Modular Regression

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Abstract

This paper develops a new framework, called modular regression, to utilize auxiliary information – such as variables other than the original features or additional data sets – in the training process of linear models. At a high level, our method follows the routine: (i) decomposing the regression task into several sub-tasks, (ii) fitting the sub-task models, and (iii) using the sub-task models to provide an improved estimate for the original regression problem. This routine applies to widely-used low-dimensional (generalized) linear models and high-dimensional regularized linear regression. It also naturally extends to missing-data settings where only partial observations are available. By incorporating auxiliary information, our approach improves the estimation efficiency and prediction accuracy compared to linear regression or the Lasso under a conditional independence assumption. For high-dimensional settings, we develop an extension of our procedure that is robust to violations of the conditional independence assumption, in the sense that it improves efficiency if this assumption holds and coincides with the Lasso otherwise. We demonstrate the efficacy of our methods with both simulated and real data sets.

1 Introduction

Suppose for a patient subject to a surgical procedure, we are interested in predicting their future health outcome $Y \in \mathbb{R}$ in two years using some features $X \in \mathbb{R}^p$ collected at the time of the surgery. The standard approach is supervised learning: The training data containing $n$ observations $\{(X_i,Y_i)\}_{i=1}^n$ from previous patients is used to pick a predictor $\hat{f}: \mathbb{R}^p \rightarrow \mathbb{R}$ that minimizes the average prediction error $\frac{1}{n} \sum_{i=1}^n \ell(f(X_i),Y_i)$ over $f \in \mathcal{F}$ for some loss function $\ell: \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ and some function class $\mathcal{F}$.

However, the long duration of the study can pose various practical challenges to this paradigm. The number of joint observations of $(X,Y)$ may be very limited because they take at least two years to collect. The training data may also contain intermediate measurements $Z$, such as the health outcome one year after their surgery. In addition, there may be some patients for which we only observe $(X,Z)$ which are easier to collect. It is also probable that another data set provides several $(Z,Y)$ samples from patients who had surgery more than two years ago, but their features $X$ were missing due to limited technology. In this case, the standard approach of empirical risk minimization only over $(X,Y)$ samples falls short in terms of making use of auxiliary variables or additional partial observations to improve the learning performance.

In this work, we aim to build a framework for flexibly incorporating auxiliary information into generic estimation and prediction procedures while maintaining rigorous guarantees. Such information may come from other variables $Z$ in addition to the original features and responses in the training process; it may
also be additional data sets that only cover a subset of variables. We will generalize the ideas of leveraging independence structures from the missing data literature to prediction problems such as (generalized) linear models, and develop more robust methods that work for general dependence patterns. Let us begin with the tasks we consider.

A common algorithmic structure. We focus on statistical learning algorithms that take the form

$$\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^{p_x}} \frac{1}{n} \sum_{i=1}^{n} \left\{ h(X_i, \theta) - Y_i X_i^\top \theta \right\},$$

(1)

where \( h: \mathcal{X} \times \mathbb{R}^{p_x} \to \mathbb{R} \) is a known function that is convex in \( \theta \), and \( p_x \in \mathbb{N} \) is the dimension of the original features. The simplest example is ordinary least squares (OLS):

$$\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^{p_x}} \frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{1}{2} \theta^\top X_i X_i^\top \theta - Y_i X_i^\top \theta \right\}.$$  

Logistic regression with \( Y \in \{0,1\} \) also satisfies (1):

$$\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^{p_x}} \frac{1}{n} \sum_{i=1}^{n} \left\{ \log(1 + \exp(X_i^\top \theta)) - Y_i X_i^\top \theta \right\}.$$  

We will later extend to other generalized linear models as we develop our method. The final example we consider is the high-dimensional \( \ell_1 \)-regularized linear regression (Tibshirani, 1996):

$$\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^{p_x}} \left\{ -\frac{1}{n} \sum_{i=1}^{n} Y_i X_i^\top \theta + \theta^\top \left( \frac{1}{2n} \sum_{i=1}^{n} X_i X_i^\top \right) \theta + \lambda \|\theta\|_1 \right\}. $$

(2)

In the situation we discuss at the beginning, the supervised learning estimators of the form (1) may not be able to utilize auxiliary data. Instead of minimizing equation (1), we propose an alternative risk minimization criterion:

$$\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^{p_x}} \left\{ \frac{1}{n} \sum_{i=1}^{n} h(X_i, \theta) - \hat{C}^\top \theta \right\},$$

where \( \hat{C} \) is a proxy term for \( C := \mathbb{E}[XY] \) computed from the data. We will see that the learning performance of \( \hat{\theta} \) is closely related to the estimation accuracy of \( \hat{C} \) for \( C \). At a high level, our idea is to replace \( \frac{1}{n} \sum_{i=1}^{n} X_i Y_i \) by a proxy \( \hat{C} \) with negligible bias and a lower variance, which translates to the improved performance of \( \hat{\theta} \). We achieve this by developing a “modular” estimator \( \hat{C} \) – whose meaning will be made precise soon – that naturally allows for flexible incorporation of auxiliary information to improve the learning performance.

We do emphasize that we still target at minimizing the same population risk as using \( \frac{1}{n} \sum_{i=1}^{n} X_i Y_i \). As a result, the estimator still converges to the same limit, such as the best linear predictor from \( X \) for \( Y \) in the OLS case.

1.1 Leveraging the dependence structure

The driving force for constructing the proxy term \( \hat{C} \) is to leverage the dependence structures among the variables. More precisely, certain conditional independence structure allows us to incorporate auxiliary information to improve efficiency while providing rigorous statistical guarantees.

Conditional independencies are often used to improve performance over saturated models. As a classical example, suppose we have i.i.d. copies of a vector \((X, Y)\) that satisfies that \( X_{-S} \) is conditionally independent of \( Y \) given \( X_S \), where \( X_S \) denotes a subset \( S \) of features, and \( X_{-S} \) stores the remaining ones. Using standard mathematical notation, we equivalently write \( X_{-S} \perp \perp Y | X_S \). It is known that running a regression of \( Y \) on \( X_S \) can have lower mean-squared error than running a regression of \( Y \) on \( X \), since the latter may have very large variance (see, e.g., Hastie et al. (2009) for more intuition). However, the former estimate may be biased.
if the conditional independence relation is not satisfied. Furthermore, even if the conditional independence relationship holds for some set $S$, the set $S$ is generally unknown. It is common to use model selection methods such as the best subset selection, Lasso, AIC, or BIC to navigate the bias-variance tradeoff.

Perhaps less widely known is that conditional independence structures of the type $Y \perp X_S | Z$ for auxiliary variables $Z$ can also be leveraged to improve estimation and prediction performance. Analogous to classical model selection strategies, we want to derive a data-driven strategy to learn and exploit such structures. To fix ideas, let us consider an extreme case where $X \perp Y | Z$.

**A naive approach.** If $X \perp Y | Z$, we can re-write

$$E[XY] = E[E[X | Z]E[Y | Z]]. \tag{3}$$

Assuming access to i.i.d. copies $\{(X_i, Y_i, Z_i)\}_{i=1}^n$, in view of (3), we can (i) estimate $E[Y | Z = z]$ via $\hat{\mu}_y(z)$, (ii) estimate $E[X | Z = z]$ via $\hat{\mu}_x(z)$ and (iii) combine these two estimates to compute $\hat{C} = \frac{1}{n} \sum_{i=1}^n \hat{\mu}_y(Z_i) \hat{\mu}_x(Z_i)$ for $C = E[XY]$. If $\hat{\mu}_x$ and $\hat{\mu}_y$ are accurate, then this estimate has smaller variance than $\frac{1}{n} \sum_{i=1}^n X_i Y_i$, as

$$\text{Var}(\hat{\mu}_y(Z) \hat{\mu}_x(Z)) \approx \text{Var}(E[Y | Z]E[X | Z]) = \text{Var}(E[XY | Z]) \leq \text{Var}(XY).$$

However, this naive approach has a pressing issue that may hinder its performance: even if (3) holds, there can be considerable bias if the estimation of $\hat{\mu}_y$ and $\hat{\mu}_x$ has slow convergence rates. In this case, $\hat{C}$ is not a good estimator for $C$ because the bias $E[\hat{C}] - C$ can be much larger than the variance of $\frac{1}{n} \sum_{i=1}^n X_i Y_i$.

**A better approach.** The bias issue can be resolved using ideas from semi-parametric statistics. When $X \perp Y | Z$, we can rewrite

$$E[XY] = E[E[X | Y | Z] + E[E[X | Z]Y] - E[E[X | Z]E[Y | Z]].$$

Again, this can be turned into an estimator by conducting three sub-tasks: (i) estimating $E[Y | Z = z]$ via $\hat{\mu}_y(z)$, (ii) estimating $E[X | Z = z]$ via $\hat{\mu}_x(z)$, and (iii) combining these two estimates via

$$\hat{C} = \frac{1}{n} \sum_{i=1}^n \hat{\mu}_y(Z_i) X_i + Y_i \hat{\mu}_x(Z_i) - \hat{\mu}_y(Z_i) \hat{\mu}_x(Z_i). \tag{4}$$

We will show that a slight variation of this approach has very favorable properties. Most importantly, even if $\hat{\mu}_y$ and $\hat{\mu}_x$ converge to the ground truth at slow speed, the bias of $\hat{C}$ in (4) can be negligible compared to its variance, and one can check that it has a lower variance than $\frac{1}{n} \sum_{i=1}^n X_i Y_i$:

$$n \cdot \text{Var}(\hat{C}) \approx \text{Var}(XY) - \text{Var} ((X - \mu_x(Z)) \cdot (Y - \mu_y(Z))) \leq \text{Var}(XY).$$

Indeed, it leads to an estimator $\hat{\theta}$ that is the most efficient (unbiased with the smallest asymptotic variance) if $X \perp Y | Z$ holds. This approach also opens a door for data fusion: The three terms in (4) only depend on pairwise observations of $(X, Z)$ or $(Z, Y)$. Thus, it can flexibly utilize additional data to improve estimation accuracy, and works even when no joint observations of $(X, Z, Y)$ are available.

There remain several issues with this improved approach. First, under the conditional independence condition, there are some nuances of how to obtain the estimators $\hat{\mu}_x$ and $\hat{\mu}_y$ to avoid bias in $\hat{C}$; we also have to prove rigorously that the proposed approach may lead to improved estimation and prediction performance for the original task. Furthermore, from a practical perspective, $Y \perp X | Z$ may not hold in general. A more realistic setting is $Y \perp X_S | Z$ for variables in an unknown subset $S$, or $E[XY] \approx E[E[Y | Z]E[X | Z]]$ instead of exact equality. In such cases, we need to carefully trade off between bias and variance. Finally, to fulfill the potentials in flexible data fusion, we need to develop concrete procedures for incorporating additional data sets with theoretical justifications. To resolve these issues, we are to develop a rigorous statistical framework to turn the ideas discussed above into a principled approach.
1.2 A modular regression framework

The derivation above gives a hint on our proposal. We will decompose the estimation of \( E[XY] \) into smaller modules – each being a sub-task that involves a subset of variables such as \((Y,X)\), \((Y,Z)\) or \((Z,X)\) – and then re-assemble the modules to construct \( \hat{C} \). This idea generalizes (4), and is visualized in Figure 1.

![Diagram](a) Conditional independencies can be leveraged to decompose statistical tasks into subtasks. (b) Modularity allows combining multiple datasets.

Figure 1: Our approach to decomposing the estimation of \( C = E[YX] \) tackles two settings that may seem different at first sight. In (a), one can leverage conditional independencies to reduce statistical uncertainty. In (b), one can use additional partial observations to increase the effective sample size.

As shown in panel (a), our method adapts to specific structures, such as conditional independence between variables, so as to ensure a properly chosen decomposition and to reduce statistical uncertainty with rigorous theoretical guarantee. Such structure can also be learned from data when it is unknown. Furthermore, by the decomposition, our method easily adapts to data availability; see panel (b) of Figure 1. As long as a data set covers the variables needed in a sub-task, it can be incorporated to increase the effective sample size. We summarize our main results as follows.

- **Modular linear regression.** We develop a generic approach for decomposing the estimation and prediction in (generalized) linear models into smaller modules. This is achieved by rewriting the estimation equation when some auxiliary variables are observed. Leveraging semi-parametric theory, we show that our approach leads to a more efficient estimator under the assumption that the auxiliary variables capture all the information for predicting the response. A similar statement holds in cases where the auxiliary variables satisfy a conditional independence criterion for only a subset of the variables.

- **High-dimensional modular regression.** By adding \( \ell_1 \)-regularization, our tools extend to the high-dimensional setting where the number of covariates grow larger than the sample size. We leverage the conditional independence assumption to develop a proxy empirical risk that has negligible bias and lower variance than the empirical risk of the Lasso. We show that this results in improved bounds for prediction accuracy asymptotically.

- **Robustness under conditional dependence.** Since the conditional independence assumption may be violated in practice, we develop an extension of our method that adapts to the conditional dependency structures among variables, and we allow such structures to be learned from data. To be more precise, the proposed procedure interpolates between conventional linear regression (non-modular) and the fully-modular approach (which is efficient under the conditional independence condition). It is robust to potential violations of the conditional independence assumption while potentially improving efficiency with rigorous statistical guarantees.

- **Data fusion.** We further develop an extension of our method that is able to combine multiple data sets. This formulation allows using additional data on sub-tasks to improve overall statistical efficiency.

The rest of the paper is organized as follows. Section 2 develops modular (generalized) linear regression in the fixed-\( p \) setting. Section 3 studies modular regression for penalized linear regression in high dimensions, and develops a robust variant that can adapt to different dependence structures. Applications to data fusion and partial observations are discussed in Section 4. Finally, we evaluate our methods on simulated datasets in Section 5 and apply them to real datasets in Section 6.
1.3 Related work

Modular regression combines evidence from sub-tasks, leveraging a “modular structure” provided by the conditional independence. One related strand is to use surrogates instead of an outcome of interest that is too difficult to measure (Fleming et al., 1994; Post et al., 2010). In particular, in the causal inference literature, when the access to some long-term outcome is limited, a series of work (Prentice, 1989; Lauritzen et al., 2004; Chen et al., 2007; VanderWeele, 2013; Athey et al., 2016, 2019; Kallus and Mao, 2020) have advocated using intermediate (short-term) outcome(s) as “surrogates” for the long-term outcome, and assumes various surrogate conditions, such as conditional independence of the long-term outcome and the treatment given the surrogates. In their context, similar to our approach, the surrogate condition is the key to “modularity”, allowing to decompose the treatment effect estimation task into sub-tasks of estimating the effect of the treatment on the intermediate outcome and estimating the effect of the intermediate outcome on the long-term outcome. Distinct from this strand of work, we work under a generic conditional independence condition and mainly focus on the regression and prediction tasks instead of treatment effect estimation. In addition, we propose a method that adapts to dependence structures in the data and is robust to violations of the conditional independence assumption.

Our framework is naturally related to missing data approaches and in particular data fusion, which combines data sets that cover different subsets of variables. The preceding paragraph is also related; for example, Athey et al. (2016, 2019) combine treatment, surrogates and the long-term outcome in separate datasets, Kallus and Mao (2020) assumes a few full treatment-surrogate-outcome triples are available as supplements, etc. More generally, there has been a surge of interest in combining different data sets, such as combining experimental and observational data for treatment effect estimation (Rosenman et al., 2022, 2020; Colnet et al., 2020), generalizing inference to different populations (Dahabreh et al., 2019; Hartman et al., 2015; Jin and Rothenhausler, 2021), so on and so forth. Many of these works require identifiability assumptions for the target estimand, which are often similar to the conditional independence condition. These works often concern treatment effect or population mean estimation, while we study the regression and prediction tasks in (high-dimensional) linear models. In addition, we also develop variants that are robust to violation of the conditional independence assumption.

In a missing data scenario, some other works study general regression estimators in settings that differ from ours. Those for high-dimensional data include Loh and Wainwright (2011) on penalized regression, Lounici (2014); Cai and Zhang (2016) on the estimation of covariance matrices, and Elsener and van de Geer (2019); Zhu et al. (2019) on sparse principal component analysis, which consider estimation when some covariates are missing at random. In contrast, we focus more on the data fusion aspect for combining data sets; we draw ideas from semiparametric statistics, and our setting needs more consideration for the dependence structure among variables. Closer to ours is the recent work of Cannings and Fan (2022) on U-statistics with low-dimensional data, which aims at devising an estimator with smaller prediction MSE by incorporating a partially missing data set. In contrast, our approach leverages the conditional independence structures among variables instead of correlation between estimators; we focus on regression problems and consider the high dimensional regime.

Our efficient modular estimator is inspired by recent progress in efficient regression adjustment (Henckel et al., 2019; Rotnitzky and Smucler, 2019) that operates under a low-dimensional graphical model. Compared to them, our framework is more general as it applies to (generalized) linear models, works for high dimensional settings, does not require knowing the graphical structure, and imposes minimal model assumptions; it is also more restricted in that we do not consider choosing the optimal covariate sets.

Our modular estimator is shown to be optimal for linear regression under the conditional independence assumption, in the sense of semiparametric efficiency (Bickel et al., 1993; Tsiatis, 2006). Thus, this work is also connected to the literature of efficient estimation for missing data. Furthermore, our estimator enjoys double robustness properties similar to the AIPW estimator (Robins et al., 1994), among many others, while our results are for linear regression which differs from the causal inference task.

The conditional independence structure has been used in a series of early works (Sargan, 1958; Hansen, 1982) to improve estimation efficiency; also related is Causeur and Dhorne (2003) on linear regression under conditional independence, which is close to related to our first modular regression algorithm in low dimensions.
However, these works assume strong parametric models such as a joint Gaussian distribution and independent Gaussian noise, while our method does not require stringent model assumptions.

**Notations.** We use the standard $O_p(\cdot)$ and $o_P(\cdot)$ notation to denote smaller order in probability. For any two sequences $\{a_n\}$ and $\{b_n\}$ of positive numbers, we denote $a_n = O(b_n)$ if $\lim_{n \to \infty} a_n/b_n < \infty$ and $\lim_{n \to \infty} b_n/a_n < \infty$; we denote $a_n = O(b_n)$ if $a_n/b_n \leq C$ for some constant $C > 0$. We use $\mathbb{P}_{X,Y,Z}$ to denote the joint distribution of $(X, Y, Z)$. For any functions $f, g : Z \to \mathbb{R}^d$, we denote their $L_2$-distance as $\|f - g\|_{L_2(\mathbb{P}_Z)}^2 = \mathbb{E}[\|f(Z) - g(Z)\|^2_2]$, where $\| \cdot \|_2$ is the Euclidean norm and the expectation is with respect to the distribution $\mathbb{P}_Z$ of $Z$. For any vector $v \in \mathbb{R}^t$ and positive definite matrix $\Sigma \in \mathbb{R}^{t \times t}$ we set $\|v\|_\Sigma^2 = v^\top \Sigma v$.

## 2 Modular linear regression in low dimensions

We first introduce our modular regression in low-dimensional linear models, allowing $X \in \mathbb{R}^{p_x}$ and $Z \in \mathbb{R}^{p_z}$ to be random vectors, where $p_x$ and $p_z$ do not grow with $n$ asymptotically. We consider a scenario where conditional independence allows for decomposing the task into sub-tasks.

**Assumption 2.1.** The joint distribution of $(X, Z, Y)$ satisfies $X \perp \right Y \mid Z$.

In this section, we use this working assumption to show how conditional independencies can be leveraged to improve estimation accuracy. It will be relaxed later in Section 3.3, where we develop a method that is robust to violations of Assumption 2.1. Intuitively, Assumption 2.1 ensures that $Z$ contains all the information in $Y$ that is relevant to $X$. While this assumption seems strong, it is reasonable in many situations and has been widely used in a variety of applications. For example, $Z$ could be an intermediate outcome in the training data that is unavailable for the test samples, while $Y$ is a long-term outcome of interest. Intermediate outcomes are widely used as a proxy in estimating long-term treatment effects (Athey et al., 2016, 2019), while we focus on regression and do not necessarily consider a causal inference problem.

### 2.1 Modular linear regression

For simplicity of exposition, we start with linear (OLS) regression to show the benefits of a modular structure. Our goal is to predict $Y \in \mathbb{R}$ by $\hat{Y} = X^\top \theta$ for some $\theta \in \mathbb{R}^{p_x}$, but we do not necessarily assume a well-posed linear model. In the training process, we have observations of i.i.d. triples $\{(X_i, Y_i, Z_i)\}_{i=1}^n$ for some auxiliary variables $Z_i \in \mathbb{R}^{p_z}$, and $X_i \in \mathbb{R}^{p_x}$ are random vectors (we view all vectors as column vectors throughout). The training and the target distributions are induced by the same distribution $\mathbb{P}_{X,Y,Z}$.

Modular regression proceeds in three steps to leverage the conditional independence structure.

1. **Decompose into sub-tasks.** First, the conditional independence structure in Assumption 2.1 allows us to decompose the estimation of $\mathbb{E}[XY]$ into sub-tasks that only involve observations of $(X, Z)$ or $(Y, Z)$.

2. **Solve the sub-tasks.** We then learn the conditional mean functions. We use cross-fitting (Chernozhukov et al., 2018) to ensure desirable statistical properties: we randomly split $\mathcal{I} = \{1, \ldots, n\}$ into two disjoint folds $\mathcal{I}_1, \mathcal{I}_2$. Then for each fold $k = 1, 2$, we fit models $\mu^x(z) : Z \to \mathbb{R}^{p_x}$ and $\mu^y(z) : Z \to \mathbb{R}$ for $\mu^x(z) = \mathbb{E}[X \mid Z = z]$ and $\mu^y(z) = \mathbb{E}[Y \mid Z = z]$ using data in $\mathcal{I}\backslash\mathcal{I}_k$.

3. **Assemble the sub-tasks.** Finally, we solve a modular least squares regression

$$\hat{\theta}_{n, \text{mod}} = \arg\min_{\theta \in \mathbb{R}^{p_x}} \left\{ \frac{1}{n} \sum_{i=1}^n \theta^\top X_i X_i^\top \theta/2 - \hat{C}_{\text{lim}} \theta \right\},$$

where we use a proxy cross-term

$$\hat{C}_{\text{lim}} = \frac{1}{n} \sum_{i=1}^n [X_i \hat{\mu}_y(Z_i) + \hat{\mu}_x(Z_i) Y_i - \hat{\mu}_x(Z_i) \hat{\mu}_y(Z_i)].$$

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With a slight abuse of notation, we write \( \hat{\mu}_y(Z_i) = \hat{\mu}_y^{(k)}(Z_i) \) and \( \hat{\mu}_x(Z_i) = \hat{\mu}_x^{(k)}(Z_i) \) for \( i \in \mathcal{I}_k \).

The procedure is summarized in Algorithm 1.

**Algorithm 1 Modular linear regression**

**Input:** Dataset \( \mathcal{I} = \{(Y_i, X_i, Z_i)_{i=1}^n \} \).

1. Randomly split \( \mathcal{I} \) into equally-sized folds \( \mathcal{I}_k, k = 1, 2 \).
2. **for** \( k = 1, 2 \) **do**
   3. Fit models \( \hat{\mu}_x^{(k)}(\cdot) \) for \( \mathbb{E}[X \mid Z = \cdot] \) using observations \( (X_i, Z_i), i \notin \mathcal{I}_k \);
   4. Fit models \( \hat{\mu}_y^{(k)}(\cdot) \) for \( \mathbb{E}[Y \mid Z = \cdot] \) using observations \( (Y_i, Z_i), i \notin \mathcal{I}_k \);
   5. Compute \( \hat{\mu}_x(Z_i) = \hat{\mu}_x^{(k)}(Z_i) \) and \( \hat{\mu}_y(Z_i) = \hat{\mu}_y^{(k)}(Z_i) \) for all \( i \in \mathcal{I}_k \).
3. **end for**
4. Compute the proxy cross-term \( \hat{C}_l \) as in (6).

**Output:** The modular linear regression \( \hat{\theta}_n^{\text{mod}} \) as in (5).

### 2.2 Double robustness and semiparametric efficiency

The modular estimator \( \hat{\theta}_n^{\text{mod}} \) is doubly robust with respect to the estimation error of \( \hat{\mu}_{xz} \) and \( \hat{\mu}_{yz} \). To be more precise, the estimator converges at \( n^{-1/2} \) rate to \( \theta^* \) and is semiparametrically efficient even when \( \hat{\mu}_{xz} \) and \( \hat{\mu}_{yz} \) are consistent with slow nonparametric rates, that is if \( \|\hat{\mu}_x - \mu_x\|_{L_2(P_x)} = o_P(n^{-1/4}) \) and \( \|\hat{\mu}_y - \mu_y\|_{L_2(P_y)} = o_P(n^{-1/4}) \). The proof of the next theorem is in Appendix B.1.

**Theorem 2.2.** Suppose \( \|\hat{\mu}_x^{(k)} - \mu_x\|_{L_2(P_x)} \cdot \|\hat{\mu}_y^{(k)} - \mu_y\|_{L_2(P_y)} = o_P(1/\sqrt{n}) \) for \( k = 1, 2 \). Assume \( \mathbb{E}[XX^\top] \succ 0 \) is finite, and entries of \( X(Y - X^\top \theta^*) \) has finite second moments. Then \( \sqrt{n}(\hat{\theta}_n^{\text{mod}} - \theta^*) \overset{d}{\to} \mathcal{N}(0, \Sigma^{\text{mod}}) \) as \( n \to \infty \), where \( \Sigma^{\text{mod}} = \text{Cov}(\phi^{\text{mod}}(X_i, Y_i, Z_i)) \) for \( \phi^{\text{mod}}(x, y, z) = \mathbb{E}[XX^\top]^{-1}(x\mu_y(z) + \mu_x(z)y - \mu_x(z)\mu_y(z) - xx^\top\theta^*) \), and \( \phi^{\text{mod}} \) is the (semiparametrically) efficient influence function for estimating \( \theta^* \).

Theorem 2.2 shows modular regression has the lowest asymptotic variance among all regular estimators (Bickel et al., 1993). We now compare it to the OLS estimator \( \hat{\theta}_n^{\text{ols}} = \arg\min_{\theta \in \mathbb{R}^p} \sum_{i=1}^n (Y_i - X_i^\top \theta)^2 \), which only uses the information in \( (X_i, Y_i) \) pairs. Assuming \( \Sigma := \mathbb{E}[XX^\top] \) is positive-definite, as \( n \to \infty \),

\[
\hat{\theta}_n^{\text{ols}} - \theta^* = \frac{1}{n} \sum_{i=1}^n \phi^{\text{ols}}(X_i, Y_i) + o_P(1/\sqrt{n})
\]

with influence function \( \phi^{\text{ols}}(x, y) = \mathbb{E}[XX^\top]^{-1}(xy - xx^\top\theta^*) \). Under Assumption 2.1, the asymptotic covariance matrix of \( \phi^{\text{mod}}(X_i, Y_i, Z_i) \) is dominated by that of \( \phi^{\text{ols}}(X_i, Y_i) \). Indeed, one can check that

\[
\text{Cov} \left( \phi^{\text{mod}}(X_i, Y_i, Z_i) \right) = \text{Cov} \left( \phi^{\text{ols}}(X_i, Y_i) \right) - \Sigma^{-1} \text{Cov} \left( (Y - \mu_y(Z))(X - \mu_x(Z)) \right) \Sigma^{-1},
\]

where \( \text{Cov}(A) \) denotes the covariance matrix for a random vector \( A \), so that \( \text{Cov} \left( (Y - \mu_y(Z))(X - \mu_x(Z)) \right) > 0 \). More efficient parameter estimation also translates to more accurate prediction: The prediction mean squared error (MSE) for an independent test sample \( (X, Y) \) is \( \mathbb{E}[(X - X^\top \hat{\theta})^2] = \mathbb{E}[(Y - X^\top \theta^*)^2] + \|\hat{\theta} - \theta^*\|_\Sigma^2 \), where the second term is smaller when \( \theta \) is the modular estimator instead of the OLS estimator. In our numerical experiments, we mostly focus on improving prediction in very noisy settings with low sample size because the improvement in \( \|\hat{\theta} - \theta^*\|_\Sigma^2 \) is more pronounced in those cases.

Many practitioners will be interested in quantifying the uncertainty of modular regression estimates. In principle, confidence intervals can be derived using the asymptotic distribution in Theorem 2.2. One may also learn and adapt to the dependence structure from data (see Section 3.3 for a related discussion). In such cases, confidence intervals have to be adjusted to account for the variation induced by estimation of the structure. In practice, one can deal with this issue by data-splitting (i.e., use one fold of data for model selection and the second for estimation) and cross-fitting (Chernozhukov et al., 2018).
Remark 2.3. To gain more intuition on the improvement in parameter estimation, we consider a one-dimensional special case where $Z = \alpha X + \epsilon_z$, $Y = \beta Z + \epsilon_y$ for $\alpha, \beta \in \mathbb{R}$. Here $X \sim N(0, \sigma_z^2)$, and $\epsilon_z \sim N(0, \sigma_z^2)$ are independent random noise. The true parameter for OLS regression is $\theta^* = \alpha \beta$. The OLS estimator $\hat{\theta}_{ols}^*$ has asymptotic variance $\sigma_{ols}^2 = \text{Var}(X)^{-2} \text{Var}(X\epsilon_2 + X\beta \epsilon_1) = \text{Var}(X)^{-1}(\sigma_z^2 + \beta^2 \sigma_z^2)$, and our modular estimator $\hat{\theta}_{mod}^*$ has asymptotic variance $\sigma_{mod}^2 = \text{Var}(X)^{-2} \text{Var}(\mu_x(Z)\epsilon_2 + X\beta \epsilon_1) = \text{Var}(X)^{-1}(\sigma_z^2 \text{Var}(\mu_x(Z))/\text{Var}(X) + \beta^2 \sigma_z^2)$. That is, the absolute improvement in asymptotic variance is $\sigma_{ols}^2 - \sigma_{mod}^2 = \sigma_z^2 \text{Var}(X-Z\mu_x)/\text{Var}(X)^2$; this quantity is large if $\sigma_z^2$ is large or $Z$ explains a small proportion of the variance in $X$, i.e., $\text{Var}(X-Z\mu_x(Z))$ is large compared to $\text{Var}(X)$. The relative improvement in asymptotic variance is $1 - \sigma_{mod}^2/\sigma_{ols}^2 = 1 - \sigma_z^2/\sigma_{ols}^2 + \beta^2$; this quantity is large if $\sigma_z^2$ is large or $\beta^2$ are small, which corresponds to (i) weak signal $\alpha, \beta$, or (ii) large noise $\alpha^2 \sigma_z^2$ and $\beta^2 \sigma_z^2$ are compared to $\sigma_z^2$ and $\sigma_z^2$ are compared to $\sigma_z^2$. In the most extreme case where $\alpha = \beta = 0$, the best prediction is 0, and we achieve the asymptotic variance $\sigma_{mod}^2 = 0$.

2.3 Modular regression in generalized linear models

The ideas outlined in the previous section also apply to generalized linear models (GLMs) as long as the estimation equation has a modular structure we mention in Section 1. We suppose for a loss function

$$\ell: \mathcal{X} \times \mathcal{Y} \times \Theta \rightarrow \mathbb{R},$$

the true parameter $\theta^* \in \Theta \subseteq \mathbb{R}^p$ is the unique minimizer of

$$\mathbb{E}[\ell(X_i, Y_i, \theta^*)], \quad \text{where} \quad \ell(x, y, \theta) = YX^\top \theta + h(x, \theta)$$

for some function $h: \mathcal{X} \times \Theta \rightarrow \mathbb{R}$ that is convex in $\theta$. As usual, a default estimator $\hat{\theta}_{ml}^*$ is the unique minimizer of the empirical loss:

$$\hat{\theta}_{ml}^* = \arg\min_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \{h(X_i, \theta) + Y_iX_i^\top \theta\},$$

(8)

Maximum likelihood estimation for generalized linear models with log links satisfies this condition in general, such as logistic regression with $\ell(x, y, \theta) = -x^\top \theta y + \log(1 + \exp(x^\top \theta))$ for $y \in \{0, 1\}$, Poisson regression with $\ell(x, y, \theta) = -x^\top \theta y + \exp(x^\top \theta)$ for $y \in \mathbb{N}$. More generally, for models such as exponential regression with $\ell(x, y, \theta) = 2\log y \cdot \theta^\top x - (\theta^\top x)^2$ for $y \in \mathbb{R}^+$, one can use the transformed outcome $\tilde{Y} := 2\log(Y)$ to make it a special case of equation (8).

We still follow the approach in Section 2.1 to obtain a more accurate estimator for $C = \mathbb{E}[XY]$. The first two steps are exactly the same as in Section 2.1. In the third step (assemble the sub-tasks), we use the proxy term $\tilde{C}_{lm}$ defined in (6), and compute the modular estimator

$$\hat{\theta}_{mod}^* = \arg\min_{\theta \in \Theta} \left\{ \frac{1}{N} \sum_{i=1}^n h(X_i, \theta) + \tilde{C}_{lm}^\top \theta \right\}.$$  

(9)

This modular estimator is again doubly-robust to the estimation error of $\hat{\mu}_x$ and $\hat{\mu}_y$, and has smaller asymptotic variance than $\hat{\theta}_{ml}^*$ under mild conditions. While the theoretical justification follows similar ideas as before, the technical conditions are slightly more involved, and we defer all the results to Appendix A.

3 Modular linear regression in high dimensions

Many prediction problems involve a huge number of predictive variables, entering the high-dimensional regime where $p_x$ grows with, and can even be large than, the sample size $n$. A popular approach to dealing with high-dimensional data is penalized regression such as the Lasso (Tibshirani, 1996). By assuming a sparse linear regression function, high-dimensional regression has been shown to be consistent under various well-conditioning assumptions on the design matrix (Candes and Tao, 2005, 2007; Van de Geer, 2007; Zhang and Huang, 2008; Bickel et al., 2009; Negahban et al., 2012).

Our modular regression idea extends naturally to the high-dimensional setting. In this section, we show that by including an $\ell_1$ penalty on top of the modular loss we develop in the preceding section, it improves
upon the Lasso by seeking for a more efficient estimation equation. Throughout this section, we assume a sparse linear model to ensure the task is tractable.

**Assumption 3.1.** There exists some $\theta^* \in \mathbb{R}^p$ with $\|\theta^*\|_0 = s$, such that $\mathbb{E}[Y \mid X] = X^T \theta^*$.

### 3.1 Regularized modular regression

We again start with cross-fitting, and let $\hat{\mu}_x^{(k)}$ and $\hat{\mu}_y^{(k)}$ be estimators for $\mu_x(\cdot) = \mathbb{E}[X \mid Z = \cdot]$ and $\mu_y(\cdot) = \mathbb{E}[Y \mid Z = \cdot]$ obtained with $\mathcal{T} \setminus \mathcal{T}_k$, and define the cross-terms exactly the same as in (6). The only difference from the previous case is that we add an $\ell_1$-regularization to encourage sparsity. We define

$$
\hat{\theta}^{\text{mod}}_n = \arg \min_{\theta \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^n \theta^T X_i X_i^T \theta / 2 - C_{\text{lin}} \theta + \lambda \|\theta\|_1 \right\}
$$

(10)

for some regularization parameter $\lambda > 0$, where $\|\theta\|_1 = \sum_{j=1}^p |\theta_j|$. The objective function in (10) is convex in $\theta$, so the optimization problem can be efficiently solved similar to the Lasso (such as coordinate-wise descent). In practice, the parameter $\lambda$ can be determined by cross validation.

### 3.2 Theoretical guarantee

It turns out that, with proper choice of $\lambda$, modular regression leads to a sharper upper bound on the estimation error. We assume a $\mu$-RSC property for the design matrix $X \in \mathbb{R}^{n \times p}$ which is standard in the literature to ensure the consistency of Lasso-type methods (Bickel et al., 2009; Negahban et al., 2012). Our theoretical analysis may be generalized to other conditions, which is beyond the scope of this work.

**Assumption 3.2.** $X \in \mathbb{R}^{n \times p}$ satisfies $\zeta$-Restricted Strong Convexity ($\zeta$-RSC) with respect to $C_3$, i.e., $\|X \Delta\|_2^2 / n \geq \zeta \|\Delta\|_2^2$ for any $\Delta \in C_3$, where $C_3 := \{ x \in \mathbb{R}^p : \|x_{S^c}\|_1 \leq 3 \|x_S\|_1 \}$, and $S = \{ j : \theta^*_j \neq 0 \}$.

We assume entries of $X$ and the response $Y$ are bounded by constants. This condition is mild since the Lasso is often implemented after normalization.

**Assumption 3.3.** $|X_{ij}| \leq 1$ and $\|\hat{\mu}_x^{(k)}(\cdot)\|_\infty \leq 1$ almost surely for $k = 1, 2$ and all $1 \leq j \leq p$. Also, $|Y_i| \leq c_0$ and $\|\hat{\mu}_y^{(k)}(\cdot)\|_\infty \leq c_0$ almost surely for $k = 1, 2$ for some constant $c_0 > 0$.

Finally, we assume the regression functions $\hat{\mu}_y^{(k)}$ and $\hat{\mu}_x^{(k)}$ are consistent with $o(n^{-1/4})$ convergence rates.

**Assumption 3.4.** Suppose $\|\hat{\mu}_y^{(k)}(\cdot) - \mu_y(\cdot)\|_{L_2(\mathbb{P}_x)} = o_P(n^{-1/4})$ for $k = 1, 2$. Also, there exists a sequence of constants $c_n \to 0$ such that for sufficiently large $n$,

$$
\max_{1 \leq j \leq p, k=1,2} \mathbb{P}\left( \|\hat{\mu}_x^{(k)}(\cdot) - \mu_x(\cdot)\|_{L_2(\mathbb{P}_x)} \geq c_n \log(1/\delta) / n^{1/4} \right) \leq \delta.
$$

(11)

Here $\hat{\mu}_x^{(k)}(\cdot)$ is the $j$-th entry of $\hat{\mu}_x^{(k)}$, an estimator for $\mu_x(\cdot) := \mathbb{E}[X_{ij} \mid Z = \cdot]$.

Assumption 3.4 slightly differs from the commonly adopted consistency conditions — which is often of the form $\|\hat{\mu}_x^{(k)} - \mu_x(\cdot)\|_{L_2(\mathbb{P}_x)} = o_P(n^{-1/4})$ — on the estimation of nuisance components. This is because we need an exponential tail bound to control all $2 \times p$, estimated functions $\{\hat{\mu}_x^{(k)}(\cdot)\}_{j=1}^p$ simultaneously. Running these many regressions may incur considerable computational cost in high dimensions; we discuss this issue and provide a computational shortcut in Section 3.4.

Many estimators in the literature obey Assumption 3.4. When $Z$ is high-dimensional (i.e., $p_z$ may grow with $n$ or be larger than $n$), if $\mathbb{E}[X_{ij} \mid Z]$ is an $s$-sparse linear function of $Z$, then (11) holds for the Lasso estimator with $c_n \approx \sqrt{s \log(p_z) / n^{1/4}}$ when the regularization parameter is properly chosen. When $Z$ is low-dimensional (i.e., $p_z$ does not grow with $n$), under the standard assumption that $\mathbb{E}[X_{ij} \mid Z]$ is sufficiently smooth, the well-established convergence results of sieve estimation can be turned into such bounds by exponential tail bounds for the concentration of empirical loss functions (Chen and Shen, 1998; Chen, 2007).

We show an improved bound for the estimation error of $\hat{\theta}_n^{\text{mod}}$ than the Lasso estimator using $(X_i, Y_i)$. The proof of Theorem 3.5 is in Appendix B.2.
Theorem 3.5. Suppose Assumptions 2.1, 3.2, 3.3 and 3.4 hold. Then there exists a sequence of constants \( \{c_n\} \) with \( c_n \to 0 \) as \( n \to \infty \), such that for any fixed \( \delta \in (0, 1) \) and any regularization parameter \( \lambda \) obeying
\[
\lambda \geq \frac{2}{n} \| \mu_y^T X + Y^T \mu_x - \mu_y^T \mu_x - (X \theta^*)^T X \|_\infty + \frac{c_n (\log(3p_\xi/\delta))^2}{\sqrt{n}},
\]
it holds with probability at least \( 1 - \delta \) that
\[
\| \hat{\theta}_n^{\text{mod}} - \theta^* \|_2 \leq \frac{3\lambda \sqrt{s}}{2\varsigma}.
\]
Here we denote \( \| z \|_\infty = \sup_j |z_j| \), \( Y, \mu_y \in \mathbb{R}^n \) are vectors whose \( i \)-th entries are \( Y_i \) and \( \mu_y(Z_i) \), and \( X, \mu_x \in \mathbb{R}^{n \times p_x} \) are matrices whose \((i, j)\)-th entries are \( X_{ij} \) and \( \mu_{x,j}(Z_i) \).

The second term in (12) arises from the estimation error in \( \hat{\mu}_y \) and \( \hat{\mu}_x \). It enjoys a double robustness property that is similar to the low-dimensional case: under the slow convergence rate in Assumption 3.4, this error is negligible compared to the first term in (12) that is typically the order of \( \Omega(\sqrt{\log p_x}/n) \) (Vershynin, 2018). The estimation error of \( \hat{\theta}_n^{\text{mod}} \) is then characterized by the first term in (12).

When \( n \) is sufficiently large such that the second term in (12) is negligible, the deviation of the first term can be decided by the variance of each entry. We define the random vector \( \epsilon_n^{\text{mod}} := X^T \theta^* X - \mu_y(Z) X - Y \mu_x(Z) + \mu_y(Z) \mu_x(Z) \in \mathbb{R}^{p_x} \). Then, in Theorem 3.5, choosing \( \lambda \asymp L \sqrt{\max_j \text{Var}(\epsilon_j^{\text{mod}})} \cdot \log(p_x)/n \) yields the estimation error
\[
\| \hat{\theta}_n^{\text{mod}} - \theta^* \|_2 \leq L \cdot \frac{\sqrt{s \log(p_x)}}{\sqrt{n} \mu} \cdot \sqrt{\max_j \text{Var}(\epsilon_j^{\text{mod}})},
\]
where \( L > 0 \) is a universal constant. On the other hand, we let \( \hat{\theta}_n^{\text{Lasso}} \) be the Lasso estimator (2). Under similar conditions like Assumption 3.2, existing results in the literature (Negahban et al., 2012) show that
\[
\| \hat{\theta}_n^{\text{Lasso}} - \theta^* \|_2 \leq \frac{3\lambda \sqrt{s}}{2\varsigma}
\]
for any regularization parameter obeying \( \lambda \geq \frac{\| \rho \|_2 \sum_{i=1}^n (Y_i - X_i^T \theta^*) X_i \|_\infty}{2n} \). We define \( \epsilon_n^{\text{Lasso}} = X(Y - X^T \theta^*) \). Similarly, choosing \( \lambda \asymp L \sqrt{\max_j \text{Var}(\epsilon_j^{\text{Lasso}})} \cdot \log(p_x)/n \) yields
\[
\| \hat{\theta}_n^{\text{Lasso}} - \theta^* \|_2 \leq L \cdot \frac{\sqrt{s \log(p_x)}}{\sqrt{n} \mu} \cdot \sqrt{\max_j \text{Var}(\epsilon_j^{\text{Lasso}})},
\]
where \( L > 0 \) is the same universal scaling as above. The bounds in (13) and (13) distinguish our modular estimator from the Lasso, as one can check that \( \text{Var}(\epsilon_n^{\text{mod}}) \leq \text{Var}(\epsilon_n^{\text{Lasso}}) \) for all \( j \). That is, modular regression reduces the uncertainty in our estimator by a constant order.

Though this is only an upper bound analysis, our numerical experiments later on confirm the improvement in estimation accuracy. In particular, we will see that the regularization parameter \( \lambda \) chosen by cross-validation is smaller for modular regression than the Lasso. Intuitively, the reduction in the noise \( \text{Var}(\epsilon_n^{\text{mod}}) \) allows cross-validation to choose a different \( \lambda \) than for the Lasso.

3.3 Robustness to the conditional independence condition

In practice, Assumption 2.1 may be violated, and the true dependence structure among the variables may be completely unknown. In this part, we derive a generalization of our modular regression framework that allows to estimate and adapt to the conditional independence structure.

To be precise, Assumption 2.1 posits that \( X_j \indep Y \mid Z \) for every \( j \). That is, \( Z \) captures all the predictive power of every \( X_j \) for \( Y \). This condition can be violated in many ways. For instance, \( Z \) may capture all the information for a subset of variables in \( X \), while others in \( X \) still have direct effects for \( Y \).

In this subsection, we assume that \( X_{\mathcal{J}_1} \indep Y \mid \{Z, X_{\mathcal{J}_2}\} \) for two (unknown) disjoint subset \( \mathcal{J}_1, \mathcal{J}_2 \) where \( \{1, \ldots, p_x\} = \mathcal{J}_1 \cup \mathcal{J}_2 \), and \( X_{\mathcal{J}_2} \) is the vector containing \( X_j \) for all \( j \in \mathcal{J}_k \). The choice of \( \mathcal{J}_2 \) can be from prior knowledge, or by estimating (consistently) the dependence structure among all the variables when joint
observations of \((X, Z, Y)\) are available. Learning the conditional independence structure is beyond the focus of this paper; popular methods in the literature include constraint-based (Spirtes et al., 2000; Margaritis and Thrun, 1999; Tsamardinos et al., 2006), score-based (Lam and Bacchus, 1994; Jordan, 1999; Friedman et al., 2013), and regression-based (Lee et al., 2006; Meinshausen and Bühlmann, 2006; Roth, 2004; Banerjee et al., 2006) ones assuming a high-dimensional graphical model, to name a few.

**Remark 3.6.** For high-dimensional linear regression, a heuristic idea is to use the Lasso for structure learning. For example, one can regress \(Y\) on \((X, Z)\) via the Lasso, and use all features in \(X\) with nonzero estimated coefficient as \(X_{\mathcal{J}_2}\). We find that this heuristic approach works well in improving estimation accuracy in our numerical experiments, see Section 5.

In the following, we outline how to use the output from a structure learning approach such as in Remark 3.6 in conjunction with the modular regression approach. The condition \(X_{\mathcal{J}_1} \perp Y \mid (Z, X_{\mathcal{J}_2})\) can be seen as a special case of Assumption 2.1 for a different choice of the conditioning set “\(Z\)”:

\[
X \perp Y \mid Z_{\text{full}}, \quad \text{where} \quad Z_{\text{full}} = (Z, X_{\mathcal{J}_2}). \tag{14}
\]

This again allows us to break the problem into sub-tasks. In learning \(\mu_y\), after data splitting, for each \(k = 1, 2\), we aim \(\hat{\mu}_y^{(k)}\) for \(\mathbb{E}[Y \mid Z_{\text{full}}]\) using data in \(\mathcal{T}_j \setminus \mathcal{I}_k\), instead of \(\mathbb{E}[Y \mid Z]\). We only learn \(\mu_x\) for \(j \in \mathcal{J}_1\): if \(j \in \mathcal{J}_1\), we let \(\hat{\mu}_{x,j}(x)\) be an estimate for \(\mathbb{E}[X_j \mid Z_{\text{full}}]\) using the data in \(\mathcal{T}_j \setminus \mathcal{I}_k\) for \(k = 1, 2\). Then for each \(i \in \mathcal{I}_k\), we compute the cross-term \(C_i\) whose \(j\)-th entry is

\[
(C_i)_j = \begin{cases} 
\mu^{(k)}_{Y}(Z_{i}^{\text{full}}) + \hat{\mu}^{(k)}_{x,j}(Z_{i}^{\text{full}})Y_i - \hat{\mu}_{x,j}(Z_{i}^{\text{full}})\hat{\mu}^{(k)}_{y}(Z_{i}^{\text{full}}), & \text{if } j \in \mathcal{J}_1, \\
\mu_{x,j}(Y_i), & \text{if } j \in \mathcal{J}_2.
\end{cases} \tag{15}
\]

Finally, we solve the same modular least squares (5) or penalized least squares (10) with \(\hat{C}_{\text{lm}} := \frac{1}{n} \sum_{i=1}^n C_i\) for the above \(C_i\). When Assumption 2.1 is violated, the original \(\hat{C}_{\text{lm}}\) defined in (6) might be biased even if the estimators for conditional expectations are correct. In contrast, the new cross-terms we derive in (15) are unbiased for \((X_i)_jY_i\) with potentially smaller variance under the generalized condition (14). Theoretical guarantee for this approach can be directly implied by Theorems 2.2 and 3.5 in view of (14) and the fact that the definition of \(C_i\) in (15) is equivalent to taking \(\hat{\mu}^{(k)}_{x,j}(Z_{i}^{\text{full}}) := (X_i)_j\), which we omit here.

This variant can be viewed as a data-driven interpolation between the fully modular regression we introduce in the preceding part and the standard OLS or Lasso. If the conditional independence condition holds for \(X_\cdot\), then utilizing the information in \(Z_{\text{full}}\) reduces the estimation error in \(\hat{\theta}_{\text{mod}}^n\); otherwise, it reduces to \(\hat{\theta}_{\text{mod}}^n\) in the low-dimensional case, and yields a similar bound as \(\hat{\theta}_{\text{lasso}}^n\) for the high-dimensional regression. Our simulation studies in Section 5 show that this approach robustly improves the estimation and prediction accuracy in cases where Assumption 2.1 is violated but the conditional independence structure (14) may be learned from the data.

### 3.4 Practical implementation via linear transformation

We now discuss a computational shortcut for high-dimensional modular regression. By using linear transformations for estimating the conditional mean functions, it reduces the computational costs and is readily compatible with standard implementation of the Lasso (e.g., glmnet R-package (Friedman et al., 2010)).

First, let us discuss why the estimator as defined in equation (10) is computationally demanding. Note that the modular estimator (10) minimizes

\[
\frac{1}{n} \{ \theta^\top X^\top X \theta / 2 - \hat{\mu}_y^\top X \theta - Y^\top \hat{\mu}_x \theta + \hat{\mu}_y^\top \hat{\mu}_x \theta \} + \lambda \| \theta \|_1 \tag{16}
\]

where \(\hat{\mu}_x \in \mathbb{R}^{n \times p_x}\) is a matrix whose \((i, j)\)-th entry stores an estimator for \(\mu_{x,j}(Z_i)\), and \(\hat{\mu}_y \in \mathbb{R}^n\) is a vector whose \(i\)-th entry is an estimator for \(\mu_y(Z_i)\). In the cross-fitting approach we outline in Section 3.1, the estimators are specified as \([\hat{\mu}_{x,i,j}] = \hat{\mu}_{x,j}^{(k)}(Z_i)\) and \([\hat{\mu}_{y,i}] = \hat{\mu}_{y}^{(k)}(Z_i)\) for \(i \in \mathcal{I}_k\). That is, we need to run \(\Omega(p_x)\) times of regression to obtain \(\hat{\mu}_{x}^{(k)}\) and \(\hat{\mu}_{y}^{(k)}\).
Here, we take a different approach to estimating $\mu_x$ and $\mu_y$:

$$\hat{\mu}_x = \Pi_x X, \quad \hat{\mu}_y = \Pi_y Y,$$

where $\Pi_x, \Pi_y \in \mathbb{R}^{n \times n}$ are symmetric matrices. Examples include OLS regression for $\Pi_x = \Pi_y = Z(Z^T Z)^{-1} Z^T$ and ridge regression (with $\ell_2$-penalty parameter $\eta$) for $\Pi_x = Z(Z^T Z + \eta I)^{-1} Z^T$, where $Z \in \mathbb{R}^{n \times p_x}$ is the data matrix, $I \in \mathbb{R}^{n \times n}$ is the identity matrix, and we call $\eta$ the ridge penalty for clarity. We then compute the modular estimator by minimizing (16), or equivalently,

$$\frac{1}{n} \left\{ \theta^T X^T X \theta / 2 - Y^T (\Pi_y + \Pi_x - \Pi_y \Pi_x) X \theta \right\} + \lambda \| \theta \|_1. \tag{17}$$

The objective (17) is equivalent to the Lasso estimator (2) applied to the design matrix $X$ and the response vector $(\Pi_y + \Pi_x - \Pi_y \Pi_x) Y$. Our modular estimator could then be computed with standard libraries or packages for the Lasso (Friedman et al., 2010). The parameters in $\Pi_x, \Pi_y$ (such as the ridge penalty) can also be chosen with cross-validation. In our real data experiments, this computation shortcut using ridge regression and cross-validated ridge penalty $\eta$ achieves a prediction accuracy that is comparable to the fully modular approach (with entry-wise regression) and better than the Lasso.

As this shortcut combines ridge regression and the Lasso, it is related to the LAVA estimator (Chernozhukov et al., 2017) that is designed for recovering sums of dense and sparse signals. We develop a different estimator than theirs, which also serves a distinct goal of improving efficiency by exploiting the conditional independence structure.

### 4 Extension to missing data

Modular regression allows for flexible combination of data sets in various missing data settings. In this part, we discuss a general scenario where we may have access to a mixture of pairwise observations $(X_i, Z_i)$ or $(Z_i, Y_i)$ and/or some tuples $(X_i, Z_i, Y_i)$. We will see that the decomposition of the regression task allows us to flexibly modify our methods in Sections 2 and 3 according to the availability of data.

The crucial fact we rely on is that (6) only involves pairwise observations of $(X, Z)$ and $(Z, Y)$, and the same for learning $\mu_x(z)$ and $\mu_y(z)$. Thus, $\hat{\theta}_n^{\text{mod}}$ is computable without any joint observation of $(X, Z, Y)$. We discuss this case in Section 4.1. When we do have access to a few $(X, Z, Y)$ observations along with observations of $(X, Z)$ and $(Z, Y)$, these can also be incorporated. We discuss this case in Section 4.2.

#### 4.1 Pairwise observations

When no joint observations of $(X, Z, Y)$ are available, the prediction of $Y$ with $X$ is impossible without identification assumptions. For this subsection, we will assume that Assumption 2.1 holds. Also, our structure learning approach outlined in Section 3.3 is no longer applicable in this case.

Suppose $I^{xz}$ and $I^{yz}$ are two index sets for $(X_i, Z_i)$ and $(Z_i, Y_i)$ observations. We randomly split each of them into two equally sized folds $I_k^{xz}, I_k^{yz}$ for $k = 1, 2$. A modification to Section 2.1 is that we use $I^{xz} \setminus I_k^{xz}$ to obtain the estimate $\hat{\mu}_x^{(k)}$ for $E[X | Z]$, and similarly $\hat{\mu}_y^{(k)}$ for $E[Y | Z]$, $k = 1, 2$. We then modify the modular cross-terms in (5) and define the modular estimator as

$$\hat{\theta}_n^{\text{mod}} = \arg\min_{\theta \in \mathbb{R}^{p_x}} \left\{ -\hat{C}_{\text{miss}}^x \theta + \frac{1}{n} \sum_{i=1}^n \theta^T X_i X_i^T \theta / 2 \right\}. \tag{18}$$

where we define

$$\hat{C}_{\text{miss}}^x := \frac{1}{n_{xz}} \sum_{i \in I^{xz}} X_i \hat{\mu}_x^{(k_i)}(Z_i) - \frac{1}{n_{yz}} \sum_{i \in I^{yz}} Y_i \hat{\mu}_y^{(k_i)}(Z_i) + \frac{1}{n_{xz} + n_{yz}} \sum_{i \in I^{xz} \cup I^{yz}} \hat{\mu}_x^{(k_i)}(Z_i) \hat{\mu}_y^{(k_i)}(Z_i). \tag{19}$$

Here for any $i \in I^{xz}$ or $i \in I^{yz}$, we use $k_i$ to denote the subfold that data $i$ lies in, and $n_{xz} = |I^{xz}|$ and $n_{yz} = |I^{yz}|$. In particular, (19) modifies the three full-sample mean terms in $\frac{1}{n} \sum_{i=1}^n C_i$ of (5) to sample mean on the separate data sets. The modular estimator in the high dimensional case can be similarly obtained by adding an $\ell_1$-regularization to equation (18).
4.2 Partially pairwise observations

Following the above setting, modular prediction can also be adapted to settings where a limited number of triple observations are available in addition to some \( (X, Z) \) and \( (Y, Z) \) pairs.

The idea is still to obtain an estimator \( \hat{C} \) for \( C = \mathbb{E}[XY] \) that makes use of all observations. In the cross-fitting step, we denote \( I, I^{xz} \) and \( I^{yz} \) as the index sets for triple, \((X, Z)\)-only, and \((Y, Z)\)-only observations. We randomly split each of them into two folds \( I_k, I_k^{xz} \) and \( I_k^{yz} \), respectively, \( k = 1, 2 \). We use \((I^{xz} \setminus I_k^{xz}) \cup (I \setminus I_k)\) to obtain the estimate \( \hat{\mu}_x^{(k)} \) for \( \mathbb{E}[X \mid Z] \), and similarly \((I^{yz} \setminus I_k^{yz}) \cup (I \setminus I_k)\) to obtain \( \hat{\mu}_y^{(k)} \) for \( \mathbb{E}[Y \mid Z] \), \( k = 1, 2 \). We define

\[
\hat{\theta}_{\text{mod}}^n = \arg\min_{\theta \in \mathbb{R}^p} \left\{ -\hat{C}_\text{part}^\top \theta + \frac{1}{n} \sum_{i=1}^n \theta^\top X_i X_i^\top \theta / 2 \right\}.
\]

where we define the proxy term as

\[
\hat{C}_\text{part} := \frac{1}{n_{xz}} + \frac{1}{n} \sum_{i \in I_x \cup I} X_i \hat{\mu}_y^{(k_i)}(Z_i) - \frac{1}{n_{yz}} + \frac{1}{n} \sum_{i \in I_y \cup I} Y_i \hat{\mu}_x^{(k_i)}(Z_i)
+ \frac{1}{n + n_{xz} + n_{yz}} \sum_{i \in I \cup I_x \cup I_y} \hat{\mu}_x^{(k_i)}(Z_i) \hat{\mu}_y^{(k_i)}(Z_i),
\]

and \( k_i \) denotes the subfold that data \( i \) lies in, and \( n_{xz} = |I^{xz}|, n_{yz} = |I^{yz}|, n = |I| \). Comparing (21) with (19), we now make use of all available pairs to compute the sample means. Similarly, the high-dimensional modular estimator can be obtained by adding \( \ell_1 \)-regularization to equation (20).

In this case, one may leverage the \((X, Z, Y)\) observations to learn the conditional independence structure. Following the notations in Section 3.3, here \( Z = Z^{\text{full}} \) consist both the original features in \( Z \) and some other features in \( X \). Thus, in (21), the second sample average for \( Y \hat{\mu}_x^{k_i}(Z_i) \) has to be computed with \( i \in I \), and the third sample average has to be computed with \( i \in I_x \cup I_{xz} \). That said, we do note that in our real data application (see Section 6.2), modular regression performs well without structure learning. Theoretically, the above procedure without structure learning may induce substantial bias in cases where conditional independence does not hold. However, in settings where we have recorded a rich set of intermediate covariates in \( Z \) (as often assumed in surrogate methods), the conditional independence assumption is often plausible or the bias is sufficiently small compared with the reduced variance.

5 Simulation studies

We evaluate our methods on simulated datasets to compare the bias, variance and overall estimation error of our methods to non-modular counterparts in both low and high dimensional settings. We also investigate the robustness to approximate conditional independence in the high dimensional setting.

5.1 Low-dimensional setting

We focus on parameter estimation in the low-dimensional setting. We are interested in estimating the population OLS parameter \( \theta^* = \arg\min_{\theta \in \mathbb{R}^p} \mathbb{E}[Y-X^\top \theta]^2 \), where \( Y \in \mathbb{R} \) is the response, and \( X \in \mathbb{R}^p \) are the covariates. We suppose in the training data we have access to \( Z \in \mathbb{R}^p \) such that \( X \perp Y \mid Z \). We fix the dimensions at \( p_x = 4, p_z = 6 \), and a small sample size at \( n = 200 \).

We design \( 2 \times 2 \) data generating processes depending on (i) whether the true relation is linear and (ii) whether the data generating process follows the graphical model \( X \rightarrow Z \rightarrow Y \) or \( X \leftarrow Z \rightarrow Y \). The details are summarized in Table 1. In all settings, \( \epsilon_z \sim N(0, \sigma_z^2) \) and \( \epsilon_y \sim N(0, \sigma_y^2) \) are independent noise, where we vary the noise strengths \( \sigma_z, \sigma_y \in \{0.1, 0.5, 1, 2\} \), and \( X \sim \text{Unif}[-1, 1] \) means all entries in \( X \) are i.i.d from \( \text{Unif}[-1, 1] \). The linear regression model is not necessarily well-specified for all settings, while the OLS parameter \( \theta^* \) is always well-defined.
In settings 1 and 2, we set $\gamma = (0.531, -0.126, 0.312, 0, 0, 0)^T \in \mathbb{R}^p$, and $B = \mathbb{R}^{p \times p_z}$ or $B = \mathbb{R}^{p \times p_z}$ is a constant matrix where 8 out of 24 entries are randomly set to 0.5 then fixed for all configurations, while the other entries are zero. In setting 3, we set $Z_{4:6} = [BX]_{4:6}$ with the same $B$ as setting 1, and $Z_3 = 0.5X_1 + 1\{X_1 > 0\}$, $Z_2 = -0.5X_3 + 1\{X_4 > 0\}$. In setting 4, we set $X_4 = [BZ]_4$ with the same $B$ as setting 2, and $X_3 = 0.5X_1 + 1\{Z_1 > 0\}, X_2 = -0.5Z_3 + 1\{Z_4 > 0\}$ and $X_3 = 1\{Z_4 > 0\}$.

We compute the OLS parameter $\hat{\theta}_{n}^{\text{ols}}$ and our modular estimator with $\hat{\mu}_y^{(k)}$ and $\hat{\mu}_z^{(k)}$ estimated with (i) cross-validated Lasso (Friedman et al., 2010), (ii) cross-validated ridge regression (Friedman et al., 2010), (iii) regression random forest from grf R-package, and (iv) linear regression. All procedures are repeated for $N = 1000$ independent runs. We evaluate the rooted mean square error (RMSE) $\mathbb{E}[(\hat{\theta}_j - \theta_j^*)^2]^{1/2}$, standard deviation $\text{sd}(\hat{\theta}_j - \theta_j^*)$ and bias $\mathbb{E}[\hat{\theta}_j - \theta_j^*]$ for each entry $1 \leq j \leq p_x$ for the five estimators $\hat{\theta}$. The patterns across the 4 entries are similar. In Figure 2, we present the RMSE for $j = 1$ in settings 1 and 4. Those for all entries and all settings are in Appendix D which convey similar messages.

![Figure 2: RMSE averaged over N = 1000 runs for estimating $\theta_1$ with n = 200. Each column corresponds to a value of $\sigma_z$. In each subplot, the z-axis (noise strength) equals $\sigma_y$, the standard deviation of noise in Y. Modular regression achieves smaller estimation error in almost all settings.](image)

Modular regression – no matter which machine learning regressor is used for $\hat{\mu}_x$ and $\hat{\mu}_y$ – achieves smaller RMSE than the plain OLS in almost all configurations. However, modular regression has a larger bias than OLS due to the additional regression (Figure 3), yet much more substantial reduction in standard deviation (Figure 4) in all settings. Also, results from setting 1 confirms Remark 2.3, where the asymptotic variance reduction grows with both $\sigma_x$ and $\sigma_y$.

A noteworthy exception is $\sigma_z = 0.1$ in setting 4, where the RMSE of modular regression with random forests is worse than that of the OLS estimator. This is because with small sample size ($n = 200$) and low noise (hence the uncertainty in $\hat{\theta}_n^{\text{ols}}$ is very small), the bias introduced by the random forest regression is large.

compared to the reduction in variance. However, when $\sigma_z$ becomes larger, the bias (Figure 3) has a smaller magnitude; this may be because we enter a signal-to-noise ratio regime that favors tree-based approaches. The impact of bias is also less substantial when we increase the sample size; Figure 12 in Appendix D plots the RMSE for estimating $\theta_1^*$ when $n = 1000$, where we see a much better performance of modular regression with random forests. Thus, we recommend using machine learning regressors for larger sample sizes.

We also note that modular regression with linear regression (green) performs better than the plain OLS in all settings (even when the true relation is nonlinear), although it is sometimes outperformed by other modular methods. This phenomenon is universal in our simulation (see Appendix D for the RMSE for all entries in all settings), hence we recommend running linear regression in practice, especially for small sample size. One can also add a few nonlinear regressors into the linear regression to further adapt to nonlinearity.

**Figure 3:** Bias for estimating $\theta_1^*$. Details are otherwise the same as Figure 2. Modular regression incurs a slightly larger bias than OLS when the sub-tasks are learned by flexible machine learning algorithms.

**Figure 4:** Standard deviation for estimating $\theta_1^*$. Details are otherwise the same as Figure 2. Modular regression leads to a substantial reduction in variance.
5.2 High-dimensional setting

We now consider two data generating processes in the high-dimensional setting, where the conditional independence structure holds only in one of them. We show that our methods outperform the Lasso in Setting 1 (with conditional independence), and is robust against the violation of conditional independence in Setting 2. Following the preceding notations, \( X \in \mathbb{R}^{p_x} \) is the covariates available in the prediction phase, while \( Z \in \mathbb{R}^{p_z} \) is only available for training data, and \( Y \in \mathbb{R} \) is the outcome. The data generating processes are visualized in Figure 5.

![Diagram](image)

(a) Setting 1: conditional independence  
(b) Setting 2: approximate conditional independence

Figure 5: Illustration of the two data generating processes.

In setting 1, we generate \( X \in \mathbb{R}^{p_x} \) where each entry is i.i.d. from \( N(0,1) \); then we generate \( Z = BX + \epsilon_z \in \mathbb{R}^{p_z} \) with i.i.d. noise \( \epsilon_z \sim N(0,1) \) given a parameter matrix \( B \in \mathbb{R}^{p_z \times p_x} \). Finally, we generate \( Y = Z^\top \gamma + \epsilon_y \) for i.i.d. random noise \( \epsilon_y \sim N(0,4) \) and some \( \gamma \in \mathbb{R}^{p_z} \). To ensure sparsity, we let \( B_{ij} = 0 \) for all \( j > s \), such that \( X_j \)'s for \( j > s \) are irrelevant for the prediction. Then for each \( j \leq s \), we randomly select 2s entries in the \( j \)-th column of \( B \) with \( B_{ij} = 0.25 \), the remainings with \( B_{ij} = 0 \). We set \( \gamma_i = 0.5 \) for \( 1 \leq i \leq s \), and \( \gamma_i = 0 \) for \( i > s \). In this way, \( Y = X^\top \theta^* + (\gamma^\top \epsilon_z + \epsilon_y) \) where \( \theta^* = B^\top \gamma \), and \( X \perp \perp Y \mid Z \).

In setting 2, we ensure a small subset of covariates in \( X \) to have direct impact on \( Y \) (the link from \( X \) to \( Y \) in Figure 5(b)). To be specific, we generate \( X \) and \( Z = BX + \epsilon_z \), where \( \{B_{ij} : j \leq s\} \) and \( \epsilon_z \) are the same as setting 1, and generate \( Y = Z^\top \gamma + X^\top \tilde{\gamma} + \epsilon_y \) for i.i.d. random noise \( \epsilon_y \sim N(0,4) \); the direct coefficient \( \tilde{\gamma} \) satisfies \( \tilde{\gamma}_i = 0 \) for \( i \leq s \) and \( \sum_{i=1}^{p_x} 1\{\tilde{\gamma}_i \geq 0\} = 5 \). In this setting, the high dimensional model \( Y = X^\top \theta^* + (\gamma^\top \epsilon_z + \epsilon_y) \) holds with \( \theta^* = B^\top \gamma + \tilde{\gamma} \), but \( X \perp \perp Y \mid Z \) does not hold exactly.

We compare the performance of our modular regression method in Section 3.1 to the Lasso; to ensure fair comparison, we run the plain Lasso using our modular method while setting \( \hat{f}_y(Z_i) := Y_i \) and \( \hat{f}_z(Z_i) := X_i \) for all \( i \), so that (10) reduces to the Lasso. We also evaluate an oracle modular regression algorithm, that is, we set \( \hat{\mu}_y := \mathbb{E}[Y \mid Z] \) and \( \hat{\mu}_x := \mathbb{E}[X_j \mid Z] \) as the ground truth. The regularization parameter \( \lambda \) for \( \ell_1 \)-penalty is chosen by 5-fold cross validation on the training data for all methods. In our modular regression algorithm, we fit \( \hat{\mu}_x \) and \( \hat{\mu}_y \) by ridge regression using the cv.glmnet function from the glmnet R-package (Friedman et al., 2010). The procedures are evaluated for \( p_x = p_z = 100 \) and \( s = 10 \). The training sample is \( n = 500 \) and we evaluate the prediction on \( n_{\text{test}} = 1000 \) test samples for a relatively accurate estimate.

5.2.1 Performance under conditional independence

In setting 1 with a well-specified high-dimensional linear model and exact conditional independence \( X \perp \perp Y \mid Z \), we evaluate (i) the parameter estimation error \( \|\hat{\theta}_j - \theta_j^*\|_2 \) where \( \hat{\theta} \) is the output of modular regression or the Lasso, as well as (ii) prediction performance in terms of excess risk \( \frac{1}{n_{\text{test}}} \sum_{i=1}^{n_{\text{test}}} (X_i^\top \hat{\theta} - X_i^\top \theta^*)^2 \) and mean squared error (MSE) \( \frac{1}{n_{\text{test}}} \sum_{i=1}^{n_{\text{test}}} (X_i^\top \hat{\theta} - Y_i)^2 \) on the test samples.

Parameter estimation. For each \( j \in [p_x] \), we evaluate the rooted mean squared error (RMSE) \( (\hat{\theta}_j - \theta_j^*)^2 \) and bias \( \mathbb{E}[(\hat{\theta}_j) - \theta_j^*] \) over \( N = 100 \) replicates. We further investigate the estimation error by bias and standard deviation of \( \hat{\theta}_j \). Figure 6 plots the RMSE (left) and bias (right) of three methods.

For nonzero entries (the blue boxplots), we observe a significant reduction in RMSE compared to the Lasso; despite the estimation error in fitting the conditional mean functions, our method is still comparable.
to the oracle counterpart, even with a smaller overall RMSE (though less stable across entries). This might be due to the instability in cross-fitting with ridge regression as \( n = 500 \) is not a large sample size. For zero entries, the RMSE are similar across three methods: while the oracle yields lower RMSE than the Lasso, the slight inflation of RMSE from modular prediction might be due to the estimation error of \( \hat{\mu}_z \) and \( \hat{\mu}_q \).

![Boxplot of RMSE (left) and bias (right) of \( \{\hat{\theta}_j: j \in [p_x]\} \), averaged over all replicates in setting 1, separately for \( \theta_j^* \neq 0 \) (nonzero entry) and \( \theta_j^* = 0 \) (zero entry). The x-axis indicates the method to obtain \( \hat{\theta}_j \). Modular regression achieves smaller RMSE and smaller bias than the Lasso for nonzero entries by attaining a different bias-variance trade-off.](image)

We find that the reduction in RMSE for nonzero entries mainly comes from the reduction in bias, as illustrated by the right panel of Figure 6. This is consistent with our theory in Theorem 3.5: The reduced variance of the proxy \( \hat{C}_m \) allows the cross-validation step to choose a model with smaller bias.

Due to limited space, we defer the corresponding plot of standard deviations to Figure 17 in Appendix D.

### Prediction.

We plot the \( N = 100 \) excess risks and MSEs averaged on the test samples in Figure 7. The left panel (excess risk) shows significant improvement in prediction accuracy of our method compared to plain Lasso: our method is slightly inferior to the oracle counterpart but the difference is relatively moderate. In the right panel, the prediction MSEs are consistent with the excess risks but the relative reduction becomes smaller because it is diluted by the irreducible variance \( \text{Var}(Y - X^\top \theta^*) \).

![Boxplot of \( N = 1000 \) empirical excess risks \( (X_i^\top \hat{\theta} - X_i^\top \theta^*)^2 \) (left) and MSEs \( (X_i^\top \hat{\theta} - Y_i)^2 \) (right) in all replicates for setting 1. The red dots are the average excess risks and MSEs over all replicates. Modular regression achieves smaller excess risk than the Lasso. The improvement in prediction MSE is less visible because the irreducible error \( \text{Var}(Y - X^\top \theta^*) \) dominates the prediction MSE.](image)
5.2.2 Robustness to approximate conditional independence

In the following, we test the robustness of our method against potential violation of the conditional independence assumption. In setting 2 where the conditional independence only approximately holds, we additionally conduct a structure learning step using Lasso.

We first run a cross-validated Lasso of $Y$ on $(X, Z)$ using the `cv.glmnet` function (Friedman et al., 2010) for model selection; all $X_j$ that are selected by this Lasso step is then merged into $Z$. For any selected $X_j$, we will skip the regression of $E[X_j | Z]$ and directly set $\hat{f}_{x,j}(Z_i) = X_{i,j}$ for all training samples. We also evaluate an oracle counterpart which uses the ground truth of the structure and the true conditional expectations for those $X_j \perp \perp Y | Z$; we skip the regression for those $X_j$ with a direct impact on $Y$, as outlined in Section 3.3.

Figure 8 plots the RMSE (left) and bias (right) of all coefficients $\theta_j$, averaged over $N = 1000$ replicates. The plot for standard deviations of $\hat{\theta}_j$ is in Figure 17 in Appendix D. We again see an improved RMSE especially for nonzero entries (blue). While the RMSE is less stable across different entries, perhaps because of the additional uncertainty introduced in the structure learning step, it is in general better than plain Lasso and comparable to the oracle. Similar to the previous setting, this reduction of RMSE mainly comes from a reduced bias as shown in the right panel of Figure 8. In general, this shows the ability of our method to adapt to approximate conditional independence and maintain certain efficiency gain.

![Figure 8: Boxplot of RMSE (left) and bias (right) of $\hat{\theta}_j$, j ∈ [p_x], averaged over all replicates. We separately plot for those $\theta^*_j \neq 0$ (nonzero entry) and $\theta^*_j = 0$ (zero entry). Modular regression achieves smaller estimation RMSE and smaller bias than the Lasso, due to a different bias-variance trade-off.](image)

We summarize the prediction performance in Figure 9. The excess risk of modular prediction lies between that of the oracle counterpart and the Lasso. Still, the relative improvement in terms of prediction MSE is present yet smaller due to the irreducible noise.

![Figure 9: Boxplot of $N = 100$ empirical excess risks $(X_i^T \hat{\theta} - X_i^T \theta^*)^2$ (left) and MSEs $(X_i^T \hat{\theta} - Y_i)^2$ (right) in all replicates for setting 2. The red dots are the average excess risks and MSEs over all replicates. Modular regression with structure learning achieves smaller excess risk and prediction MSE than the Lasso.](image)
6 Real data analysis

6.1 Dataset overview

We apply our method to the English Longitudinal Study of Ageing dataset (Oldfield et al., 2021). Starting in 2002, the study repeatedly collected data from a representative sample of the English population to understand the ageing dynamics in England. The waves of data consistently measure several modules of features such as health trajectories, disability and healthy life expectancy, the economic and financial situations, cognition and mental health, etc. We use the Wave 7 and Wave 9 data, collected in 2014 and 2018, respectively, restricted to people who are present in both waves.

We consider predicting the future health outcomes of people based on their current available features. The Wave 7 data is used as covariates. We divide all variables into two main categories: health (both mental and physical) and social conditions (including household demographics, financial, work and social situations). After pre-processing through one-hot encoding for categorial and string-valued variables and filtering out some highly imbalanced variables, the health and social categories contain 184 and 888 features, respectively. We take the selectivity variable from Wave 9 data as the response $Y$: the reported overall health situation ranging from 1 (excellent) to 5 (poor). We treat the outcome as a continuous variable.

6.2 Real data application

We take the covariates in the social category as $X \in \mathbb{R}^{p_x}$ for $p_x = 888$, and those in the health category as $Z \in \mathbb{R}^{p_z}$ for $p_z = 184$. Our procedure is geared towards settings with high noise. To simulate such a setting, we smooth the discrete response $Y$ by adding i.i.d. noise drawn from $N(0, 4)$. The task is to predict $Y$ using $X$, while $Z$ may be available during the training process. This is a practical setting where health conditions $(Z)$ may be more costly or difficult to evaluate, hence only available in pre-collected data.

We consider a missing data scenario to evaluate the performance of our method where one only has access to a limited number $n$ of $(X, Y, Z)$ triples as well as $n_{xz}$ observations for $(X, Z)$ and $n_{yz}$ observation for $(Z, Y)$ pairs in the training phase. This mimics a realistic scenario where it is difficult to obtain full observations simultaneously but modular data are more easily accessible. When $n_{xz} = n_{yz} = 0$, it reduces to the standard full-observation setting. While it is more difficult to test for conditional independence and the modeling assumptions with limited joint observations, we could still use our framework to merge the individual datasets and improve out-of-sample prediction. We focus on the prediction MSE on the test sample because no ground truth is available. We consider two scenarios for data availability:

(i) Fixed $n$ and varying $n_{xz}$ and $n_{yz}$. We fix $n = 200$, and the number of pair observations varies as $n_{xz} = n_{yz} = n \cdot \rho$ for $\rho \in \{0.5, 1, 5, 10\}$.

(ii) Fixed $n + n_{xz} + n_{yz}$ and varying proportion. We fix the total sample size $n + n_{xz} + n_{yz} = 1000$, while varying the proportion of joint observations by $n = 1000 \cdot \rho, n_{xz} = n_{yz}$ for $\rho \in \{0.05, 0.1, 0.2, 0.5, 0.8, 1\}$.

We evaluate our modular regression approach outlined in Section 4 that utilizes the partial observations, where we use 2-fold cross-fitting to obtain $\hat{\mu}_x$ and $\hat{\mu}_y$ from 1) the Lasso using cv.glmnet (10-fold cross-validation), 2) ridge regression using cv.glmnet (10-fold cross-validation), and 3) random forests using grf R-package. The parameter $\lambda$ for $\ell_1$-regularization is chosen by 10-fold cross-validation with the 1se criterion, implemented in the same way as that in the cv.glmnet R function, i.e., we select the largest $\lambda$ within one se of CV error from the smallest CV error. We use the modular regression without structure learning. These implementations are compared to the default Lasso using cv.glmnet fitted over the $(X, Y)$ joint observations, also using 1se criterion for 10-fold validation. Here we omit the results for our methods and the Lasso using the min option (selecting minimum CV error) for cross-validation because the Lasso performs far less stable in this case. The average prediction MSEs over $N = 100$ independent runs are in Figure 10.

The left panel in Figure 10 shows the results for setting (i), where Lasso uses a fixed number of joint observations. As the number of auxiliary observations increases, our modular regression achieves smaller prediction error, showing quite substantial improvement due to incorporating auxiliary observations.
The right panel presents those for setting (ii). Naturally, the performance of the Lasso (blue, dashed line) improves as $\rho$, the proportion of joint observations, increases. Our modular regression, with all of the three regressors, outperforms the Lasso by utilizing auxiliary observations, including $\rho = 1$ without missing data. Surprisingly, keeping the total sample size fixed, we do not see much variation in the performance of modular regression (all solid lines) as $\rho$ varies: the performance with only 5% joint observations is comparable to that with more than 50% joint observations. Our method achieves very similar effective sample size as full observations on this dataset. On the other hand, this phenomenon also indicates that we are in a regime where the irreducible error in $Y$ is large compared to the learnable part. In the next part, we are to utilize semi-synthetic data to evaluate the performance of our method in a setting with slightly stronger signal.

### 6.3 Semi-synthetic data

As discussed in Section 3.4, a naive implementation of our procedure is computationally prohibitive in high-dimensional settings. Thus, in the following, we evaluate the shortcut described in Section 3.4 and compare it with the standard cross-fitting implementation. We keep the choice of $X$ and $Z$ as before, and randomly subsample without replacement the training and test folds, where we observe $(X, Z, Y)$ for $n = 1000$ training data, but only $X$ for $n_{test} = 1794$ test sample. This is a scenario where only those easier-to-measure social-related covariates are available at the time of prediction, while the pre-collected training data contain both health and social covariates.

**Data generating process.** As the signal-to-noise ratio in the original data (for both $(X, Y)$ and $(Z, Y)$ regression) is extremely low, we enhance the signal with the following synthetic data generating process to draw a more informative comparison. We standardize all features using the original dataset, from which we subsample a set of observations aside from the training and test data. On this set, we run the Lasso for $Y$ given $Z$ which finds 13 nonzero regression coefficients, and for $Y$ given $X$ which finds 12 nonzero coefficients; we then reorder the features so that $Z_{1:13}$ and $X_{1:12}$ have with nonzero coefficients. For each $j \in \{1, \ldots, 12\}$, we run a Lasso for $X_j$ over $Z_{1:13}$ on this fold, and store all coefficients in the $j$-th column of a matrix $\hat{B} \in \mathbb{R}^{13 \times 12}$.

We generate the training and testing data by $Z_i = Z_{i}^{\text{org}} + \epsilon_i^x$, where $Z_{i}^{\text{org}}$ is the original observation, and $\epsilon_i^x \sim N(0, \sigma^2_x)$ is independent noise. We then compute $\mu_x(Z_i) = 2.5 \cdot \hat{B}^\top Z_{i,1:13}$, and generate $X_{i,1:12} = \mu_x(Z_i) + \epsilon_i^x$, where $\epsilon_i^x \in \mathbb{R}^{12}$ is i.i.d. noise from $N(0, 0.25 \cdot 1_{12})$ to match the standardized variance in $X$, and $X_{13:p}$ are obtained by permuting each columns in the (standardized) original data matrices. Finally, we generate $Y_i = \mu_y(Z_i) + \epsilon_i^y$, where $\mu_y(Z_i) = Z_i^\top \gamma$ where the first 12 entries in $\gamma \in \mathbb{R}^{p_x}$ equals 0.5 while the others equal to zero, and $\epsilon_i^y \sim N(0, 4)$ is the i.i.d. random noise. This setup ensures $X \perp \perp Y \mid Z$, but the
sparse linear model $E[Y | X] = X^\top \theta^*$ does not necessarily hold, and the true parameters $\theta^*$ are not available. We thus focus on the prediction performance. We vary the signal-to-noise ratio by setting $\sigma_z \in \{1, 2\}$.

**Methods.** We evaluate two implementations of the modular regression:

(i) Cross fitting in Section 3.1. We use two-fold cross-fitting with cross-validated Lasso and ridge regression to form $\hat{\mu}_x$ and $\hat{\mu}_y$, and then use 10-fold cross-validation to decide the penalty parameter $\lambda$ in (10) by either (a) min: minimal CV error or (b) 1se: the same as the default implementation in `cv.glmnet` R function which selects the largest $\lambda$ within one se of CV error for stable performance.

(ii) Projection shortcut in Section 3.4. We use ridge projection with regularization parameters $(\eta_x, \eta_y)$ for $\Pi_y, \Pi_x$, and then run `cv.glmnet` (with both (a) min and (b) 1se choice of cross-validation) for $X$ and $(\Pi_y + \Pi_x - \Pi_x \Pi_y)Y$, where $(\eta_x, \eta_y)$ are chosen by 10-fold cross-validation to minimize CV error.

The above two implementations are compared to two baselines:

(iii) Oracle modular regression. Set $\hat{\mu}_x$ and $\hat{\mu}_y$ as the ground truth, and then the same as (i).

(iv) Standard Lasso. Run `cv.glmnet` on $(X,Y)$ with both (a) min and (b) 1se cross-validation.

**Results.** The boxplots for all methods with $N = 100$ independent runs are in Figure 11, where we compare the performance under different cross-validation options.

![Boxplots of prediction MSEs on the test data](image)

Figure 11: Boxplots of prediction MSEs on the test data. Each subplot summarizes methods with one cross validation option (1se or min) under one value of $\sigma_z$. Method stands for the projection shortcut (mod), and cross-fitting with Lasso (cfmod.Lasso) and ridge regression (cfmod.ridge). The Lasso (Lasso) and oracle modular regression (orc) with the corresponding cv options are plotted for comparison. The oracle modular regression substantially reduces MSE; the cross-fitting implementation with Lasso and ridge regression is comparable to the oracle; the projection shortcut is slightly inferior but still improves upon the Lasso.

The patterns across different values of $\sigma_z$ are similar. Among the baselines, the Lasso with minimal CV error is more accurate than 1se (see the blue boxplots in the last two columns versus in the first two columns), while the oracle modular regression always achieves smaller prediction MSE than the Lasso with the corresponding CV option (the grey boxplots).

Our modular regression method performs reasonably well when the conditional mean functions $\mu_x(\cdot)$ and $\mu_y(\cdot)$ are estimated. When they are estimation by (i) ridge projection shortcut, modular regression with both min (see the last column) and 1se (see the second column) improves upon the Lasso, although it is sometimes less accurate than the oracle. This shows the projection shortcut in Section 3.4 is a reliable alternative to the more computationally intensive cross-fitting approach. When they are estimated by (ii) cross fitting (see the first and third columns), our method improves upon the original Lasso with both Lasso (green) and ridge regression (yellow) as the regressor, and the performance is comparable to the oracle. The
Lasso as the regressor is slightly better than the ridge regression; this may be due to the true sparse linear data generating process. In general, for the (ii) implementation, cross-validation with \( \min \) CV error achieves smaller test MSE than \( 1se \), while the latter sees larger improvement upon the Lasso.

7 Discussion

In this work, we propose the modular regression framework and show that conditional independence structures between variables can be used to decompose statistical tasks into sub-tasks. We develop decomposition techniques for linear models in both low and high dimensional settings. We show that such decomposition can improve efficiency and allow to combine different datasets for a single estimation or prediction task with rigorous statistical guarantees. In practice, the conditional independence conditions for decomposition may be violated, leading to a bias-variance trade-off. We also develop a robust implementation of our method to adapt to potentially more complicated dependence structures.

Looking ahead, statistical tasks that allow for decomposition may go well beyond the cases studied in this work, and the assumptions for decomposition may vary with the nature of the tasks. For instance, in high dimensional graphical models, the edges between variables that indicate independence may be sparse, and conditional independence may not hold exactly for two disjoint sets (e.g., our \( X \in \mathbb{R}^{p_x} \) and \( Z \in \mathbb{R}^{p_z} \)). For example, in biological applications, there may exist several paths from \( X \) to \( Y \) rather than being fully mediated by \( Z \). The dependence among the features and the response may still be sparse, but additional efforts are needed in order to leverage potential independence structures to improve estimation efficiency. In addition, the data fusion technique may be further extended: In this work we have discussed incorporating auxiliary datasets for sub-tasks. In practice, one may have access to many auxiliary datasets that cover different sets of features. Developing a framework to systematically combine multiple datasets may also be an interesting direction to pursue. Finally, our theoretical results in high dimensions only cover the sparse setting \( (p \gg n \gg \log p \text{ with } s \leq \sqrt{n}) \). In this regime, both the LASSO and the modular estimator are eventually consistent, and the role of conditional independence is to lower the variance of residuals. Its role in modern asymptotic regimes such as \( p/n \to \rho \) for some fixed \( \rho > 0 \) remains an interesting unanswered question.


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A Deferred theoretical results

This section presents the omitted theorem and proof for modular generalized linear regression in Section 2.3.

**Assumption A.1.** \( \theta^* \in \Theta \) for a compact set \( \Theta \). Also, \( \ell(x,y,\theta) \) is three-times-differentiable and convex in \( \theta \in \Theta \). Let \( \nabla_{\theta} h(x,\theta) \in \mathbb{R}^{p_x} \) denote the first-order derivative of \( h(x,\theta) \) in \( \theta \), and similarly \( \nabla_{\theta}^2 h(x,\theta) \in \mathbb{R}^{p_x \times p_x} \) the second-order, and \( \nabla_{\theta}^3 h(x,\theta) \in \mathbb{R}^{p_x \times p_x \times p_x} \) the third-order ones. There exists some \( m(\mathcal{X}) \) such that \( \mathbb{E}[L(X)] < \infty \), and \( \| \nabla_{\theta} h(x,\theta) - \nabla_{\theta} h(x,\theta') \| \leq L(x) \cdot \| \theta - \theta' \| \) for any \( \theta,\theta' \in \Theta \). Also, there exists some \( \mu(\mathcal{X}) \) such that \( \mathbb{E}[m(X)] < \infty \), and \( \| \nabla_{\theta}^h h(x,\theta) \|_{L_2} \leq m(x) \cdot \| \theta - \theta' \| \) for any \( \theta,\theta' \in \Theta \).

**Theorem A.2.** Suppose Assumptions 2.1 and A.1 hold, and \( \| \hat{\mu}_x^{(k)}(\theta) - \mu_x(z) \|_{L_2} \leq o_P(1) \) for \( k = 1, 2 \). Let \( \hat{\theta}^{\text{mod}} \) be the unique minimizer of (9), and \( \theta^* \) be the unique minimizer of (7). Let \( \mu_x(z) = \mathbb{E}[X|Z_i=z] \) and \( \mu_y(z) = \mathbb{E}[Y|Z_i=z] \). Define the influence function \( \phi(X_i,Y_i,Z_i) \). Then \( \sqrt{n}(\hat{\theta}^{\text{mod}} - \theta^*) \rightarrow N(0, \text{Cov}(\phi(X_i,Y_i,Z_i))) \) and \( \sqrt{n}(\hat{\theta}^{\text{mod}} - \theta^*) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \phi(X_i,Y_i,Z_i) + o_P(1) \) as \( n \rightarrow \infty \). Furthermore, \( \phi(X_i,Y_i,Z_i) \) is the efficient influence function for estimating \( \theta^* \) under the model space obeying Assumption 2.1.

**Proof of Theorem A.2.** The proof idea is similar to that of Jin and Rothenhäusler (2021, Proposition E.2 and Theorem 3.11). We write \( \ell(X_i,Y_i,Z_i,\theta) = [\hat{\mu}_x(Z_i)g(Y_i) + f(X_i)\hat{\mu}_y(Z_i) - \hat{\mu}_x(Z_i)\hat{\mu}_y(Z_i)] - \theta + h(X_i,\theta) \). We first show that \( \hat{\theta}^{\text{mod}} \rightarrow \theta^* \) as \( n \rightarrow \infty \). Since the score function \( s \) is differentiable and convex in \( \theta \), equivalently, \( \hat{\theta}^{\text{mod}} \in \Theta \) is the unique solution to

\[
\hat{L}_n(\theta) := \frac{1}{n} \sum_{i=1}^n \nabla \ell(X_i,Y_i,Z_i,\theta) = \frac{1}{n} \sum_{i=1}^n \left[ \hat{\mu}_x(Z_i)g(Y_i) + f(X_i)\hat{\mu}_y(Z_i) - \hat{\mu}_x(Z_i)\hat{\mu}_y(Z_i) + \nabla h(X_i,\theta) \right] = 0,
\]

while the population parameter \( \theta^* \) is the unique solution to

\[
L(\theta) := \mathbb{E}[\nabla \ell(X_i,Y_i,\theta)] = \mathbb{E}[g(Y_i)f(X_i) + \nabla h(X_i,\theta)] = 0.
\]

We also define the empirical score at any \( \theta \in \Theta \) as

\[
\hat{L}_n(\theta) = \frac{1}{n} \sum_{i=1}^n \left[ \hat{\mu}_x(Z_i)g(Y_i) + f(X_i)\hat{\mu}_y(Z_i) - \hat{\mu}_x(Z_i)\hat{\mu}_y(Z_i) + \nabla h(X_i,\theta) \right].
\]

Then for any fixed \( \theta \in \Theta \), we note that

\[
\hat{L}_n(\theta) - \hat{L}_n(\theta) = \frac{1}{n} \sum_{i=1}^n \left[ \mu_x(Z_i)g(Y_i) + f(X_i)\mu_y(Z_i) - \mu_x(Z_i)\mu_y(Z_i) - g(Y_i)f(X_i) \right]
\]

\[
= \frac{1}{n} \sum_{k=1}^2 \sum_{i \in \mathcal{X}} \left[ \mu_x^{(k)}(Z_i)g(Y_i) + f(X_i)\mu_y^{(k)}(Z_i) - \mu_x^{(k)}(Z_i)\mu_y^{(k)}(Z_i) - g(Y_i)f(X_i) \right].
\]

Similar to the proof of Theorem 2.2 (see equation (24)), under the given consistency condition for \( \mu_x^{(k)} \) and \( \mu_y^{(k)} \), we know \( \sup_{\theta \in \Theta} |\hat{L}_n(\theta) - \hat{L}_n(\theta)| = o_P(1) \). Furthermore, the law of large numbers implies \( \frac{1}{n} \sum_{i=1}^n \hat{L}_n(\theta) = o_P(1) \) for any fixed \( \theta \in \Theta \). Therefore, \( |\hat{L}_n(\theta) - L(\theta)| = o_P(1) \) for any fixed \( \theta \in \Theta \).

Since \( \Theta \) is compact and \( \nabla h(x,\theta) \) is \( L(x) \)-Lipschitz in \( \theta \in \Theta \) for any \( x \in \mathcal{X} \), we know that for any \( \theta,\theta' \in \Theta \), by the triangular inequality,

\[
|\hat{L}_n(\theta) - \hat{L}_n(\theta')| \leq \frac{1}{n} \sum_{i=1}^n L(X_i) \cdot \| \theta - \theta' \|
\]

where \( \frac{1}{n} \sum_{i=1}^n L(X_i) = o_P(1) \) since \( \mathbb{E}[L(X)] < \infty \). Thus, for any fixed \( \epsilon > 0 \), there exists a finite subset \( \{\theta_1, \ldots, \theta_{N_\epsilon}\} \) of \( \Theta \) such that \( \sup_{\theta} \inf_{1 \leq i \leq N_\epsilon} |\hat{L}_n(\theta) - \hat{L}_n(\theta_i)| \leq \epsilon \). Similar arguments applied to \( L(\theta) \), together
with the convergence, implies \( \sup_{\theta \in \Theta} |\hat{L}_n(\theta) - L(\theta)| = o_P(1) \). Thus we have \( \sup_{\theta \in \Theta} |\hat{L}_n^{\mod}(\theta) - L(\theta)| = o_P(1) \).

On the other hand, the compactness of \( \Theta \) and the uniqueness of \( \theta^* \) as a solution to \( L(\theta) = 0 \) implies the well-separatedness condition (c.f. Van der Vaart (2000, Theorem 5.9)): for any \( \epsilon > 0 \), one could find some \( \delta > 0 \) such that \( \inf_{\theta} \|\theta - \theta^*\| \geq \delta |L(\theta)| \geq 2\epsilon \). Since \( \sup_{\theta \in \Theta} |\hat{L}_n^{\mod}(\theta) - L(\theta)| = o_P(1) \), for any fixed \( \epsilon > 0 \), one could find some \( \delta > 0 \) such that for \( n \) sufficiently large, \( \mathbb{P}(\inf_{\theta} \|\theta - \theta^*\| \geq \delta |\hat{L}_n^{\mod}(\theta)| > \epsilon) \geq 1 - \epsilon \), i.e., \( \mathbb{P}(|\hat{L}_n^{\mod} - \theta^*| \leq \delta) \geq 1 - \epsilon \). This proves \( \hat{L}_n^{\mod} - \theta^* = o_P(1) \).

We now proceed to show the asymptotic normality of \( \hat{L}_n^{\mod} \). Recall that \( \tilde{I}_n^{\mod}(\hat{L}_n^{\mod}) = 0 \). Taylor expansion around \( \theta^* \) then gives

\[
0 = \tilde{I}_n^{\mod}(\theta^*) + \nabla_{\theta} \tilde{I}_n^{\mod}(\theta^*)(\hat{L}_n^{\mod}(\theta^*) - \theta^*) + 1/2 \cdot (\hat{L}_n^{\mod}(\theta^*) - \theta^*) \nabla_{\theta}^2 \tilde{I}_n^{\mod}(\hat{L}_n^{\mod}(\theta^*)) (\hat{L}_n^{\mod}(\theta^*) - \theta^*)
\]

(22)

for some \( \tilde{I}_n^{\mod} \) that lies on the segment between \( \hat{L}_n^{\mod} \) and \( \theta^* \), which implies \( \tilde{I}_n^{\mod} = \theta^* + o_P(1) \). Here \( \nabla_{\theta} \tilde{I}_n^{\mod} \in \mathbb{R}^{p_x \times p_x} \) and \( \nabla_{\theta}^2 \tilde{I}_n^{\mod} \in \mathbb{R}^{p_x \times p_x \times p_x} \) are second and third order derivative of \( \sum_{i=1}^n \tilde{I}(X_i, Y_i, Z_i, \theta) \). By definition

\[ \nabla_{\theta} \tilde{I}_n^{\mod}(\theta) = \frac{1}{n} \sum_{i=1}^n \nabla_{\theta}^2 h(X_i, \theta), \quad \nabla_{\theta}^2 \tilde{I}_n^{\mod}(\theta) = \frac{1}{n} \sum_{i=1}^n \nabla_{\theta}^3 h(X_i, \theta). \]

The law of large numbers imply \( \nabla_{\theta} \tilde{I}_n^{\mod}(\theta^*) = \mathbb{E}[\nabla_{\theta}^2 h(X_i, \theta^*)] + o_P(1) \) where \( o_P(1) \) means a matrix whose every entry is \( o_P(1) \), hence \( \nabla_{\theta} \tilde{I}_n^{\mod}(\theta^*) \) is invertible for sufficiently large \( n \). Also, by the Lipschitz condition of \( \nabla_{\theta}^3 h(x, \theta) \) and the triangular inequality, we have

\[ |\nabla_{\theta}^2 \tilde{I}_n^{\mod}(\theta^*) - \nabla_{\theta}^2 \tilde{I}_n^{\mod}(\tilde{L}_n^{\mod}(\theta^*))| \leq \frac{1}{n} \sum_{i=1}^n m(X_i) \|\theta^* - \tilde{L}_n^{\mod}(\theta^*)\| = o_P(1) \]

since \( \mathbb{E}[m(X_i)] < \infty \). Hence \( \nabla_{\theta}^2 \tilde{I}_n^{\mod}(\tilde{L}_n^{\mod}(\theta^*)) = O_P(1) \). Returning to (22), we have

\[
0 = \tilde{I}_n^{\mod}(\theta^*) + \{ \mathbb{E}[\nabla_{\theta}^2 h(X_i, \theta^*)] + o_P(1) \} (\hat{L}_n^{\mod}(\theta^*) - \theta^*) + O_P(\|\hat{L}_n^{\mod} - \theta^*\|^2)
\]

\[
= \tilde{I}_n^{\mod}(\theta^*) + \{ \mathbb{E}[\nabla_{\theta}^2 h(X_i, \theta^*)] + o_P(1) \} (\hat{L}_n^{\mod}(\theta^*) - \theta^*)
\]

and thus

\[
\hat{L}_n^{\mod}(\theta^*) = \mathbb{E}[\nabla_{\theta}^2 h(X_i, \theta^*)]^{-1} \tilde{I}_n^{\mod}(\theta^*) + o_P(1/\sqrt{n}).
\]

Finally, we note that under the consistency condition of \( \hat{L}_n^{(k)} \) and \( \hat{L}_n^{(k)} \), similar to the proof of Theorem 2.2, one could show that

\[
\tilde{I}_n^{\mod}(\theta^*) = \frac{1}{n} \sum_{i=1}^n \left[ \mu_x(Z_i)g(Y_i) + f(X_i)\mu_y(Z_i) - \mu_x(Z_i)\mu_y(Z_i) + \nabla_{\theta} h(X_i, \theta^*) \right] + o_P(1/\sqrt{n}).
\]

Because \( X \perp Y \mid Z \), we have \( \mathbb{E}[\mu_x(Z_i)g(Y_i) + f(X_i)\mu_y(Z_i) - \mu_x(Z_i)\mu_y(Z_i) + \nabla_{\theta} h(X_i, \theta^*)] = \mathbb{E}[\nabla_{\theta} s(X_i, Y_i, \theta^*)] = 0 \), hence \( \tilde{I}_n^{\mod}(\theta^*) = O_P(1/\sqrt{n}) \), which, combined with (23), implies

\[
\hat{L}_n^{\mod}(\theta^*) = \mathbb{E}[\nabla_{\theta}^2 h(X_i, \theta^*)]^{-1} \tilde{I}_n^{\mod}(\theta^*) + o_P(1/\sqrt{n})
\]

\[
= \frac{1}{n} \sum_{i=1}^n \mathbb{E}[\nabla_{\theta}^2 h(X_i, \theta^*)]^{-1} \left[ \mu_x(Z_i)g(Y_i) + f(X_i)\mu_y(Z_i) - \mu_x(Z_i)\mu_y(Z_i) + \nabla_{\theta} h(X_i, \theta^*) \right] + o_P(1/\sqrt{n}).
\]

We thus complete the proof of the asymptotic expansion of \( \hat{L}_n^{\mod} \) in Theorem A.2.

Finally, the efficient influence function for estimating \( \theta^* \) among all models obeying \( X \perp Y \mid Z \) can be obtained by, similar to Theorem 2.2, projecting the influence function of \( \hat{L}_n^{\mod} \) onto the tangent space \( T = T_1 \oplus T_2 \oplus T_3 \) where \( T_j \) is defined as in (25). Standard M-estimator theory (Van der Vaart, 2000) gives

\[ \hat{\theta}_n^{\mod} - \theta^* = \frac{1}{n} \sum_{i=1}^n \phi^{\mod}(X_i, Y_i) + o_P(1/\sqrt{n}) \]

where

\[ \phi^{\mod}(x, y) = \mathbb{E}[\nabla_{\theta}^2 h(X_i, \theta^*)]^{-1} \left[ g(Y_i)f(X_i) + \nabla_{\theta} h(X_i, \theta^*) \right]. \]

The projection follows exactly the same idea as Theorem A.2 and one could see \( \phi \) is the efficient influence function. We thus complete the proof of Theorem A.2.
B Technical proofs

B.1 Proof of Theorem 2.2

Proof of Theorem 2.2. Recall that \( \theta^* \) is the least-squares estimator \( \theta^* = \arg \min_{\theta \in \mathbb{R}^p} \mathbb{E}[(Y - X^\top \theta)^2] \). The estimation equation gives

\[
\hat{\theta}_n^{\text{ols}} - \theta^* = \left( \sum_{i=1}^{n} X_i X_i^\top \right)^{-1} \sum_{i=1}^{n} X_i Y_i - \theta^* = \left( \frac{1}{n} \sum_{i=1}^{n} X_i X_i^\top \right)^{-1} \frac{1}{n} \sum_{i=1}^{n} X_i (Y_i - X_i^\top \theta^*).
\]

Since \( X_i(Y_i - X_i^\top \theta^*) \) has finite second moment and we know \( \mathbb{E}[X(Y - X^\top \theta^*)] = 0 \) by the optimality of \( \theta^* \), we have \( \frac{1}{n} \sum_{i=1}^{n} X_i(Y_i - X_i^\top \theta^*) = O_P(1/\sqrt{n}) \), where \( O_P(1/\sqrt{n}) \) represents a random vector whose each entry is \( O_P(1/\sqrt{n}) \). Since \( X_iX_i^\top \) has finite expectation \( \mathbb{E}[XX^\top] > 0 \), we have

\[
\left( \frac{1}{n} \sum_{i=1}^{n} X_i X_i^\top \right)^{-1} = \left( \mathbb{E}[XX^\top] + o_P(1) \right)^{-1} = \left( \mathbb{E}[XX^\top] \right)^{-1} + o_P(1),
\]

where \( o_P(1) \) stands for a random matrix whose all entries converge in probability to zero. We thus have

\[
\hat{\theta}_n^{\text{ols}} - \theta^* = \left( \mathbb{E}[XX^\top] \right)^{-1} + o_P(1) \frac{1}{n} \sum_{i=1}^{n} X_i(Y_i - X_i^\top \theta^*)
= \frac{1}{n} \sum_{i=1}^{n} \left( \mathbb{E}[XX^\top] \right)^{-1} X_i(Y_i - X_i^\top \theta^*) + o_P(1) \times O_P(1/\sqrt{n})
= \frac{1}{n} \sum_{i=1}^{n} \phi^{\text{ols}}(X_i, Y_i) + o_P(1/\sqrt{n}),
\]

where

\[
\phi^{\text{ols}}(x, y) = \mathbb{E}[XX^\top]^{-1} x(y - x^\top \theta^*).
\]

For our modular estimator, we first note the closed form solution

\[
\hat{\theta}_n^{\text{mod}} - \theta^* = \left( \sum_{i=1}^{n} X_i X_i^\top \right)^{-1} \sum_{i=1}^{n} C_i - \theta^* = \left( \sum_{i=1}^{n} X_i X_i^\top \right)^{-1} \sum_{i=1}^{n} (C_i - X_iX_i^\top \theta^*).
\]

We now show that under the conditions in Theorem 2.2, one has

\[
\frac{1}{n} \sum_{i=1}^{n} (C_i - X_iX_i^\top \theta^*) = \frac{1}{n} \sum_{i=1}^{n} (C_i^* - X_iX_i^\top \theta^*) + o_P(1/\sqrt{n}), \quad (24)
\]

where \( C_i^* = X_i \mu_y(Z_i) + \mu_x(Z_i) Y_i - \mu_x(Z_i) \mu_y(Z_i) \). To see this, by rearranging the terms, we have \( \frac{1}{n} \sum_{i=1}^{n} (C_i - C_i^*) = (i) + (ii) + (iii) \), where we define

\[
(i) = \frac{1}{n} \sum_{k=1}^{2} \sum_{i \in I_k} \{X_i - \mu_x(Z_i)\} \{\hat{\mu}_y^{(k)}(Z_i) - \mu_y(Z_i)\},

(ii) = \frac{1}{n} \sum_{k=1}^{2} \sum_{i \in I_k} \{\hat{\mu}_x^{(k)}(Z_i) - \mu_x(Z_i)\} \{Y_i - \mu_y(Z_i)\},

(iii) = \frac{1}{n} \sum_{k=1}^{2} \sum_{i \in I_k} \{\hat{\mu}_x^{(k)}(Z_i) - \mu_x(Z_i)\} \{\hat{\mu}_y^{(k)}(Z_i) - \mu_y(Z_i)\}.
\]
We first bound the summation in (i). For each $k$, because $\hat{\mu}_y^{(k)}$ is obtained from the independent fold $I \setminus I_k$, for any $i \in I_k$, by the tower property,

$$E[\{X_i - \mu_x(Z_i)\}\{\hat{\mu}_y^{(k)}(Z_i) - \mu_y(Z_i)\} \mid I \setminus I_k] = E[\{X_i - \mu_x(Z_i)\} \mid I \setminus I_k] E[\{\hat{\mu}_y^{(k)}(Z_i) - \mu_y(Z_i)\} \mid I \setminus I_k] = 0,$$

and they are i.i.d. copies conditional on $I \setminus I_k$ with conditional variance

$$E[\{X_i - \mu_x(Z_i)\}^2 \{\hat{\mu}_y^{(k)}(Z_i) - \mu_y(Z_i)\}^2 \mid I \setminus I_k] = o_P(1).$$

The Markov’s inequality thus implies

$$\frac{1}{n} \sum_{i \in I_k} \{X_i - \mu_x(Z_i)\}\{\hat{\mu}_y^{(k)}(Z_i) - \mu_y(Z_i)\} = o_P(1/\sqrt{n}),$$

hence (i) = $o_P(1/\sqrt{n})$. Similar arguments also apply to (ii) and yield (ii) = $o_P(1/\sqrt{n})$. Finally, conditional on $I \setminus I_k$, for any $i \in I_k$, by the Cauchy-Schwarz inequality,

$$\left| \sum_{i \in I_k} \{\hat{\mu}_x^{(k)}(Z_i) - \mu_x(Z_i)\}\{\hat{\mu}_y^{(k)}(Z_i) - \mu_y(Z_i)\} \right| \leq \left[ \sum_{i \in I_k} \{\hat{\mu}_x^{(k)}(Z_i) - \mu_x(Z_i)\}^2 \right]^{1/2} \cdot \left[ \sum_{i \in I_k} \{\hat{\mu}_y^{(k)}(Z_i) - \mu_y(Z_i)\}^2 \right]^{1/2}.$$

By the Markov’s inequality, we have

$$\sum_{i \in I_k} \{\hat{\mu}_x^{(k)}(Z_i) - \mu_x(Z_i)\}^2 = o_P \left( |I_k| \cdot E \left[ \{\hat{\mu}_x^{(k)}(Z_i) - \mu_x(Z_i)\}^2 \mid I \setminus I_k \right] \right) = o_P \left( n \cdot \|\hat{\mu}_x^{(k)} - \mu_x\|_{L_2(P_2)}^2 \right).$$

With similar arguments applied to the second summation, we arrive at

$$\left| \sum_{i \in I_k} \{\hat{\mu}_x^{(k)}(Z_i) - \mu_x(Z_i)\}\{\hat{\mu}_y^{(k)}(Z_i) - \mu_y(Z_i)\} \right| \leq o_P \left( n \cdot \|\hat{\mu}_x^{(k)} - \mu_x\|_{L_2(P_2)} \|\hat{\mu}_y^{(k)} - \mu_y\|_{L_2(P_2)} \right).$$

Combining $k = 1, 2$, we have

(iii) = $o_P \left( \|\hat{\mu}_x^{(k)} - \mu_x\|_{L_2(P_2)} \|\hat{\mu}_y^{(k)} - \mu_y\|_{L_2(P_2)} \right) = o_P(1/\sqrt{n})$

by the conditions in Theorem 2.2. Putting together our bounds on the three terms, we prove the claim in (24). Note that $E[C_i^* - X_iX_i^T \theta^*] = 0$, hence $\frac{1}{n} \sum_{i=1}^n (C_i^* - X_iX_i^T \theta^*) = O_P(1/\sqrt{n})$, thus

$$\hat{\theta}_n^{\text{mod}} - \theta^* = \left[ \frac{1}{n} \sum_{i=1}^n X_iX_i^T \right]^{-1} \cdot \frac{1}{n} \sum_{i=1}^n (C_i - X_iX_i^T \theta^*)$$

$$= \left[ E[XX^T]^{-1} + o_P(1) \right] \cdot \left[ \frac{1}{n} \sum_{i=1}^n (C_i^* - X_iX_i^T \theta^*) + o_P(1/\sqrt{n}) \right]$$

$$= \frac{1}{n} \sum_{i=1}^n E[XX^T]^{-1} (C_i^* - X_iX_i^T \theta^*) + o_P(1/\sqrt{n}).$$

That is, we obtain the asymptotic linear expansion $\hat{\theta}_n^{\text{mod}} - \theta^* = \frac{1}{n} \sum_{i=1}^n \phi^{\text{mod}}(X_i, Y_i, Z_i) + o_P(1/\sqrt{n})$, where the influence function is given by

$$\phi^{\text{mod}}(x, y, z) = E[XX^T]^{-1} (x\mu_y(z) + \mu_x(z)y - \mu_x(z)\mu_y(z) - xx^T \theta^*).$$

The Central Limit Theorem thus gives the asymptotic distribution $\sqrt{n}(\hat{\theta}_n^{\text{mod}} - \theta^*) \overset{d}{\rightarrow} N(0, \Sigma^{\text{mod}})$ where $\Sigma^{\text{mod}} = \text{Cov}(\phi^{\text{mod}}(X_i, Y_i, Z_i)).$

We now proceed to show that $\phi^{\text{mod}}(X_i, Y_i, Z_i)$ is the efficient influence function for estimating $\theta^*$ under the current distribution $P$. Our argument is similar to that of (Rotnitzky and Scaucler, 2019, Lemma 9).
and (Tsiatis, 2006, Theorem 4.5). We let \( \mathcal{P} \) denote the collection of all distributions obeying Assumption 2.1, so \( \mathcal{P} \in \mathcal{P} \). For any \( \mathcal{P} \in \mathcal{P} \), let \( p \) denote the density of \( P \) with respect to the base measure \( \mu \). Then the joint density \( p(x, y, z) \) decomposes as

\[
p(x, y, z) = p(z)p(x | z)p(y | z),
\]

where \( p(z) \) is the marginal density of \( Z \), \( p(x | z) \) is the conditional density of \( P_{X \mid Z} \), and \( p(y | z) \) is the conditional density of \( P_{Y \mid Z} \). By (Van der Laan and Robins, 2003, Lemma 1.6), the tangent space of \( \mathcal{P} \) at \( \mathcal{P} \) is given by \( \mathcal{T} = \mathcal{T}_1 \oplus \mathcal{T}_2 \oplus \mathcal{T}_3 \), where \( \{\mathcal{T}_j\}_{j=1}^3 \) are orthogonal spaces. More specifically, \( \mathcal{T}_1 \) is the closed linear span of scores of one-dimensional regular parametric submodel \( \gamma \mapsto p(z; \gamma)p(x | z)p(y | z) \), \( \mathcal{T}_2 \) is that of the parametric submodel \( \gamma \mapsto p(x | z; \gamma)p(y | z) \), and \( \mathcal{T}_3 \) is that of the parametric submodel \( \gamma \mapsto p(y | z; \gamma)p(z) \). Similar to (Tsiatis, 2006, Theorem 4.5), these subspaces can be equivalently represented as

\[
\mathcal{T}_1 = \{ f(Z) \mapsto \mathbb{R}^{p_z} : \mathbb{E}[f(Z)] = 0 \},
\]

\[
\mathcal{T}_2 = \{ f(X, Z) \mapsto \mathbb{R}^{p_z} : \mathbb{E}[f(X, Z) | Z] = 0 \},
\]

\[
\mathcal{T}_3 = \{ f(Y, Z) \mapsto \mathbb{R}^{p_z} : \mathbb{E}[f(Y, Z) | Z] = 0 \},
\]

(25)

where all the functions in them are additionally square integrable.

By standard semiparametric theory (Tsiatis, 2006), the efficient influence function, denoted as \( \phi^s \), can be obtained by the projection of \( \phi^{ols} \) onto the tangent space \( \mathcal{T} \). That is, \( \phi^s(x, y, z) = \phi^1_s(x) + \phi^2_s(y, z) + \phi^3_s(y) \), where \( \phi^j_s \) is the projection of \( \phi^{ols} \) onto \( \mathcal{T}_j \) defined in (25). Hence

\[
\phi^s(X, Y, Z) = \mathbb{E}[\phi^{ols}(X, Y) | Z] - \mathbb{E}[\phi^{ols}(X, Y)|Y, Z]
\]

\[
\quad - \mathbb{E}[\phi^{ols}(X, Y) | Z] + \mathbb{E}[\phi^{ols}(X, Y)|X, Z] - \mathbb{E}[\phi^{ols}(X, Y)|X, Z]
\]

\[
\quad \quad = \mathbb{E}[X X^\top]^{-1}\{ \mathbb{E}[X (Y - X^\top \theta^*) | X, Z] + \mathbb{E}[X (Y - X^\top \theta^*) | Y, Z]
\]

\[
\quad \quad \quad \quad - \mathbb{E}[X (Y - X^\top \theta^*) | Z] - \mathbb{E}[X (Y - X^\top \theta^*) | Z] = \mathbb{E}[X X^\top]^{-1}\{ \mathbb{E}[X | Y | Z] - \mathbb{E}[X X^\top \theta^* + \mathbb{E}[X | Z] - \mathbb{E}[X X^\top \theta^* | Z] - \mathbb{E}[X Y | Z] + \mathbb{E}[X X^\top \theta^* | Z]}
\]

\[
\quad \quad \quad \quad \quad \quad \quad = \mathbb{E}[X X^\top]^{-1}\{ \mathbb{E}[X | Y | Z] - \mathbb{E}[X X^\top \theta^* + \mathbb{E}[X | Z] Y - \mathbb{E}[X | Z]|E[Y | Z]}
\]

\[
\quad \quad \quad \quad = \phi^{mod}(X, Y, Z),
\]

where the first and second equalities are from the projection onto subspaces, the third equality uses the fact that \( \mathbb{E}[X (Y - X^\top \theta^*)] = 0 \) and the tower property, and the fourth equality uses the conditional independence in Assumption 2.1. We thus conclude the proof of Theorem 2.2. \( \square \)

### B.2 Proof of Theorem 3.5

**Proof of Theorem 3.5.** For notational simplicity, throughout the proof we write \( \hat{\theta}^{mod} \) as \( \hat{\theta} \). Denote \( \Delta = \hat{\theta} - \theta^* \), and let \( X \in \mathbb{R}^{n \times p_x} \) be the design matrix. We define the vector

\[
G = \sum_{i=1}^n C_i \in \mathbb{R}^{p_x},
\]

where we recall the definition of \( C_i \) in (6). Since \( \hat{\theta} \) is the minimizer of (10), we have

\[
\frac{1}{2n} \hat{\theta}^\top X^\top X \hat{\theta} - \frac{1}{n} G^\top \hat{\theta} + \lambda \| \hat{\theta} \|_1 \leq \frac{1}{2n} (\theta^*)^\top X^\top X \theta^* - \frac{1}{n} G^\top \theta^* + \lambda \| \theta^* \|_1,
\]

which implies

\[
\frac{1}{2n} \Delta^\top X^\top X \Delta \leq \frac{1}{n} (\theta^*)^\top X^\top X - G, \Delta \| \theta^* \|_1 - \lambda \| \hat{\theta} \|_1.
\]

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Let $S$ be the set of indices for nonzero entries of $\theta^*$, and $\theta_S$ be the subvector containing all entries with indices in $S$. Then
\[
\|\theta^*\|_1 - \|\hat{\theta}\|_1 = \|\theta_S^*\|_1 - \|\hat{\theta}_S\|_1 - \|\hat{\theta}_{S^c}\|_1 \leq \|\Delta_S\|_1 - \|\Delta_{S^c}\|_1,
\]
where the last inequality uses triangular inequality and the fact that $\theta_{S^c}^* \equiv 0$. We thus have
\[
\frac{1}{2n} \Delta^T X^T X \Delta \leq \frac{1}{n} \langle (\theta^*)^T X^T X - G, \Delta \rangle + \lambda \|\Delta_S\|_1 - \lambda \|\Delta_{S^c}\|_1 \\
\leq \frac{1}{n} \|\Delta\|_1 \| (\theta^*)^T X^T X - G \|_{\infty} + \lambda \|\Delta_S\|_1 - \lambda \|\Delta_{S^c}\|_1.
\]
(26)
The first implication is that, as the left-handed side is non-negative, once $\lambda \geq \frac{2}{n} \|(\theta^*)^T X^T X - G\|_{\infty}$, we have
\[
0 \leq \frac{\lambda}{2} \|\Delta\|_1 + \lambda \|\Delta_S\|_1 - \lambda \|\Delta_{S^c}\|_1,
\]
hence
\[
\Delta \in C_3 = \{ x \in \mathbb{R}^p: \|x_{S^c}\|_1 \leq 3\|s_S\|_1 \}.
\]
By Assumption 3.2, (26) further implies
\[
\zeta \|\Delta\|_2^2 \leq \frac{\lambda}{2} \|\Delta\|_1 + \lambda \|\Delta_S\|_1 - \lambda \|\Delta_{S^c}\|_1 \leq \frac{3\lambda}{2} \|\Delta_S\|_1 \leq \frac{3\lambda}{2} \sqrt{k} \|\Delta\|_2,
\]
where $k = |S| = \|\theta^*\|_0$ is the sparsity level. To summarize, under Assumption 3.2, the solution $\hat{\theta}$ satisfies
\[
\|\hat{\theta} - \theta^*\|_2 \leq \frac{3\lambda \sqrt{k}}{2\zeta},
\]
(27)
for any regularization parameter $\lambda \geq \frac{2}{n} \|(\theta^*)^T X^T X - G\|_{\infty}$. We now write $\hat{\mu}_y \in \mathbb{R}^n$ as the vector whose $i$-th entry is $\hat{\mu}_y^{(k)}(Z_i)$ for $i \in \mathcal{I}_k$, and $\hat{\mu}_x \in \mathbb{R}^{n \times p_x}$ whose $(i,j)$-th entry is $\hat{\mu}_x^{(k)}(Z_i)$ for $i \in \mathcal{I}_k$. Similarly, $\mu_y \in \mathbb{R}^n$ and $\mu_x \in \mathbb{R}^{n \times p_x}$ record the ground truth of these regression functions. The error term is then
\[
(\theta^*)^T X^T X - G = (\theta^*)^T X^T X - \hat{\mu}_y^T X - Y^T \hat{\mu}_x + \hat{\mu}_y \hat{\mu}_x \\
= (Y - \mu_y)^T (X - \mu_x) + (X \theta^* - Y)^T X \\
+ (\mu_y - \hat{\mu}_y)^T (X - \mu_x) + (Y - \mu_y)^T (\mu_x - \hat{\mu}_x) + (\mu_y - \hat{\mu}_y)^T (\mu_x - \hat{\mu}_x).
\]
(28)
For any constant $\delta \in (0,1)$, we define the event
\[
\mathcal{E}_{\text{est}}^{n,\delta} = \left\{ \|\hat{\mu}_x^{(k)} - \mu_{x,j}\|_{L_2(\mathcal{P}^2)} \|\hat{\mu}_y^{(k)} - \mu_y\|_{L_2(\mathcal{P}^2)} \leq \frac{4c_n \log(3p_x/\delta)^{1/4}}{n^{1/4}}, \forall 1 \leq j \leq p_x, \forall k = 1,2 \right\}.
\]
(29)
Then under Assumption 3.4, for any constant $\delta \in (0,1)$, taking a union bound over $2p_x + 2 \leq 3p_x$ estimated functions for $1 \leq j \leq p_x$ and $k = 1,2$, we know that $\mathbb{P}(\mathcal{E}_{\text{est}}^{n,\delta}) \geq 1 - \delta$.

We now proceed to analyze each entry $j \in \{1,\ldots,p_x\}$ of the above error term. First,
\[
\mathbb{E} \left[ (\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i))(X_{i,j} - \mu_{x,j}(Z_i)) \right] = \mathbb{E} \left[ (\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i)) \left| \mathcal{I} \setminus \mathcal{I}_k \right. \right] = 0
\]
for each $k = 1,2$, conditional on $\mathcal{I} \setminus \mathcal{I}_k$, the terms in the summation $(\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i))(X_{i,j} - \mu_{x,j}(Z_i))$, $i \in \mathcal{I}_k$ are mutually independent with mean zero, since
\[
\mathbb{E} \left[ (\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i)) (X_{i,j} - \mu_{x,j}(Z_i)) \left| \mathcal{I} \setminus \mathcal{I}_k \right. \right] = \mathbb{E} \left[ \left( \mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i) \right) \cdot \mathbb{E} \left[ X_{i,j} - \mu_{x,j}(Z_i) \left| Z_i, \mathcal{I} \setminus \mathcal{I}_k \right. \right. \right] = 0
\]

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by the tower property. Also, the absolute value of each term is bounded below $4c_0$ by the boundedness in Assumption 3.3. We now define the event

$$\mathcal{E}_{ct}^{1,k}(\delta) = \left\{ \sum_{i \in I_k} (\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i))(X_{i,j} - \mu_{x,j}(Z_i)) \right\} \leq \max \left\{ 16c_0 \log(2/\delta)/3, 2\epsilon_1 \sqrt{|I_k| \log(2/\delta)} \right\},$$

where we define

$$\epsilon_2^2 = 4 \sup_{k=1,2} \|\mu_y - \hat{\mu}_y^{(k)}\|_{L_2(^p\mathbb{R})}^2 \geq \mathbb{E} \left[ (\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i))^2 (X_{i,j} - \mu_{x,j}(Z_i))^2 \right| \mathcal{I}\setminus I_k].$$

The Bernstein’s inequality in Lemma C.1, implies $\mathbb{P}(\mathcal{E}_{ct}^{1,k} | \mathcal{I}\setminus I_k) \leq \delta$. Marginalizing out the conditional probability and taking a union bound over $k = 1, 2$, we know that $\mathbb{P}(\mathcal{E}_{ct}^{1}(\delta)) \geq 1 - \delta$ for any constant $\delta$, where we define $\mathcal{E}_{ct}^{1}(\delta) = \mathcal{E}_{ct}^{1,1}(\delta/2) \cup \mathcal{E}_{ct}^{1,2}(\delta/2)$. That is, with probability at least $1 - \delta$,

$$\left| \frac{1}{n} \left[ (\mu_y - \hat{\mu}_y)(X - \mu_x) \right] \right| \leq \max \left\{ \frac{16c_0 \log(4/\delta)}{3n}, \epsilon_1 \sqrt{\frac{2 \log(4/\delta)}{n}} \right\}. \quad (30)$$

For each fixed $j$, applying exactly the same arguments to

$$\frac{1}{n} \left[ (Y - \mu_y)^\top (X - \mu_x) \right]_j = \frac{1}{n} \sum_{k=1}^2 \sum_{i \in I_k} (Y_i - \mu_y(Z_i))(\mu_{x,j}(Z_i) - \hat{\mu}_{x,j}(Z_i)),$$

with probability at least $1 - \delta$,

$$\left| \frac{1}{n} \left[ (Y - \mu_y)^\top (X - \mu_x) \right] \right| \leq \max \left\{ \frac{16c_0 \log(4/\delta)}{3n}, c_0 \epsilon_2 \epsilon_{2,j} \sqrt{\frac{2 \log(4/\delta)}{n}} \right\}, \quad (31)$$

where we define $\epsilon_{2,j} = 2 \sup_{k=1,2} \|\mu_{x,j} - \hat{\mu}_{x,j}^{(k)}\|_{L_2(^p\mathbb{R})}$. The third term is

$$\frac{1}{n} \left[ (\mu_y - \hat{\mu}_y)(X - \mu_x) \right]_j = \frac{1}{n} \sum_{k=1}^2 \sum_{i \in I_k} (\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i))(\mu_{x,j}(Z_i) - \hat{\mu}_{x,j}^{(k)}(Z_i)).$$

Here for each $k = 1, 2$, conditional on $\mathcal{I}\setminus I_k$, each term $(\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i))(\mu_{x,j}(Z_i) - \hat{\mu}_{x,j}^{(k)}(Z_i))$, $i \in I_k$ in the above summation is i.i.d. whose expectation is bounded as

$$\mathbb{E} \left[ (\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i))(\mu_{x,j}(Z_i) - \hat{\mu}_{x,j}^{(k)}(Z_i)) \right| \mathcal{I}\setminus I_k] \leq \|\mu_y - \hat{\mu}_y^{(k)}\|_{L_2(^p\mathbb{R})} \|\mu_{x,j} - \hat{\mu}_{x,j}^{(k)}\|_{L_2(^p\mathbb{R})} \leq \epsilon_1 \epsilon_{2,j} / 4.$$

Meanwhile, their second moments are bounded as

$$\mathbb{E} \left[ (\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i))^2 (\mu_{x,j}(Z_i) - \hat{\mu}_{x,j}^{(k)}(Z_i))^2 \right| \mathcal{I}\setminus I_k] \leq 4 \|\mu_y - \hat{\mu}_y^{(k)}\|_{L_2(^p\mathbb{R})}^2 \leq \epsilon_1^2$$

according to the boundedness in Assumption 3.3. Combining the above two bounds and invoking the Bernstein’s inequality in Lemma C.1, it holds with probability at least $1 - \delta$ that

$$\left| \sum_{i \in I_k} (\mu_y(Z_i) - \hat{\mu}_y^{(k)}(Z_i))(\mu_{x,j}(Z_i) - \hat{\mu}_{x,j}^{(k)}(Z_i)) \right| \leq |I_k| \epsilon_1 \epsilon_{2,j} / 4 + \max \left\{ 16c_0 \log(2/\delta)/3, 2\epsilon_1 \sqrt{|I_k| \log(2/\delta)} \right\}.$$

Taking a union bound for $k = 1, 2$ implies that with probability at least $1 - \delta$,

$$\left| \frac{1}{n} \left[ (\mu_y - \hat{\mu}_y)^\top (X - \mu_x) \right] \right| \leq \frac{\epsilon_1 \epsilon_{2,j}}{4} + \max \left\{ \frac{16c_0 \log(4/\delta)}{3n}, \epsilon_1 \sqrt{\frac{2 \log(4/\delta)}{n}} \right\}. \quad (32)$$
Putting together (30), (31) and (32), we know that with probability at least \(1 - \delta/2\),
\[
\|\left(\mu_y - \hat{\mu}_y\right)^\top (X - \mu_x) + (Y - \mu_y)^\top (\mu_x - \hat{\mu}_x) + (\mu_y - \hat{\mu}_y)^\top (\mu_x - \hat{\mu}_x)\|_\infty \\
\leq \frac{\epsilon_1 \epsilon_2 \delta}{4} + 2 \max \left\{ \frac{16c_0 \log(24/\delta)}{3n}, \frac{\epsilon_1 \sqrt{2 \log(24/\delta)}}{n}, \frac{\epsilon_0 \epsilon_2 \delta}{3n}, \frac{2 \log(24/\delta)}{n} \right\}.
\]
Further taking a union bound over the above event and (29) for \(\xi_{est}^{n,3/2}\), and using the fact that \(\max\{a, b\} \leq a + b\) for \(a, b \geq 0\), we know it holds with probability at least \(1 - \delta\) that
\[
\|\left(\mu_y - \hat{\mu}_y\right)^\top (X - \mu_x) + (Y - \mu_y)^\top (\mu_x - \hat{\mu}_x) + (\mu_y - \hat{\mu}_y)^\top (\mu_x - \hat{\mu}_x)\|_\infty \\
\leq 4c_n^2 (\log(3p_x/\delta))^2 \frac{\sqrt{n}}{n} + 16c_0 \log(24/\delta) \frac{2 + c_0 \log(3p_x/\delta) \sqrt{2 \log(24/\delta)}}{n^{3/4}}.
\]
Recalling (28) and letting
\[
\tilde{c}_n = 4c_n^2 + 16c_0 / \sqrt{n} + (2 + c_0) / n^{1/4},
\]
we have \(\tilde{c}_n \to 0\) as \(n \to \infty\) and with probability at least \(1 - \delta\),
\[
\frac{1}{n} \| (\hat{\theta}^*)^\top X^\top X - G \|_\infty \leq \frac{1}{n} \| (Y - \mu_y)^\top (X - \mu_x) + (X \theta^* - Y)^\top X \|_\infty + \frac{\tilde{c}_n (\log(3p_x/\delta))^2}{\sqrt{n}}.
\]
Combining this high-probability bound with (27), we know that
\[
\mathbb{P} \left( \| \hat{\theta} - \theta^* \|_2 \leq \frac{3\lambda \sqrt{\delta}}{2\epsilon}, \quad \forall \lambda \geq \frac{2}{n} \| (Y - \mu_y)^\top (X - \mu_x) + (X \theta^* - Y)^\top X \|_\infty + \frac{2\tilde{c}_n (\log(3p_x/\delta))^2}{\sqrt{n}} \right) \\
\geq \mathbb{P} \left( \frac{1}{n} \| (\hat{\theta}^*)^\top X^\top X - G \|_\infty \leq \frac{1}{n} \| (Y - \mu_y)^\top (X - \mu_x) + (X \theta^* - Y)^\top X \|_\infty + \frac{\tilde{c}_n (\log(3p_x/\delta))^2}{\sqrt{n}} \right) \geq 1 - \delta,
\]
which proves (12).
\[\square\]

### C Supporting lemmas

**Lemma C.1** (Bernstein’s inequality). Suppose \(X_1, \ldots, X_n\) are independent zero-mean random variables such that \(|X_i| \leq M\) almost surely for some constant \(M > 0\). Then for any constant \(t > 0\),
\[
\mathbb{P} \left( \left| \sum_{i=1}^{n} X_i \right| \geq t \right) \leq 2 \exp \left( - \frac{t^2}{2 \sum_{i=1}^{n} \mathbb{E}[X_i^2] + 2Mt/3} \right).
\]
That is, for any \(\delta \in (0, 1)\), with probability at least \(1 - \delta\), it holds that
\[
\left| \sum_{i=1}^{n} X_i \right| \leq \max \left\{ 2 \sqrt{\sum_{i=1}^{n} \mathbb{E}[X_i^2] \log(2/\delta)}, 4M \log(2/\delta)/3 \right\}.
\]

### D Deferred simulation results

#### D.1 Low-dimensional simulation

Figure 12 plots the RMSE for estimating \(\theta^*_1\) in settings 1 and 4 with sample size \(n = 1000\); this is in comparison to Figure 2. Figures 13 to 16 present the RMSE for all entries of \(\theta^*\) in all settings.
Figure 12: Bias for estimating $\theta^*_1$ when $n = 1000$. Details are otherwise the same as Figure 2.

Figure 13: RMSE for estimating $\theta^*_1$. Details are otherwise the same as Figure 2.
Figure 14: RMSE for estimating $\theta_2^*$. Details are otherwise the same as Figure 2.
Figure 15: RMSE for estimating $\theta_3^\ast$. Details are otherwise the same as Figure 2.
D.2 High-dimensional simulation

Figure 16: RMSE for estimating $\theta_4^\ast$. Details are otherwise the same as Figure 2.

Figure 17: Boxplot of standard deviations for all $\hat{\theta}_j$, $j \in [p_x]$ over $N = 1000$ replicates in setting 1 (left) and setting 2 (right). Other details of the plot are the same as Figure 6.