M := K(L + n\lambda_1 I)^{-1}L. \)

**Proof.** It follows from (13) that the structural function \( g^* \in \mathcal{G} \) satisfies
\[
(C_{XW}(C_W + \lambda_1 I)^{-1}C_{WX} + \lambda_2 L)g^* = C_{XW}(C_W + \lambda_1 I)^{-1}b.
\]
Replacing the population quantities with the empirical counterparts \( \hat{C}_{XW} = \frac{1}{n} \Phi \Sigma \Sigma^{\top}, \hat{C}_{W} = \frac{1}{n} \Sigma \Sigma^{\top}, \) and \( b = \frac{1}{n} \Sigma \gamma \) yields
\[
(\Phi \Sigma^{\top} (\Sigma \Sigma^{\top} + n\lambda_1 I)^{-1} \Sigma \Sigma^{\top} + n\lambda_2 L)g^*
= \Phi \Sigma^{\top} (\Sigma \Sigma^{\top} + n\lambda_1 I)^{-1} \Sigma \gamma.
\]
Using the identity \( \Sigma^{\top} (\Sigma \Sigma^{\top} + n\lambda_2 L)^{-1} \Sigma \Sigma^{\top} = (\Sigma^{\top} \Sigma + n\lambda_1 I)^{-1} \Sigma \Sigma^{\top} \), we can write the above equation as
\[
(\Phi \Sigma^{\top} (\Sigma \Sigma^{\top} + n\lambda_1 I)^{-1} \Sigma \Sigma^{\top} + n\lambda_2 \Sigma^{\top})g^*
= \Phi \Sigma^{\top} (\Sigma \Sigma^{\top} + n\lambda_1 I)^{-1} \Sigma \gamma.
\]
By Lemma 6, \( g^* = \Phi \beta \) for some \( \beta \in \mathbb{R}^n. \) Substituting back into the equation above yields
\[
\Phi (L + n\lambda_1 I)^{-1} L \Phi \beta + n\lambda_2 \Phi \beta
= \Phi (L + n\lambda_1 I)^{-1} L \gamma.
\]
The identity \( (\Sigma^{\top} \Sigma + n\lambda_1 I)^{-1} \Sigma \Sigma^{\top} = (\Sigma^{\top} \Sigma + n\lambda_1 I)^{-1} \Sigma \Sigma^{\top} \) gives
\[
(\Phi (L + n\lambda_1 I)^{-1} L \Phi) \beta + n\lambda_2 \Phi \beta
= \Phi (L + n\lambda_1 I)^{-1} L \gamma.
\]
Multiplying both sides of the equation by \( \Phi^{\top} \) gives
\[
\Phi^{\top} \Phi (L + n\lambda_1 I)^{-1} L \Phi \beta + n\lambda_2 \Phi^{\top} \Phi \beta
= \Phi^{\top} \Phi (L + n\lambda_1 I)^{-1} L \gamma.
\]

Setting \( M = K(L + n\lambda_1 I)^{-1} L \) yields the result. \( \square \)

**F Proof of Consistency**

Before diving into the proof, we set up the notation and outline prior results that will be used in the proof.
Notation. For ease of understanding, we will use the following notation throughout the proof:

\[
\begin{align*}
\mathcal{R} & := C_{XW}C_{W}^{-1}C_{WX} \\
\hat{\mathcal{R}} & := \hat{C}_{XW}\hat{C}_{W}^{-1}\hat{C}_{WX} \\
\mathcal{R}_{\lambda_1} & := C_{XW}(C_{W} + \lambda_1 I)^{-1}C_{WX} \\
\hat{\mathcal{R}}_{\lambda_1} & := \hat{C}_{XW}((\hat{C}_{W} + \lambda_1 I)^{-1}\hat{C}_{WX} \\
\mathcal{C}_{\lambda_1} & := C_{W} + \lambda_1 I \\
\hat{\mathcal{C}}_{\lambda_1} & := \hat{C}_{W} + \lambda_1 I \\
\end{align*}
\]

We use the following equality heavily in our proof.

\[
(B^{-1} - A^{-1}) = B^{-1}(A - B)A^{-1}.
\] (17)

Proof. Recall the assumption that \(C_{W}^{-1}\) and \((C_{XW}C_{W}^{-1}C_{W}^{T})^{-1}\) exist. For the sake of simplicity, we also assume that \(|C_{W}^{-1}|_{op} \leq \frac{1}{\delta^2}\) and \(|(C_{XW}C_{W}^{-1}C_{W}^{T})^{-1}|_{op} \leq \frac{1}{\delta^2}\). We denote \((C_{W} + \lambda I)^{-1}\) as \(C_{W,\lambda}^{-1}\) and \(\hat{C}_{W,\lambda}^{-1}\) as its empirical counterpart. Hence we have our empirical estimate:

\[
\hat{g}_{\lambda} = (\hat{\mathcal{R}}_{\lambda_1} + \lambda_2 I)^{-1}\hat{C}_{XW}\hat{C}_{\lambda_1}^{-1}b.
\]

Similarly, under our assumption, the true population function:

\[
g^{*} = \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b.
\]

Our goal is the bound the difference of \(\hat{g}_{\lambda}\) and \(g^{*}\) in RKHS norm. Now, let us consider the following \(|\hat{g}_{\lambda} - g^{*}|_{\mathcal{A}}\):

\[
|\hat{g}_{\lambda} - g^{*}|_{\mathcal{A}} = ||(\hat{\mathcal{R}}_{\lambda_1} + \lambda_2 I)^{-1}\hat{C}_{XW}\hat{C}_{\lambda_1}^{-1}b - \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
\leq ||(\hat{\mathcal{R}}_{\lambda_1} + \lambda_2 I)^{-1}\hat{C}_{XW}\hat{C}_{\lambda_1}^{-1}b - (\mathcal{R} + \lambda_2 I)^{-1}\mathcal{C}_{W}C_{\lambda_1}^{-1}b||_{\mathcal{A}} \\
+||(\mathcal{R}_{\lambda_1} + \lambda_2 I)^{-1}\mathcal{C}_{XW}C_{\lambda_1}^{-1}b - \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
\]

Bounding \(T_{21}\): Let us consider \(T_{21}\) first.

\[
T_{21} = \|((\mathcal{R}_{\lambda_1} + \lambda_2 I)^{-1}\mathcal{C}_{XW}C_{\lambda_1}^{-1}b - \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
= \lambda_2\|((\mathcal{R}_{\lambda_1} + \lambda_2 I)^{-1}\mathcal{C}_{XW}C_{\lambda_1}^{-1}b - \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
\leq \lambda_2\|((\mathcal{R}_{\lambda_1} + \lambda_2 I)^{-1}\mathcal{C}_{XW}C_{\lambda_1}^{-1}b - \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
\leq \lambda_2\|((\mathcal{R}_{\lambda_1} + \lambda_2 I)^{-1}(\mathcal{C}_{XW}C_{\lambda_1}^{-1}C_{WX} + C_{\lambda_1}^{T})b - \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
= \mathcal{R}_{\lambda_1}^{2}\|\mathcal{C}_{XW}C_{\lambda_1}^{-1}b||_{\mathcal{A}} \\
\leq \lambda_2\|\mathcal{R}_{\lambda_1}^{2}\|\mathcal{C}_{XW}C_{\lambda_1}^{-1}b||_{\mathcal{A}} \\
\leq \frac{\lambda_2}{\delta^2}\|\mathcal{C}_{XW}C_{\lambda_1}^{-1}b||_{\mathcal{A}} \\
\leq \frac{\lambda_2}{\delta^2}\|\mathcal{C}_{XW}C_{\lambda_1}^{-1}b||_{\mathcal{A}} \\
\]

Equation 17.

Hence, \(T_{21} = O(\lambda_2)\). From the above argument it is also clear that there exists a positive constant \(c\) such that \(\|\mathcal{C}_{XW}C_{\lambda_1}^{-1}b||_{\mathcal{A}}, \|\mathcal{C}_{XW}C_{\lambda_1}^{-1}b||_{\mathcal{A}} \leq C\).

Bounding \(T_{22}\): Let us now consider the term \(T_{22}\).

\[
T_{22} = \|\mathcal{R}_{\lambda_1}^{-1}\mathcal{C}_{XW}C_{\lambda_1}^{-1}b - \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
\leq \mathcal{R}_{\lambda_1}^{-1}\|\mathcal{C}_{XW}C_{\lambda_1}^{-1}b - \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
+\mathcal{R}_{\lambda_1}^{-1}\|\mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
\leq \mathcal{R}_{\lambda_1}^{-1}\|\mathcal{C}_{XW}C_{\lambda_1}^{-1}b - \mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
+\mathcal{R}_{\lambda_1}^{-1}\|\mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
\leq \mathcal{R}_{\lambda_1}^{-1}\||\mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
+\mathcal{R}_{\lambda_1}^{-1}\||\mathcal{R}^{-1}C_{XW}C_{W}^{-1}b||_{\mathcal{A}} \\
\]

Further, we have:

\[
T_{22} \leq \frac{\lambda C}{\delta^2}\||\mathcal{R}^{-1}C_{XW}C_{\lambda_1}^{-1}C_{WX}||_{\mathcal{A}} \\
+\||\mathcal{R}^{-1}C_{XW}(C_{\lambda_1}^{-1} - C_{W}^{-1})b||_{\mathcal{A}} \\
\]

Let us consider now the following term in the above inequality:

\[
||\mathcal{R}_{\lambda_1}^{-1}||_{op} \leq ||\mathcal{R}^{-1}||_{op} + ||\mathcal{R}_{\lambda_1}^{-1} - \mathcal{R}^{-1}||_{op} \\
\leq \frac{1}{\delta^2} + ||\mathcal{R}_{\lambda_1}^{-1} - \mathcal{R}^{-1}||_{op} \\
\leq \frac{1}{\delta^2} + ||\mathcal{R}_{\lambda_1}^{-1}||_{op}||\mathcal{R}^{-1}||_{op}||\mathcal{R}_{\lambda_1} - \mathcal{R}||_{op} \\
= \frac{1}{\delta^2} + ||\mathcal{R}_{\lambda_1}^{-1}||_{op}||\mathcal{R}^{-1}||_{op}||\mathcal{C}_{XW}(C_{\lambda_1}^{-1} - C_{W}^{-1})C_{WX}||_{op} \\
= \frac{1}{\delta^2} + \lambda_1||\mathcal{R}_{\lambda_1}^{-1}||_{op}||\mathcal{R}^{-1}||_{op}||\mathcal{C}_{XW}(C_{\lambda_1}^{-1} - C_{W}^{-1})C_{WX}||_{op} \\
\]

Now, \(||\mathcal{C}_{XW}C_{\lambda_1}^{-1}C_{WX}||_{op} \leq \frac{\epsilon}{\delta^2}\) similarly \(||\mathcal{C}_{XW}(C_{\lambda_1}^{-1} - C_{W}^{-1})b||_{\mathcal{A}} \leq \frac{\epsilon}{\delta^2}\) for some positive
real numbers $\hat{c}$ and $\hat{c}$. Hence,

$$\|R_{\lambda_1}^{-1}\|_{op} \leq \frac{1}{\delta_2} + \frac{\lambda_1 \hat{c}}{\delta_1 \delta_2} \|R_{\lambda_2}^{-1}\|_{op} \Rightarrow \|R_{\lambda_1}^{-1}\|_{op} \leq \frac{1/\delta_2}{1 - \frac{\lambda_1 \hat{c}}{\delta_1 \delta_2}}$$

Hence, if $\lambda_1 \to 0$ fast enough then

$$T_{22} \leq \lambda_1 \hat{C}$$  (22)

for a positive real number $\hat{C}$. This implies $T_{22} = O(\lambda_1)$.

**Bounding $T_1$:** Now, we will consider the first term for our evaluation.

$$T_1 = ||(R_{\lambda_1} + \lambda_2 I)^{-1} \hat{C}_{XW} C_{\lambda_1}^{-1} \hat{b} - (R_{\lambda_1} + \lambda_2 I)^{-1} C_{XW} C_{\lambda_1}^{-1} b||_G$$

$$\leq ||(R_{\lambda_1} + \lambda_2 I)^{-1} \hat{C}_{XW} C_{\lambda_1}^{-1} b||_G$$

$$\leq \|C_{XW} C_{\lambda_1}^{-1} b\|_G$$  (23)

**Bounding $T_{11}$:** Consider the following term:

$$T_{11} = ||(R_{\lambda_1} + \lambda_2 I)^{-1} \hat{C}_{XW} C_{\lambda_1}^{-1} \hat{b} - (R_{\lambda_1} + \lambda_2 I)^{-1} C_{XW} C_{\lambda_1}^{-1} \hat{b}||_G$$

$$\leq \|C_{XW} C_{\lambda_1}^{-1} \hat{b}\|_G \|C_{XW} C_{\lambda_1}^{-1} \hat{b} - C_{XW} C_{\lambda_1}^{-1} \hat{b}\|_G$$

$$\leq \frac{C}{\lambda_1 \lambda_2^2} \|R_{\lambda_1} - R_{\lambda_1'}\|_{op}$$

for some positive constant $C$. Now,

$$\|C_{XW} C_{\lambda_1}^{-1} \hat{C}_{XW} - C_{XW} C_{\lambda_1}^{-1} C_{XW}\|_{op}$$

$$\leq \|\hat{C}_{XW} C_{\lambda_1}^{-1} \hat{C}_{XW} - C_{XW} C_{\lambda_1}^{-1} \hat{C}_{XW}\|_{op}$$

$$+ \|\hat{C}_{XW} C_{\lambda_1}^{-1} \hat{C}_{XW} - C_{XW} C_{\lambda_1}^{-1} C_{XW}\|_{op}$$

$$\leq \|\hat{C}_{XW} (C_{\lambda_1}^{-1} - C_{\lambda_1}^{-1}) \hat{C}_{XW}\|_{op}$$

$$+ \|\hat{C}_{XW} C_{\lambda_1}^{-1} \hat{C}_{XW} - C_{XW} C_{\lambda_1}^{-1} C_{XW}\|_{op}$$

$$\leq \|\hat{C}_{XW} C_{\lambda_1}^{-1} \hat{C}_{XW} - C_{XW} C_{\lambda_1}^{-1} C_{XW}\|_{op}$$

$$+ \|\hat{C}_{XW} C_{\lambda_1}^{-1} \hat{C}_{XW} - C_{XW} C_{\lambda_1}^{-1} C_{XW}\|_{op}$$

From the $\sqrt{m}$ consistency of covariance and cross-covariance operator, we have:

$$\|\hat{C}_{XW} C_{\lambda_1}^{-1} \hat{C}_{XW} - C_{XW} C_{\lambda_1}^{-1} C_{XW}\|_{op} = O\left(\frac{1}{\lambda_1 \sqrt{m}}\right)$$

Hence, as far as $\lambda_1 \lambda_2^2$ goes slower to $0$ then $1/\sqrt{m}$ then $T_{11}$ converges to zero asymptotically.