ddml: Double/debiased machine learning in Stata

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Abstract. We introduce the package `ddml` for Double/Debiased Machine Learning (DDML) in Stata. Estimators of causal parameters for five different econometric models are supported, allowing for flexible estimation of causal effects of endogenous variables in settings with unknown functional forms and/or many exogenous variables. `ddml` is compatible with many existing supervised machine learning programs in Stata. We recommend using DDML in combination with stacking estimation which combines multiple machine learners into a final predictor. We provide Monte Carlo evidence to support our recommendation.

Keywords: st0001, causal inference, machine learning, doubly-robust estimation

1 Introduction

Identification of causal effects frequently relies on an unconfoundedness assumption, requiring that treatment or instrument assignment is sufficiently random given observed control covariates. Estimation of causal effects in these settings then involves conditioning on the controls. Unfortunately, estimators of causal effects that are insufficiently flexible to capture the effect of confounds generally do not produce consistent estimates of causal effects even when unconfoundedness holds. For example, Blandhol et al. (2022) highlight that TSLS estimands obtained after controlling linearly for confounds do not generally correspond to weakly causal effects even when instruments are valid conditional on controls. Even in the ideal scenario where theory provides a small number of relevant controls, theory rarely specifies the exact nature of confounding. Thus, applied empirical researchers wishing to exploit unconfoundedness assumptions to learn causal effects face a nonparametric estimation problem.

Traditional nonparametric estimators suffer greatly under the curse of dimensionality and are quickly impractical in the frequently encountered setting with multiple observed covariates.[1] These difficulties leave traditional nonparametric estimators essentially inapplicable in the presence of increasingly large and complex data sets, e.g.

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1. For example, the number of coefficients in polynomial series regression with interaction terms increases exponentially in the number of covariates.

textual confounders as in Roberts et al. (2020) or digital trace data (Hangartner et al. 2021). Tools from supervised machine learning have been put forward as alternative estimators. These approaches are often more robust to the curse of dimensionality via the exploitation of regularization assumptions. A prominent example of a machine learning-based causal effects estimator is Post-Double Selection Lasso (PDS-Lasso) of Belloni et al. (2014), which fits auxiliary lasso regressions of the outcome and treatment(s), respectively, against a menu of transformed controls. Under an approximate sparsity assumption, which posits that the DGP can be approximated well by a relatively small number of terms included in the menu, this approach allows for precise treatment effect estimation. The lasso can also be used for approximating optimal instruments (Belloni et al. 2012). Lasso-based approaches for estimation of causal effects have become a popular strategy in applied econometrics (e.g. Gilchrist and Sands 2016; Dhar et al. 2022), partially facilitated by the availability of software programs in Stata (`pdslasso`, Ahrens et al. 2018; StataCorp 2019) and R (`hdm`, Chernozhukov et al. 2016).

Although approximate sparsity is a weaker regularization assumption than assuming a linear functional form that depends on a known low-dimensional set of variables, it may not be suitable in a wide range of applications. For example, Giannone et al. (2021) argue that approximate sparsity may provide a poor description in several economic examples. There is thus a potential benefit to expanding the set of regularization assumptions and correspondingly considering a larger set of machine learners including, for example, random forests, gradient boosting, and neural networks. While the theoretical properties of these estimators are an active research topic (see, e.g., Athey et al. 2019; Farrell et al. 2021), machine learning methods are widely adopted in industry and practice for their empirical performance. To facilitate their application for causal inference in common econometric models, Chernozhukov et al. (2018) propose Double/Debiased Machine Learning (DDML), which exploits Neyman orthogonality of estimating equations and cross-fitting to formally establish asymptotic normality of estimators of causal parameters under relatively mild convergence rate conditions on nonparametric estimators.

DDML increases the set of machine learners that researchers can leverage for estimation of causal effects. Deciding which learner is most suitable for a particular application is difficult, however, since researchers are rarely certain about the structure of the underlying data generating process. A practical solution is to construct combinations of a diverse set of machine learners using stacking (Wolpert 1992; Breiman 1996). Stacking is a meta learner given by a weighted sum of individual machine learners (the "base learners"). When the weights corresponding to the base learners are chosen to maximize out-of-sample predictive accuracy, this approach hedges against the risk of relying on any particular poorly suited or ill-tuned machine learner.

In this article, we introduce the Stata package `ddml`, which implements DDML for Stata.[2] `ddml` adds to a small number of programs for causal machine learning in Stata (Ahrens et al. 2018, StataCorp 2019, StataCorp 2021). We briefly summarize the four main features of the program:

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2. This article refers to version v1.4.2 of `ddml`.

1. `ddml` supports flexible estimators of causal parameters in five econometric models: (1) the Partially Linear Model, (2) the Interactive Model (for binary treatment), (3) the Partially Linear IV Model, (4) the Flexible Partially Linear IV Model, and (5) the Interactive IV Model (for binary treatment and instrument).

2. `ddml` supports data-driven combinations of multiple machine learners via stacking by leveraging `pystacked` (Ahrens et al. 2022), our complementary Stata frontend relying on the Python library *scikit-learn* (Pedregosa et al. 2011; Buitinck et al. 2013). `ddml` also supports two novel approaches to pairing DDML with stacking introduced in Ahrens et al. (2023): short-stacking takes a short-cut by leveraging the cross-fitted predicted values for estimating the stacking weights and pooled stacking enforces common weights across cross-fitting folds.

3. Aside from `pystacked`, `ddml` can be used in combination with many other existing supervised machine learning programs available in or via Stata. `ddml` has been tested with `lassopack` (Ahrens et al. 2020), `rforest` (Schonlau and Zou 2020), `svmachines` (Guenther and Schonlau 2018), and `parsnip` (Huntington-Klein 2021). Indeed, the requirements for compatibility with `ddml` are minimal: Any `eclass` program with the Stata-typical "`reg y x`" syntax, support for `if` conditions and post-estimation `predict` is compatible with `ddml`.

4. `ddml` provides flexible multi-line syntax and short one-line syntax. The multi-line syntax offers a wide range of options, guides the user through the DDML algorithm step-by-step, and includes auxiliary programs for storing, loading and displaying additional information. We also provide a complementary one-line version called `qddml` ('quick' `ddml`), which uses a similar syntax as `pdslasso` and `ivlasso` (Ahrens et al. 2018).

The article proceeds as follows. Section 2 outlines DDML for the Partially Linear and Interactive Models under conditional unconfoundedness assumptions. Section 3 outlines DDML for Instrumental Variables (IV) models. Section 4 discusses how stacking can be combined with DDML and provides evidence from Monte Carlo simulations illustrating the advantages of DDML with stacking. Section 5 explains the features, syntax and options of the program. Section 6 demonstrates the program's usage with two applications.

2 DDML with Conditional Unconfoundedness

This section discusses DDML for the Partially Linear Model and the Interactive Model in turn. The exposition follows Chernozhukov et al. (2018). Both models are special cases of the general causal model

$$Y = f_0(D, \boldsymbol{X}, U), \tag{1}$$

where f_0 is a structural function, Y is the outcome, D is the variable of interest, $\boldsymbol{X}$ are observed covariates, and U are all unobserved determinants of Y (i.e., other than D and

$\boldsymbol{X}$).[3] The key difference between the Partially Linear Model and the Interactive Model is their position in the trade-off between functional form restrictions on f_0 and restrictions on the joint distribution of observables $(D, \boldsymbol{X})$ and unobservables U. For both models, we highlight key parameters of interest, state sufficient identifying assumptions, and outline the corresponding DDML estimator. A random sample $\{(Y_i, D_i, \boldsymbol{X}_i)\}_{i=1}^n$ from $(Y, D, \boldsymbol{X})$ is considered throughout.

2.1   The Partially Linear Model (`partial`)

The Partially Linear Model imposes the estimation model

$$Y = \theta_0 D + g_0(\boldsymbol{X}) + U \tag{2}$$

where θ_0 is a fixed unknown parameter. The key feature of the model is that the controls $\boldsymbol{X}$ enter through the unknown and potentially nonlinear function g_0. Note that D is not restricted to be binary and may be discrete, continuous or mixed. For simplicity, we assume that D is a scalar, although `ddml` allows for multiple treatment variables in the Partially Linear Model.

The parameter of interest is θ_0, the causal effect of D on Y.[4] The key identifying assumption is given in Assumption 1.[5]

Assumption 1 (Conditional Orthogonality) $E[Cov(U, D|\boldsymbol{X})] = 0$.

To show identification of θ_0, consider the score

$$\psi(\boldsymbol{W}; \theta, m, \ell) = \Big(Y - \ell(\boldsymbol{X}) - \theta\big(D - m(\boldsymbol{X})\big)\Big)\big(D - m(\boldsymbol{X})\big), \tag{3}$$

where $\boldsymbol{W} \equiv (Y, D, \boldsymbol{X})$, and ℓ and m are nuisance functions. Letting $m_0(\boldsymbol{X}) \equiv E[D|\boldsymbol{X}]$ and $\ell_0(\boldsymbol{X}) \equiv E[Y|\boldsymbol{X}]$, note that

$$E\left[\psi(\boldsymbol{W}; \theta_0, m_0, \ell_0)\right] = 0$$

by Assumption 1. When in addition $E[Var(D|\boldsymbol{X})] \neq 0$, we get

$$\theta_0 = \frac{E\left[\big(Y - \ell_0(\boldsymbol{X})\big)\big(D - m_0(\boldsymbol{X})\big)\right]}{E\left[(D - m_0(\boldsymbol{X}))^2\right]}. \tag{4}$$

3. Since in (1), $(D, \boldsymbol{X}, U)$ jointly determine Y, the model is also dubbed the "all causes model" (see, e.g., Heckman and Vytlacil 2007). Note that the model can equivalently be put into potential outcome notation with potential outcomes defined as $Y(d) \equiv f_0(d, \boldsymbol{X}, U)$.

4. The interpretation of θ_0 can be generalized. For example, the results of Angrist and Krueger (1999) imply that in the general causal model (1), θ_0 is a positively weighted average of causal effects (e.g., conditional average treatment effects) under stronger identifying assumptions. The basic structure can also be used to obtain valid inference on objects of interest, such as projection coefficients, in the presence of high-dimensional data or nonparametric estimation without requiring a causal interpretation.

5. Discussions of Partially Linear Model typically show identification under the stronger assumption that $E[U|D, \boldsymbol{X}] = 0$. We differentiate here to highlight differences between the Partially Linear Model and Interactive Model.

Equation (4) is constructive in that it motivates estimation of θ_0 via a simple two-step procedure: First, estimate the conditional expectation of Y given $\boldsymbol{X}$ (i.e., ℓ_0) and of D given $\boldsymbol{X}$ (i.e., m_0) using appropriate nonparametric estimators (e.g., machine learners). Second, residualize Y and D by subtracting their respective conditional expectation function (CEF) estimates, and regress the resulting CEF residuals of Y on the CEF residuals of D. This approach is fruitful when the estimation error of the first step does not propagate excessively to the second step. DDML leverages two key ingredients to control the impact of the first step estimation error on the second step estimate: 1) second step estimation based on Neyman orthogonal scores and 2) cross-fitting. As shown in Chernozhukov et al. (2018), this combination facilitates the use of any nonparametric estimator that converges sufficiently quickly in the first and potentially opens the door for the use of many machine learners.

Neyman orthogonality refers to a property of score functions ψ that ensures local robustness to estimation errors in the first step. Formally, it requires that the Gateaux derivative with respect to the nuisance functions evaluated at the true values is mean-zero. In the context of the partially linear model, this condition is satisfied for the moment condition (3):

$$\partial_r \left\{ E \left[\psi(W; \theta_0, m_0 + r(m - m_0), \ell_0 + r(\ell - \ell_0)) \right] \right\} |_{r=0} = 0,$$

where the derivative is with respect to the scalar r and evaluated at $r = 0$. Heuristically, we can see that this condition alleviates the impact of noisy estimation of nuisance functions as local deviations of the nuisance functions away from their true values leave the moment condition unchanged. We refer to Chernozhukov et al. (2018) for a detailed discussion but highlight that all score functions discussed in this article are Neyman orthogonal.

Cross-fitting ensures independence between the estimation error from the first step and the regression residual in the second step. To implement cross-fitting, we randomly split the sample into K evenly-sized folds, denoted as $I_1, \ldots, I_K$. For each fold k, the conditional expectations ℓ_0 and m_0 are estimated using only observations *not* in the kth fold – i.e., in $I_k^c \equiv I \setminus I_k$ – resulting in $\hat{\ell}_{I_k^c}$ and $\hat{m}_{I_k^c}$, respectively, where the subscript I_k^c indicates the subsample used for estimation. The out-of-sample predictions for an observation i in the kth fold are then computed via $\hat{\ell}_{I_k^c}(\boldsymbol{X}_i)$ and $\hat{m}_{I_k^c}(\boldsymbol{X}_i)$. Repeating this procedure for all K folds then allows for computation of the DDML estimator for θ_0:

$$\hat{\theta}_n = \frac{\frac{1}{n} \sum_{i=1}^n \left(Y_i - \hat{\ell}_{I_{k_i}^c}(\boldsymbol{X}_i) \right) \left(D_i - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i) \right)}{\frac{1}{n} \sum_{i=i}^n \left(D_i - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i) \right)^2}, \tag{5}$$

where k_i denotes the fold of the ith observation.[6]

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6. We here omit the constant from the estimation stage. Since the residualized outcome and treatment may not be exactly mean-zero in finite samples, `ddml` includes the constant by default in the estimation stage of partially linear models.

We summarize the DDML algorithm for the Partially Linear Model in Algorithm 1:[7]

❏ **Algorithm 1. DDML for the Partially Linear Model.**

Split the sample $\{(Y_i, D_i, \boldsymbol{X}_i)\}_{i=1}^n$ randomly in K folds of approximately equal size. Denote I_k the set of observations included in fold k and I_k^c its complement.

1. For each $k \in \{1, \ldots, K\}$:

   a. Fit a CEF estimator to the sub-sample I_k^c using Y_i as the outcome and $\boldsymbol{X}_i$ as predictors. Obtain the out-of-sample predicted values $\hat{\ell}_{I_k^c}(\boldsymbol{X}_i)$ for $i \in I_k$.

   b. Fit a CEF estimator to the sub-sample I_k^c using D_i as the outcome and $\boldsymbol{X}_i$ as predictors. Obtain the out-of-sample predicted values $\hat{m}_{I_k^c}(\boldsymbol{X}_i)$ for $i \in I_k$.

2. Compute (5).

❏

Chernozhukov et al. (2018) give conditions on the joint distribution of the data, in particular on g_0 and m_0, and properties of the nonparametric estimators used for CEF estimation, such that $\hat{\theta}_n$ is consistent and asymptotically normal. Standard errors are equivalent to the conventional linear regression standard errors of $Y_i - \hat{\ell}_{I_{k_i}^c}(\boldsymbol{X}_i)$ on $D_i - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)$. `ddml` computes the DDML estimator for the Partially Linear Model using Stata's `regress`. All standard errors available for linear regression in Stata are also available in `ddml`, including different heteroskedasticity and cluster-robust standard errors.[8]

Remark 1: Number of folds. The number of cross-fitting folds is a necessary tuning choice. Theoretically, any finite value is admissable. Chernozhukov et al. (2018, Remark 3.1) report that four or five folds perform better than only using $K = 2$. Based on our simulation experience, we find that more folds tends to lead to better performance as more data is used for estimation of conditional expectation functions, especially when the sample size is small. We believe that more work on setting the number of folds would be useful, but believe that setting $K = 5$ provides is likely a good baseline in many settings.

Remark 2: Cross-fitting repetitions. DDML relies on randomly splitting the sample into K folds. We recommend running the cross-fitting procedure more than once using different random folds to assess randomness introduced via the sample splitting. `ddml` facilitates this using the `rep(integer)` options, which automatically estimates the same model multiple times and combines the resulting estimates to obtain the final estimate. By default, `ddml` reports the median over cross-fitting repetitions. `ddml` also supports the average of estimates. Specifically, let $\hat{\theta}_n^{(r)}$ denote the DDML estimate from the rth cross-fit repetition and $\hat{s}_n^{(r)}$ its associated standard error estimate with $r = 1, \ldots, R$.

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7. Algorithm 1 corresponds to the 'DML2' algorithm in Chernozhukov et al. (2018). Chernozhukov et al. (2018, Remark 3.1) recommend 'DML2' over the alternative 'DML1' algorithm, which fits the final estimator by fold.

8. See `help regress##vcetype` for available options.

The aggregate median point estimate and associated standard error are defined as

$$\breve{\theta}_n = \text{median}\left(\left(\hat{\theta}_n^{(r)}\right)_{r=1}^R\right) \quad \text{and} \quad \breve{s}_n = \sqrt{\text{median}\left(\left((\hat{s}_n^{(r)})^2 + (\hat{\theta}_n^{(r)} - \breve{\theta}_n)^2\right)_{r=1}^R\right)}.$$

The aggregate mean point estimates and associated standard error are calculated as

$$\bar{\hat{\theta}}_n = \frac{1}{R}\sum_{r=1}^R \hat{\theta}_n^{(r)} \quad \text{and} \quad \bar{\hat{s}}_n = \sqrt{\text{hmean}\left(\left((\hat{s}_n^{(r)})^2 + (\hat{\theta}_n^{(r)} - \bar{\hat{\theta}}_n)^2\right)_{r=1}^R\right)},$$

where hmean() is the harmonic mean.[9]

Remark 3: Cluster-dependence and folds. Under cluster-dependence, we recommend randomly assigning folds by cluster; see `fcluster(`*varname*`)`.

2.2   The Interactive Model (`interactive`)

The Interactive Model is given by

$$Y = g_0(D, \boldsymbol{X}) + U \tag{6}$$

where D takes values in $\{0, 1\}$. The key deviations from the Partially Linear Model are that D must be a scalar binary variable and that D is not required to be additively separable from the controls $\boldsymbol{X}$. In this setting, the parameters of interest we consider are

$$\theta_0^{\text{ATE}} \equiv E[g_0(1, \boldsymbol{X}) - g_0(0, \boldsymbol{X})]$$
$$\theta_0^{\text{ATET}} \equiv E[g_0(1, \boldsymbol{X}) - g_0(0, \boldsymbol{X})|D = 1],$$

which correspond to the average treatment effect (ATE) and average treatment effect on the treated (ATET), respectively.

Assumptions 2 and 3 below are sufficient for identification of the ATE and ATET. Note the conditional mean independence condition stated here is stronger than the conditional orthogonality assumption sufficient for identification of θ_0 in the Partially Linear Model.

Assumption 2 (Conditional Mean Independence) $E[U|D, \boldsymbol{X}] = 0$.

Assumption 3 (Overlap) $\Pr(D = 1|\boldsymbol{X}) \in (0, 1)$ *with probability 1.*

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9. The harmonic mean of $x_1, \ldots, x_n$ is defined as $\text{hmean}(x_1, \ldots, x_n) = n\left(\sum_{i=1}^n \frac{1}{x_i}\right)^{-1}$. We use the harmonic mean as it is less sensitive to outlier values.

Under assumptions 2 and 3, we have

$$E[Y|D, \boldsymbol{X}] = E[g_0(D, \boldsymbol{X})|D, \boldsymbol{X}] + E[U|D, \boldsymbol{X}] = g_0(D, \boldsymbol{X}),$$

so that identification of the ATE and ATET immediately follows from their definition.[10]

In contrast to Section 2.1, second-step estimators are not directly based on the moment conditions used for identification. Additional care is needed to ensure local robustness to first-stage estimation errors (i.e., Neyman orthogonality). In particular, the Neyman orthogonal score for the ATE that Chernozhukov et al. (2018) consider is the efficient influence function of Hahn (1998)

$$\psi^{\mathrm{ATE}}(\boldsymbol{W}; \theta, g, m) = \frac{D(Y - g(1, \boldsymbol{X}))}{m(\boldsymbol{X})} - \frac{(1 - D)(Y - g(0, \boldsymbol{X}))}{1 - m(\boldsymbol{X})} + g(1, \boldsymbol{X}) - g(0, \boldsymbol{X}) - \theta,$$

where $\boldsymbol{W} \equiv (Y, D, \boldsymbol{X})$. Similarly for the ATET,

$$\psi^{\mathrm{ATET}}(\boldsymbol{W}; \theta, g, m, p) = \frac{D(Y - g(0, \boldsymbol{X}))}{p} - \frac{m(\boldsymbol{X})(1 - D)(Y - g(0, \boldsymbol{X}))}{p(1 - m(\boldsymbol{X}))} - \theta.$$

Importantly, for $g_0(D, \boldsymbol{X}) \equiv E[Y|D, \boldsymbol{X}]$, $m_0(\boldsymbol{X}) \equiv E[D|\boldsymbol{X}]$, and $p_0 \equiv E[D]$, Assumptions 2 and 3 imply

$$E[\psi^{\mathrm{ATE}}(\boldsymbol{W}; \theta_0^{\mathrm{ATE}}, g_0, m_0)] = 0$$
$$E[\psi^{\mathrm{ATET}}(\boldsymbol{W}; \theta_0^{\mathrm{ATET}}, g_0, m_0, p_0)] = 0;$$

and we also have that the Gateaux derivative of each condition with respect to the nuisance parameters (g_0, m_0, p_0) is zero.

As before, the DDML estimators for the ATE and ATET leverage cross-fitting. The DDML estimators of the ATE and ATET based on ψ^{ATE} and ψ^{ATET} are

$$\hat{\theta}_n^{\mathrm{ATE}} = \frac{1}{n} \sum_{i=1}^n \left(\frac{D_i(Y_i - \hat{g}_{I_{k_i}^c}(1, \boldsymbol{X}_i))}{\hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)} - \frac{(1 - D_i)(Y_i - \hat{g}_{I_{k_i}^c}(0, \boldsymbol{X}_i))}{1 - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)} \right. \tag{7}$$
$$\left. + \hat{g}_{I_{k_i}^c}(1, \boldsymbol{X}_i) - \hat{g}_{I_{k_i}^c}(0, \boldsymbol{X}_i) \right),$$

$$\hat{\theta}_n^{\mathrm{ATET}} = \frac{1}{n} \sum_{i=1}^n \left(\frac{D_i(Y_i - \hat{g}_{I_{k_i}^c}(0, \boldsymbol{X}_i))}{\hat{p}_{I_{k_i}^c}} - \frac{\hat{g}_{I_{k_i}^c}(0, \boldsymbol{X}_i)(1 - D_i)(Y_i - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i))}{\hat{p}_{I_{k_i}^c}(1 - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i))} \right), \tag{8}$$

where $\hat{g}_{I_k^c}$ and $\hat{m}_{I_k^c}$ are cross-fitted estimators for g_0 and m_0 as defined in Section 2.1. Since D is binary, the cross-fitted values $\hat{g}_{I_k^c}(1, \boldsymbol{X})$ and $\hat{g}_{I_k^c}(0, \boldsymbol{X})$ are computed by only

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10. In the defined Interactive Model under Assumption 2, the heterogeneity in treatment effects that the ATE and ATET average over is fully observed since U is additively separable. Under stronger identifying assumptions, the DDML ATE and ATET estimators outlined here also apply to the ATE and ATET in the general causal model (1) that average over both observed and unobserved heterogeneity. See, e.g., Belloni et al. (2017).

using treated and untreated observations, respectively. $\hat{p}_{I_k^c}$ is a cross-fitted estimator of the unconditional treatment probability.

`ddml` supports heteroskedasticity and cluster-robust standard errors for $\hat{\theta}_n^{\text{ATE}}$ and $\hat{\theta}_n^{\text{ATET}}$. The algorithm for estimating the ATE and ATET are conceptually similar to Algorithm 1. We delegate the detailed outline to Appendix A. Mean and median aggregation over cross-fitting repetitions are implemented as outlined in Remark 2.

3   DDML with Instrumental Variables

This section outlines the Partially Linear IV Model, the Flexible Partially Linear IV Model, and the Interactive IV Model. The discussion is again based on Chernozhukov et al. (2018). As in the previous section, each model is a special case of the general causal model (1). The discussion in this section differs from the preceding section in that identifying assumptions leverage instrumental variables $\boldsymbol{Z}$. The two partially linear IV models assume strong additive separability as in (2), while the Interactive IV Model allows for arbitrary interactions between the treatment D and the controls $\boldsymbol{X}$ as in (6). The Flexible Partially Linear IV Model allows for approximation of optimal instruments[11] as in Belloni et al. (2012) and Chernozhukov et al. (2015a), but relies on a stronger independence assumption than the Partially Linear IV Model. Throughout this discussion, we consider a random sample $\{(Y_i, D_i, \boldsymbol{X}_i, \boldsymbol{Z}_i)\}_{i=1}^n$ from $(Y, D, \boldsymbol{X}, \boldsymbol{Z})$.

3.1   Partially Linear IV Model (`iv`)

The Partially Linear IV Model considers the same functional form restriction on the causal model as the Partially Linear Model in Section 2.1. Specifically, the Partially Linear IV Model maintains

$$Y = \theta_0 D + g_0(\boldsymbol{X}) + U,$$

where θ_0 is the unknown parameter of interest.[12]

The key deviation from the Partially Linear Model is that the identifying assumptions leverage instrumental variables Z, instead of directly restricting the dependence of D and U. For ease of exposition, we focus on scalar-valued instruments in this section but we emphasize that `ddml` for Partially Linear IV supports multiple instrumental variables and multiple treatment variables.

Assumptions 4 and 5 below are sufficient orthogonality and relevance conditions, respectively, for identification of θ_0.

Assumption 4 (Conditional IV Orthogonality) $E[Cov(U, Z|\boldsymbol{X})] = 0.$

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11. We only accommodate approximation of optimal instruments under homoskedasticity. The instruments are valid more generally but are not optimal under heteroskedasticity. Obtaining optimal instruments under heteroskedasticity would require estimating conditional variance functions.
12. As in Section 2.1, the interpretation of θ_0 can be generalized under stronger identifying assumptions. See Angrist et al. (2000).

Assumption 5 (Conditional Linear IV Relevance) $E[Cov(D, Z|\boldsymbol{X})] \neq 0$.

To show identification, consider the score function

$$\psi(\boldsymbol{W}; \theta, \ell, m, r) = \Big(Y - \ell(\boldsymbol{X}) - \theta(D - m(\boldsymbol{X}))\Big)\Big(Z - r(\boldsymbol{X})\Big),$$

where $\boldsymbol{W} \equiv (Y, D, \boldsymbol{X}, Z)$. Note that for $\ell_0(\boldsymbol{X}) \equiv E[Y|\boldsymbol{X}]$, $m_0(\boldsymbol{X}) \equiv E[D|\boldsymbol{X}]$, and $r_0(\boldsymbol{X}) \equiv E[Z|\boldsymbol{X}]$, Assumption 4 implies $E[\psi(\boldsymbol{W}; \theta_0, \ell_0, m_0, r_0)] = 0$. We will also have that the Gateux derivative of $E[\psi(\boldsymbol{W}; \theta_0, \ell_0, m_0, r_0)]$ with respect to the nuisance functions (ℓ_0, m_0, r_0) will be zero. Rewriting $E[\psi(\boldsymbol{W}; \theta_0, \ell_0, m_0, r_0)] = 0$ then results in a Wald expression given by

$$\theta_0 = \frac{E\left[\big(Y - \ell_0(\boldsymbol{X})\big)\big(Z - r_0(\boldsymbol{X})\big)\right]}{E\left[\big(D - m_0(\boldsymbol{X})\big)\big(Z - r_0(\boldsymbol{X})\big)\right]}, \tag{9}$$

where Assumption 5 is used to ensure a non-zero denominator.

The DDML estimator based on Equation (9) is given by

$$\hat{\theta}_n = \frac{\frac{1}{n}\sum_{i=1}^n \left(Y_i - \hat{\ell}_{I_{k_i}^c}(\boldsymbol{X}_i)\right)\left(Z_i - \hat{r}_{I_{k_i}^c}(\boldsymbol{X}_i)\right)}{\frac{1}{n}\sum_{i=i}^n \left(D_i - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)\right)\left(Z_i - \hat{r}_{I_{k_i}^c}(\boldsymbol{X}_i)\right)}, \tag{10}$$

where $\hat{\ell}_{I_k^c}$, $\hat{m}_{I_k^c}$, and $\hat{r}_{I_k^c}$ are appropriate cross-fitted CEF estimators.

Standard errors corresponding to $\hat{\theta}_n$ are equivalent to the IV standard errors where $Y_i - \hat{\ell}_{I_{k_i}^c}(\boldsymbol{X}_i)$ is the outcome, $D_i - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)$ is the endogenous variable, and $Z_i - \hat{r}_{I_{k_i}^c}(\boldsymbol{X}_i)$ is the instrument. `ddml` supports conventional standard errors available for linear instrumental variable regression in Stata, including heteroskedasticity and cluster-robust standard errors. Mean and median aggregation over cross-fitting repetitions are implemented as outlined in Remark 2. In the case where we have multiple instruments or endogenous regressors, we adjust the algorithm by residualizing each instrument and endogenous variable as above and applying two-stage least squares with the residualized outcome, endogenous variables, and instruments.

3.2 Flexible Partially Linear IV Model (`fiv`)

The Flexible Partially Linear IV Model considers the same parameter of interest as the Partially Linear IV Model. The key difference here is that identification is based on a stronger independence assumption which allows for approximating optimal instruments using nonparametric estimation, including machine learning, akin to Belloni et al. (2012) and Chernozhukov et al. (2015a). In particular, the Flexible Partially Linear IV Model leverages a conditional mean independence assumption rather than an orthogonality assumption as in Section 3.1. As in Section 3.1, we state everything in the case of a scalar D.

Assumption 6 (Conditional IV Mean Independence) $E[U|\boldsymbol{Z}, \boldsymbol{X}] = 0$.

Assumption 6 implies that for any function $\tilde{p}(\boldsymbol{Z}, \boldsymbol{X})$, it holds that

$$E\left[\left(Y - \ell_0(X) - \theta(D - m_0(\boldsymbol{X}))\right)\left(\tilde{p}(\boldsymbol{Z}, \boldsymbol{X}) - E\left[\tilde{p}(\boldsymbol{Z}, \boldsymbol{X})|\boldsymbol{X}\right]\right)\right] = 0, \qquad (11)$$

where $\ell_0(\boldsymbol{X}) = E[Y|\boldsymbol{X}]$ and $m_0(\boldsymbol{X}) = E[D|\boldsymbol{X}]$. Identification based on (11) requires that there exists some function $\tilde{p}$ such that

$$E\left[Cov(D, \tilde{p}(\boldsymbol{Z}, \boldsymbol{X})|\boldsymbol{X})\right] \neq 0. \qquad (12)$$

A sufficient assumption is that D and $\boldsymbol{Z}$ are not mean independent conditional on $\boldsymbol{X}$. This condition allows setting $\tilde{p}(\boldsymbol{Z}, \boldsymbol{X}) = E[D|\boldsymbol{Z}, \boldsymbol{X}]$ which will then satisfy (12).[13] Assumption 7 is a consequence of this non-mean independence.

Assumption 7 (Conditional IV Relevance) $E[Var(E[D|\boldsymbol{Z}, \boldsymbol{X}]|\boldsymbol{X})] \neq 0$.

Consider now the score function

$$\psi(\boldsymbol{W}; \theta, \ell, m, p) = \left(Y - \ell(\boldsymbol{X}) - \theta(D - m(\boldsymbol{X}))\right)\left(p(\boldsymbol{Z}, \boldsymbol{X}) - m(\boldsymbol{X})\right),$$

where $\boldsymbol{W} \equiv (Y, D, \boldsymbol{X}, \boldsymbol{Z})$. Note that for $\ell_0(\boldsymbol{X}) \equiv E[Y|\boldsymbol{X}]$, $m_0(\boldsymbol{X}) \equiv E[D|\boldsymbol{X}]$, and $p_0(\boldsymbol{Z}, \boldsymbol{X}) \equiv E[D|\boldsymbol{Z}, \boldsymbol{X}]$, Assumption 6 and the law of iterated expectations imply $E[\psi(\boldsymbol{W}; \theta_0, \ell_0, m_0, p_0)] = 0$ and the Gateaux differentiability condition holds. Rewriting then results in a Wald expression given by

$$\theta_0 = \frac{E\left[\left(Y - \ell_0(\boldsymbol{X})\right)\left(p_0(\boldsymbol{Z}, \boldsymbol{X}) - m_0(\boldsymbol{X})\right)\right]}{E[\left(D - m_0(\boldsymbol{X})\right)\left(p_0(\boldsymbol{Z}, \boldsymbol{X}) - m_0(\boldsymbol{X})\right)]}, \qquad (13)$$

where Assumption 7 ensures a non-zero denominator.

The DDML estimator based on the moment solution (13) is given by

$$\hat{\theta}_n = \frac{\frac{1}{n}\sum_{i=1}^n \left(Y_i - \hat{\ell}_{I_{k_i}^c}(\boldsymbol{X}_i)\right)\left(\hat{p}_{I_{k_i}^c}(\boldsymbol{Z}_i, \boldsymbol{X}_i) - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)\right)}{\frac{1}{n}\sum_{i=i}^n \left(D_i - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)\right)\left(\hat{p}_{I_{k_i}^c}(\boldsymbol{Z}_i, \boldsymbol{X}_i) - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)\right)}, \qquad (14)$$

where $\hat{\ell}_{I_k^c}$, $\hat{m}_{I_k^c}$, and $\hat{p}_{I_k^c}$ are appropriate cross-fitted CEF estimators.

In simulations, we find that the finite sample performance of the estimator in (14) improves when the law of iterated expectations applied to $E[p_0(\boldsymbol{Z}, \boldsymbol{X})] = m_0(\boldsymbol{X})$ is explicitly approximately enforced in estimation. As a result, we propose an intermediate step to the previously considered two-step DDML algorithm: Rather than estimating the conditional expectation of D given $\boldsymbol{X}$ directly, we estimate it by projecting first-step estimates of the conditional expectation of $p_0(\boldsymbol{Z}, \boldsymbol{X})$ onto $\boldsymbol{X}$ instead. Algorithm 2 outlines the LIE-compliant DDML algorithm for computation of (14).

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13. The choice $\tilde{p}(\boldsymbol{Z}, \boldsymbol{X}) = E[D|\boldsymbol{Z}, \boldsymbol{X}]$ results in the optimal instrument, in the sense of semi-parametric efficiency, under homoskedasticity.

❏ **Algorithm 2. LIE-compliant DDML for the Flexible Partially Linear IV Model.**

Split the sample $\{(Y_i, D_i, \boldsymbol{X}_i, \boldsymbol{Z}_i)\}_{i=1}^n$ randomly in K folds of approximately equal size. Denote I_k the set of observations included in fold k and I_k^c its complement.

1. For each $k \in \{1, \ldots, K\}$:

   a. Fit a CEF estimator to the sub-sample I_k^c using Y_i as the outcome and $\boldsymbol{X}_i$ as predictors. Obtain the out-of-sample predicted values $\hat{\ell}_{I_k^c}(\boldsymbol{X}_i)$ for $i \in I_k$.

   b. Fit a CEF estimator to the sub-sample I_k^c using D_i as the outcome and $(\boldsymbol{Z}_i, \boldsymbol{X}_i)$ as predictors. Obtain the out-of-sample predicted values $\hat{p}_{I_k^c}(\boldsymbol{Z}_i, \boldsymbol{X}_i)$ for $i \in I_k$ and in-sample predicted values $\hat{p}_{I_k^c}(\boldsymbol{Z}_i, \boldsymbol{X}_i)$ for $i \in I_k^c$.

   c. Fit a CEF estimator to the sub-sample I_k^c using the in-sample predicted values $\hat{p}_{I_k^c}(\boldsymbol{Z}_i, \boldsymbol{X}_i)$ as the outcome and X_i as predictors. Obtain the out-of-sample predicted values $\hat{m}_{I_k^c}(\boldsymbol{X}_i)$ for $i \in I_k$.

2. Compute (14).

❏

Standard errors corresponding to $\hat{\theta}_n$ in (14) are the same as in Section 3.1 where the instrument is now given by $\hat{p}_{I_{k_i}^c}(\boldsymbol{Z}_i, \boldsymbol{X}_i) - \hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)$. Mean and median aggregation over cross-fitting repetitions are as outlined in Remark 2.

3.3   Interactive IV Model (`interactiveiv`)

The Interactive IV Model considers the same causal model as in Section 2.2; specifically

$$Y = g_0(D, \boldsymbol{X}) + U$$

where D takes values in $\{0, 1\}$. The key difference from the Interactive Model is that this section considers identification via a binary instrument Z representing assignment to treatment.

The parameter of interest we target is

$$\theta_0 = E\left[g_0(1, \boldsymbol{X}) - g_0(0, \boldsymbol{X}) \mid p_0(1, \boldsymbol{X}) > p_0(0, \boldsymbol{X})\right], \tag{15}$$

where $p_0(Z, \boldsymbol{X}) \equiv \Pr(D = 1 | Z, \boldsymbol{X})$. Here, θ_0 is a local average treatment effect (LATE). Note that in contrast to the LATE developed in Imbens and Angrist (1994), we follow the exposition in Chernozhukov et al. (2018) where "local" does not strictly refer to compliers but instead observations with a higher propensity score – i.e., a higher probability of complying.[14]

Identification again leverages Assumptions 6 and 7 made in the context of the Flexible Partially Linear IV Model. In addition, we assume that the propensity score is

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14. Identification of the conventional complier-focused LATE is achieved under stronger conditional independence and monotonicity assumptions not introduced in this paper. Under these stronger assumptions, the DDML LATE estimator outlined here targets the conventionally considered LATE parameter.

weakly monotone with probability one, and that the support of the instrument is independent of the controls.

Assumption 8 (Monotonicity) $p_0(1, \boldsymbol{X}) \geq p_0(0, \boldsymbol{X})$ *with probability 1.*

Assumption 9 (IV Overlap) $\Pr(Z = 1|\boldsymbol{X}) \in (0, 1)$ *with probability 1.*

Assumptions 6-9 imply that

$$\theta_0 = \frac{E\left[\ell_0(1, \boldsymbol{X}) - \ell_0(0, \boldsymbol{X})\right]}{E\left[p_0(1, \boldsymbol{X}) - p_0(0, \boldsymbol{X})\right]}, \tag{16}$$

where $\ell_0(Z, \boldsymbol{X}) \equiv E[Y|Z, \boldsymbol{X}]$, verifying identification of the LATE θ_0. Akin to Section 6, however, estimators of θ_0 should not directly be based on Equation (16) because the estimating equations implicit in obtaining (16) do not satisfy Neyman-orthogonality. Hence, a direct estimator of θ_0 obtained by plugging nonparametric estimators in for nuisance functions in (16) will potentially be highly sensitive to the first step nonparametric estimation error. Rather, we base estimation on the Neyman orthogonal score function

$$\psi(\boldsymbol{W}; \theta, \ell, p, r) = \frac{Z(Y - \ell(1, \boldsymbol{X}))}{r(\boldsymbol{X})} - \frac{(1-Z)(Y - \ell(0, \boldsymbol{X}))}{1 - r(\boldsymbol{X})} + \ell(1, \boldsymbol{X}) - \ell(0, \boldsymbol{X})$$
$$+ \left[\frac{Z(D - p(1, \boldsymbol{X}))}{r(\boldsymbol{X})} - \frac{(1-Z)(D - p(0, \boldsymbol{X}))}{1 - r(\boldsymbol{X})} + p(1, \boldsymbol{X}) - p(0, \boldsymbol{X})\right] \times \theta$$

where $\boldsymbol{W} \equiv (Y, D, \boldsymbol{X}, Z)$. Note that under Assumptions 6-9 and for $\ell_0(Z, \boldsymbol{X}) \equiv E[Y|Z, \boldsymbol{X}]$, $p_0(Z, \boldsymbol{X}) \equiv E[D|Z, \boldsymbol{X}]$, and $r_0(\boldsymbol{X}) \equiv E[Z|\boldsymbol{X}]$, we have $E[\psi(\boldsymbol{W}; \theta_0, \ell_0, p_0, r_0)] = 0$ and can verify that its Gateaux derivative with respect to the nuisance functions local to their true values is also zero.

The DDML estimator based on the orthogonal score ψ is then

$$\hat{\theta}_n =$$
$$\frac{\frac{1}{n} \sum_i \left(\frac{Z_i(Y_i - \hat{\ell}_{I_{k_i}^c}(1, \boldsymbol{X}_i))}{\hat{r}_{I_{k_i}^c}(\boldsymbol{X}_i)} - \frac{(1-Z_i)(Y_i - \hat{\ell}_{I_{k_i}^c}(0, \boldsymbol{X}_i))}{1 - \hat{r}_{I_{k_i}^c}(\boldsymbol{X}_i)} + \hat{\ell}_{I_{k_i}^c}(1, \boldsymbol{X}_i) - \hat{\ell}_{I_{k_i}^c}(0, \boldsymbol{X}_i) \right)}{\frac{1}{n} \sum_i \left(\frac{Z_i(D_i - \hat{p}_{I_{k_i}^c}(1, \boldsymbol{X}_i))}{\hat{r}_{I_{k_i}^c}(\boldsymbol{X}_i)} - \frac{(1-Z_i)(D_i - \hat{p}_{I_{k_i}^c}(0, \boldsymbol{X}_i))}{1 - \hat{r}_{I_{k_i}^c}(\boldsymbol{X}_i)} + \hat{p}_{I_{k_i}^c}(1, \boldsymbol{X}_i) - \hat{p}_{I_{k_i}^c}(0, \boldsymbol{X}_i) \right)}, \tag{17}$$

where $\hat{\ell}_{I_k^c}$, $\hat{p}_{I_k^c}$, and $\hat{r}_{I_k^c}$ are appropriate cross-fitted CEF estimators. Since Z is binary, the cross-fitted values $\hat{\ell}_{I_k^c}(1, \boldsymbol{X})$ and $\hat{p}_{I_k^c}(1, \boldsymbol{X})$, as well as $\hat{\ell}_{I_k^c}(0, \boldsymbol{X})$ and $\hat{p}_{I_k^c}(0, \boldsymbol{X})$ are computed by using only assigned and unassigned observations, respectively.

`ddml` supports heteroskedasticity and cluster-robust standard errors for $\hat{\theta}_n$. Mean and median aggregation over cross-fitting repetitions are implemented as outlined in Remark 2.

4   The choice of machine learner

Chernozhukov et al. (2018) show that DDML estimators are asymptotically normal when used in combination with a general class of machine learners satisfying a relatively weak convergence rate requirement for estimating the CEFs. While asymptotic properties of common machine learners remain an highly active research area, recent advances provide convergence rates for special instances of many machine learners, including lasso (Bickel et al. 2009; Belloni et al. 2012), random forests (Wager and Walther 2016; Wager and Athey 2018; Athey et al. 2019), neural networks (Schmidt-Hieber 2020; Farrell et al. 2021), and boosting (Luo et al. 2022). It seems likely that many popular learners will fall under the umbrella of suitable learners as theoretical results are further developed. However, we note that currently known asymptotic properties do not cover a wide range of learners, such as very deep and wide neural networks and deep random forests, as they are currently implemented in practice.

The relative robustness of DDML to the first-step learners leads to the question of which machine learner is the most appropriate for a given application. It is *ex ante* rarely obvious which learner will perform best. Further, rather than restricting ourselves to one learner, we might want to combine several learners into one final learner. This is the idea behind stacking generalization, or simply "stacking", due to Wolpert (1992) and Breiman (1996). Stacking allows one to accommodate a diverse set of base learners with varying tuning and hyper-tuning parameters. It thus provide a convenient framework for combining and identifying suitable learners, thereby reducing the risk of misspecification. Ahrens et al. (2023) introduce short-stacking which reduces the computational cost of pairing DDML and stacking drastically, as well as pooled stacking which enforces common weights across cross-fitting folds.

We discuss stacking approaches to DDML estimation in Section 4.1. Section 4.2 demonstrates the performance of DDML in combination with stacking approaches using a simulation.

4.1   DDML and stacking

Our discussion of stacking in the context of DDML focuses on the Partially Linear Model in (2), but we highlight that DDML and stacking can be combined in the same way for all other models supported in `ddml`. Suppose we consider J machine learners, referred to as base learners, to estimate the CEFs $\ell_0(\boldsymbol{X}) \equiv E[Y|\boldsymbol{X}]$ and $m_0(\boldsymbol{X}) \equiv E[D|\boldsymbol{X}]$. The set of base learners could, for example, include cross-validated lasso and ridge with alternative sets of predictors, gradient boosted trees with varying tree depth and feed-forward neural nets with varying number of hidden layers and neurons. Generally, we recommend considering a relatively large and diverse set of base learners, and including some learners with alternative tuning parameters.

We randomly split the sample into K cross-fitting folds, denoted as $I_1, \ldots, I_K$. In each cross-fitting step k, we define the training sample as $I_k^c \equiv T_k$, comprising all observations excluding the cross-fitting hold-out fold k. This training sample is further

divided into V cross-validation folds, denoted as $T_{k,1}, \ldots, T_{k,V}$. The stacking regressor fits a final learner to the training sample T_k using the cross-validated predicted values of each base learner as inputs. A typical choice for the final learner is constrained least squares (CLS) which restricts the weights to be positive and sum to one. The stacking objective function for estimating $\ell_0(\boldsymbol{X})$ using the training sample T_k is then defined as:

$$\min_{w_{k,1}, \ldots, w_{k,J}} \sum_{i \in T_k} \left(Y_i - \sum_{j=1}^{J} w_{k,j} \hat{\ell}^{(j)}_{T^c_{k,v(i)}}(\boldsymbol{X}_i) \right)^2, \qquad \text{s.t. } w_{k,j} \geq 0, \; \sum_{j=1}^{J} |w_{k,j}| = 1, \quad (18)$$

where $w_{k,j}$ are referred to as stacking weights. We use $\hat{\ell}^{(j)}_{T^c_{k,v(i)}}(\boldsymbol{X}_i)$ to denote the cross-validated predicted value for observation i, which is obtained from fitting learner j on the sub-sample $T^c_{k,v(i)} \equiv T_k \setminus T_{k,v(i)}$, i.e., the sub-sample excluding the fold $v(i)$ into which observation i falls. The stacking predicted values are obtained as $\sum_j \hat{w}_{k,j} \hat{\ell}^{(j)}_k(\boldsymbol{X}_i)$ where each learner j is fit on the step-k training sample T_k. The objective function for estimating $m_0(\boldsymbol{X})$ is defined accordingly.

CLS frequently performs well in practice and facilitates the interpretation of stacking as a weighted average of base learners (Hastie et al. 2009). It is, however, not the only sensible choice of combining base learners. For example, stacking could instead select the single learner with the lowest quadratic loss, i.e., by imposing the constraint $w_{k,j} \in \{0,1\}$ and $\sum_{k,j} w_{k,j} = 1$. We refer to this choice as "single best" and include it in our simulation experiments. We implement stacking for DDML using `pystacked` (Ahrens et al. 2022).

Pooled stacking. A variant of stacking specific to DDML is *pooled stacking*. Standard stacking fits the final learner K separate times, once in each cross-fitting step, yielding K separate sets of stacking weights $\hat{w}_{k,j}$ for the J learners. With DDML pooled stacking, we can impose the additional constraint in (18) that the weights are the same across all cross-fit folds, $\hat{w}_{k,j} = \hat{w}_j, \forall\, k$. By returning a single set of stacking weights, pooled stacking imposes an additional degree of regularization and facilitates interpretation but suffers from the same high computational cost as pairing DDML with (regular) stacking.

Short-stacking. Stacking and pooled stacking rely on cross-validation. In the context of DDML we can also exploit the cross-*fitted* predicted values directly for stacking. That is, we can directly apply CLS to the cross-fitted predicted values for estimating $\ell_0(\boldsymbol{X})$ (and similarly $m_0(\boldsymbol{X})$):

$$\min_{w_1, \ldots, w_J} \sum_{i=1}^{n} \left(Y_i - \sum_{j=1}^{J} w_j \hat{\ell}^{(j)}_{I^c_{k(i)}}(\boldsymbol{X}_i) \right)^2, \qquad \text{s.t. } w_j \geq 0, \; \sum_{j=1}^{J} |w_j| = 1$$

We refer to this form of stacking that utilizes the cross-fitted predicted values as *short-stacking* as it takes a short-cut. This is to contrast it with regular stacking which estimates the stacking weights for each cross-fitting fold k. The main advantage of

short-stacking relative to standard stacking is the lower computational cost, because short-stacking does not require the fitting of the j learners on sub-samples to obtain the cross-validated predicted values $\hat{\ell}^{(j)}_{T^c_{k,v(i)}}(\boldsymbol{X}_i)$ needed for standard stacking. Furthermore, short-stacking (like pooled stacking) also produces a single set of weights for the entire sample, which facilitates interpretation and implies a higher degree of regularization. A potential disadvantage of short-stacking is that it is more susceptible to over-fitting issues since stacking weights and structural parameters are estimated using the same cross-fitted predicted values. We thus recommend only considering short-stacking in regular settings where the number of candidate learners is small relative to N (see also the discussion in Ahrens et al. 2023). Algorithm A.4 in the Appendix summarizes the short-stacking algorithm for the Partially Linear Model.[15]

4.2 Monte Carlo simulation

To illustrate the advantages of DDML with stacking, we generate artificial data based on the Partially Linear Model

$$Y_i = \theta_0 D_i + c_Y g(\boldsymbol{X}_i) + \sigma_Y(D_i, \boldsymbol{X}_i)\varepsilon_i \tag{19}$$

$$D_i = c_D g(\boldsymbol{X}_i) + \sigma_D(\boldsymbol{X}_i)u_i \tag{20}$$

where both ε_i and u_i are independently drawn from the standard normal distribution. We set the target parameter to $\theta_0 = 0.5$ and the sample size to either $n = 100$ or $n = 1000$. The controls $\boldsymbol{X}_i$ are drawn from the multivariate normal distribution with $N(0, \boldsymbol{\Sigma})$ where $\Sigma_{ij} = (0.5)^{|i-j|}$. The number of controls is set to $p = \dim(\boldsymbol{X}_i) = 50$, except in DGP 5 where $p = 7$. The constants c_Y and c_D are chosen such that the R^2 in (19) and (20) are approximately equal to 0.5. To induce heteroskedasticity, we set

$$\sigma_D\left(\boldsymbol{X}_i\right) = \sqrt{\frac{(1 + g(\boldsymbol{X}_i))^2}{\frac{1}{n}\sum_i (1 + g(\boldsymbol{X}_i))^2}} \quad \text{and} \quad \sigma_Y\left(D_i, \boldsymbol{X}_i\right) = \sqrt{\frac{(1 + \theta_0 D_i + g(\boldsymbol{X}_i))^2}{\frac{1}{n}\sum_i (1 + \theta_0 D_i + g(\boldsymbol{X}_i))^2}}$$

The nuisance function $g(\boldsymbol{X}_i)$ is generated using five exemplary DGPs, which cover linear and nonlinear processes with varying degrees of sparsity and varying number of observed covariates:

DGP 1: $g(\boldsymbol{X}_i) \quad = \sum_j 0.9^j X_{ij}$

DGP 2: $g(\boldsymbol{X}_i) \quad = X_{i1}X_{i2} + X_{i3}^2 + X_{i4}X_{i5} + X_{i6}X_{i7} + X_{i8}X_{i9} + X_{i10} + X_{i11}^2 + X_{i12}X_{i13}$

DGP 3: $g(\boldsymbol{X}_i) \quad = \mathbb{1}\{X_{i1} > 0.3\}\mathbb{1}\{X_{i2} > 0\}\mathbb{1}\{X_{i3} > -1\}$

DGP 4: $g(\boldsymbol{X}_i) \quad = X_{i1} + \sqrt{|X_{i2}|} + \sin(X_{i3}) + 0.3X_{i4}X_{i5} + X_{i6} + 0.3X_{i7}^2$

DGP 5: $g(\boldsymbol{X}_i) \quad = $ same as DGP 4 with $p = 7$

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15. While short-stacking can be applied in a similar fashion to other conditional expectations, a complication arises in the Flexible Partially Linear IV Model where the cross-fitted predicted values of $E[D|\boldsymbol{X}]$ depend on $E[D|\boldsymbol{X}, \boldsymbol{Z}]$. We describe the algorithm that accounts for this in the Appendix; see Algorithm A.5.

DGP 1 is a linear design involving many negligibly small parameters. While not exactly sparse, the design can be approximated well through a sparse representation. DGP 2 is linear in the parameters and exactly sparse, but includes interactions and second-order polynomials. DGPs 3-5 are also exactly sparse but involve complex nonlinear and interaction effects. DGP 4 and 5 are identical, except that DGP 5 does not add nuisance covariates that are unrelated to Y and D.

We consider DDML with the following supervised machine learners for cross-fitting the CEFs:[16]

1.-2. Cross-validated lasso & ridge with untransformed base controls
3.-4. Cross-validated lasso & ridge with 5th-order polynomials of base controls but no interactions (referred to as 'Poly 5')
5.-6. Cross-validated lasso & ridge with second-order polynomials and all first order interaction terms (referred to as 'Poly 2 + Inter.')
   7. Random forests (RF) with low regularization: base controls, maximum tree depth of 10, 500 trees and approximately $\sqrt{p}$ features considered at each split
   8. RF with medium regularization: same as 7., but with maximum tree depth of 6
   9. RF with high regularization: same as 7., but with maximum tree depth of 2
  10. Gradient boosted trees (GB) with low regularization: base controls, 1000 trees and a learning rate of 0.3. We enable early stopping which uses a 20% validation sample to decide whether to stop the learning algorithm. Learning is terminated after 5 iterations with no meaningful improvement in the mean-squared loss of the validation sample.[17]
  11. GB with medium regularization: same as 10., but with learning rate of 0.1
  12. GB with high regularization: same as 10., but with learning rate of 0.01
  13. Feed-forward neural net with base controls and two layers of size 20

We use the above set of learners as base learners for DDML with stacking approaches. Specifically, we estimate DDML using stacking, short-stacking and pooled stacking which we combine with CLS and the single-best learner. We set the number of folds to $K = 20$ if $n = 100$, and $K = 5$ if $n = 1000$. That is, we adapt the number of folds K to the total sample size n to ensure that the CEF estimators are trained on sufficiently large training samples.

For comparison, we report results for OLS and PDS-lasso with base controls, PDS-Lasso with Poly 5, PDS-Lasso with Poly 2 + Interactions, and an oracle estimator using the full sample.[18] The oracle estimator presumes knowledge of the function $g(\boldsymbol{X})$, and obtains estimates by regressing Y on the two variables D and $g(\boldsymbol{X})$.

We report simulation median absolute bias (MAB) and coverage rates of 95% confidence intervals (CR) for DGPs 1-3 in Table 1. We delegate results for DGPs 4 and 5, including a brief discussion, to Appendix B. DDML estimators leveraging stacking approaches perform favorably in comparison to individual base learners in terms of bias

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16. All base learners have been implemented using `pystacked`. We use the defaults of `pystacked` for parameter values and settings not mentioned here.
17. We use a tolerance level of 0.01 to measure improvements.
18. The PDS-Lasso estimators set tuning parameters using the default in `pdslasso`.

and coverage. The relative performance of stacking approaches seems to improve as the sample size increases, likely reflecting that the stacking weights are more precisely estimated in larger small samples. For $n = 1000$, the bias of stacking with CLS is at least as low as the bias of the best-performing individual learner under DGP 1-2, while only gradient boosting and neural net yield a lower bias than stacking under DGP 3.

Results for coverage are similar with stacking-based estimates being comparable with the best performing feasible estimates and the oracle when $n = 1000$. With $n = 100$, coverage of confidence intervals for stacking-based estimators are inferior to coverages for a small number of the individual learners but still competitive and superior than most learners. Looking across all results, we see that stacking provides robustness to potentially very bad performance that could be obtained from using a single poorly performing learner.

There are overall little performance differences among the six stacking estimators considered., suggesting that short-stacking has a substantial practical advantage due to its lower computational cost. Ahrens et al. (2023) report that short-stacking reduces the compute time by a factor of $1/V$ where V is the number of cross-validation folds. There is some evidence that the single-best selector outperforms CLS in very small sample sizes in DGPs 2-3, but not in DGP 1 (and also not in DGPs 4-5, see Table B.1). We suspect that the single-best selector works better in scenarios where there is one base learner that clearly dominates.

The mean-squared prediction errors (MSPE) and the average stacking weights, which we report in Tables B.2 and B.3 in the Appendix, provide further insights into how stacking with CLS functions. CLS assigns large stacking weights to base learners with a low MSPE, which in turn are associated with a low bias. Importantly, stacking assigns zero or close-to-zero weights to poorly specified base learners such as the highly regularized random forest, which in all three DGPs ranks among the individual learners with highest MSPE and highest bias. The robustness to misspecified and ill-chosen machine learners, which could lead to misleading inference, is indeed one of our main motivations for advocating stacking approaches to DDML.

DDML with stacking approaches also compares favorably to conventional full-sample estimators. In the relatively simple linear DGP 1, DDML with stacking performs similarly to OLS and the infeasible oracle estimator—both in terms of bias and coverage—for $n = 100$ and $n = 1000$. In the more challenging DGPs 2 and 3, the bias of DDML with stacking is substantially lower than the biases of OLS and the PDS-Lasso estimators. While the bias and size distortions of DDML with stacking are still considerable in comparison to the infeasible oracle for $n = 100$, they are close to the oracle for $n = 1000$. The results overall highlight the flexibility of DDML with stacking to flexibly approximate a wide range of DGPs provided a diverse set of base learners is chosen.

Table 1: Bias and Coverage Rates in the Linear and Nonlinear DGPs

	DGP 1				DGP 2				DGP 3			
	n = 100		n = 1000		n = 100		n = 1000		n = 100		n = 1000	
	MAB	CR	MAB	CR	MAB	CR	MAB	CR	MAB	CR	MAB	CR
Full sample:												
Oracle	0.113	0.915	0.036	0.944	0.090	0.915	0.032	0.934	0.117	0.890	0.036	0.944
OLS (Base)	0.130	0.886	0.037	0.942	0.286	0.375	0.288	0.	0.224	0.617	0.209	0.007
PDS-Lasso (Base)	0.133	0.840	0.037	0.941	0.295	0.276	0.287	0.	0.227	0.588	0.209	0.006
PDS-Lasso (Poly 5)	0.148	0.768	0.038	0.935	0.219	0.465	0.106	0.327	0.228	0.583	0.198	0.016
PDS-Lasso (Poly 2 + Inter.)	0.158	0.742	0.039	0.931	0.200	0.549	0.033	0.922	0.231	0.591	0.176	0.058
DDML methods:												
Base learners												
OLS	0.134	0.710	0.038	0.930	0.286	0.226	0.288	0.	0.226	0.424	0.209	0.006
Lasso with CV (Base)	0.116	0.893	0.037	0.950	0.286	0.312	0.288	0.	0.221	0.617	0.210	0.008
Ridge with CV (Base)	0.123	0.888	0.038	0.941	0.291	0.288	0.289	0.458	0.246	0.542	0.219	0.002
Lasso with CV (Poly 5)	0.127	0.843	0.039	0.940	0.144	0.762	0.092	0.188	0.202	0.635	0.193	0.025
Ridge with CV (Poly 5)	0.139	0.794	0.050	0.864	0.178	0.620	0.125	0.925	0.265	0.478	0.221	0.002
Lasso with CV (Poly 2 + Inter.)	0.137	0.816	0.042	0.925	0.155	0.718	0.036	0.308	0.214	0.623	0.184	0.048
Ridge with CV (Poly 2 + Inter.)	0.158	0.695	0.095	0.505	0.152	0.685	0.112	0.015	0.191	0.645	0.265	0.
Random forest (Low)	0.179	0.728	0.098	0.566	0.249	0.438	0.196	0.005	0.229	0.619	0.110	0.447
Random forest (Medium)	0.186	0.718	0.128	0.317	0.252	0.431	0.222	0.	0.232	0.612	0.140	0.227
Random forest (High)	0.237	0.565	0.227	0.007	0.270	0.362	0.269	0.	0.259	0.520	0.230	0.002
Gradient boosting (Low)	0.103	0.906	0.039	0.924	0.126	0.802	0.080	0.578	0.118	0.885	0.038	0.938
Gradient boosting (Medium)	0.126	0.860	0.048	0.881	0.197	0.598	0.144	0.125	0.137	0.838	0.045	0.906
Gradient boosting (High)	0.239	0.544	0.154	0.142	0.277	0.338	0.258	0.	0.205	0.665	0.079	0.715
Neural net	0.137	0.773	0.152	0.131	0.106	0.843	0.075	0.534	0.107	0.882	0.037	0.865
Meta learners												
Stacking: CLS	0.117	0.898	0.037	0.949	0.169	0.683	0.037	0.918	0.169	0.742	0.048	0.892
Stacking: Single best	0.119	0.907	0.037	0.949	0.149	0.744	0.036	0.925	0.157	0.781	0.045	0.902
Short-stacking: CLS	0.116	0.892	0.037	0.948	0.170	0.671	0.037	0.920	0.165	0.754	0.046	0.897
Short-stacking: Single best	0.117	0.899	0.037	0.950	0.141	0.756	0.036	0.925	0.157	0.784	0.045	0.908
Pooled stacking: CLS	0.117	0.895	0.038	0.949	0.188	0.625	0.037	0.922	0.181	0.731	0.047	0.896
Pooled stacking: Single best	0.117	0.894	0.037	0.950	0.173	0.656	0.036	0.925	0.181	0.725	0.045	0.906

Notes: The table reports median absolute bias (MAB) and coverage rate of a 95% confidence interval (CR). We employ standard errors robust to heteroskedasticity. For comparison, we report the following full sample estimators: infeasible Oracle, OLS, PDS-Lasso with base and two different expanded sets of covariates. DDML estimators use 20 folds for cross-fitting if $n = 100$, and 5 folds if $n = 1000$. Meta-learning approaches rely on all listed base learners. Results are based on 1,000 replications. Results for DGPs 4 and 5 can be found in Table B.1 in the Appendix.

5 The program

In this section, we provide an overview of the ddml package. We introduce the syntax and workflow for the main programs in Section 5.1. Section 5.2 lists the options. Section 5.3 covers the simplified one-line program qddml. We provide an overview of supported machine learning programs in Section 5.4. Finally, Section 5.5 adds a note on how to ensure replication with ddml.

5.1 Syntax: ddml

The ddml estimation proceeds in four steps.

Step 1: Initialize ddml and select model.

ddml init *model* $\left[\right.$, mname(*name*) vars(*varlist*) kfolds(*integer*)

   fcluster(*varname*) foldvar(*varlist*) reps(*integer*) tabfold vars(*varlist*) $\left.\right]$

where *model* selects between the Partially Linear Model (partial), the Interactive Model (interactive), the Partially Linear IV Model (iv), the Flexible Partially Linear IV Model (fiv), and the Interactive IV Model (interactiveiv). This step creates a persistent Mata object with the name provided by mname(*name*) in which model specifications and estimation results will be stored. The default name is *m0*.

At this stage, the user-specified folds for cross-fitting can be set via integer-valued Stata variables (see foldvar(*varlist*)). By default, observations are randomly assigned to folds and kfolds(*integer*) determines the number of folds (the default is 5). Cluster-randomized fold splitting is supported (see fcluster(*varname*)). The user can also select the number of times to fully repeat the cross-fitting procedure (see rep(*integer*)).

Step 2: Add supervised machine learners for estimating conditional expectations.

In this second step, we select the machine learning programs for estimating CEFs.

ddml *cond_exp* $\left[\right.$, mname(*name*) vname(*varname*) learner(*name*) vtype(*string*)

   predopt(*string*) $\left.\right]$: *command depvar vars* $\left[\right.$, *cmdopt* $\left.\right]$

where *cond_exp* selects the conditional expectation to be estimated by the machine learning program *command*. At least one learner is required for each conditional expectation. Table 2 provides an overview of which conditional expectations are required by each model. The program *command* is a supervised machine learning program such as cvlasso or pystacked (see compatible programs in Section 5.4). The options *cmdopt* are specific to that program.

cond_exp	partial	interactive	iv	fiv	interactiveiv
E[Y|X]	✓		✓	✓	
E[Y|X,D]		✓			
E[Y|X,Z]					✓
E[D|X]	✓	✓	✓	✓	
E[D|Z,X]				✓	✓
E[Z|X]			✓		✓

Table 2: The table lists the conditional expectations which need to be specified for each model.

Step 3: Perform cross-fitting.

This step implements the cross-fitting algorithm. Each learner is fit iteratively on training folds and out-of-sample predicted values are obtained. Cross-fitting is the most time-consuming step, as it involves fitting the selected machine learners repeatedly.

ddml crossfit $\left[\right.$, mname(*name*) shortstack poolstack nostdstack

finalest(*name*) $\left.\right]$

Step 4: Estimate causal effects.

In the last step, we estimate the parameter of interest for all combination of learners added in Step 2.

ddml estimate $\left[\right.$, mname(*name*) robust cluster(*varname*) vce(*vcetype*) atet

trim shortstack poolstack finalest(*name*) $\left.\right]$

To report and post selected results, we can use ddml estimate with the replay option:

ddml estimate $\left[\right.$, replay mname(*name*) spec(*integer or string*) rep(*integer or*

string) fulltable notable allest $\left.\right]$

Utilities

ddml describe provides information about the model setup and or results:

ddml describe $\left[\right.$, mname(*name*) sample learners crossfit estimates all $\left.\right]$

ddml stores many internal results on associate arrays, notably the various stacking weights. These can be retrieved using ddml extract:

ddml extract $\big[$ *objectname* , mname(*name*) show(*name*) ename(*name*)
    vname(*varname*) stata keys key1(*string*) key2(*string*) key3(*string*)
    subkey1(*string*) subkey2(*string*) $\big]$

ddml export saves the estimated conditional expectations and other variables to a CSV
file:

ddml export *filename* $\big[$, mname(*name*) addvars(*varlist*) $\big]$

5.2   Options

Step 1 options: Initialization.

mname(*name*) name of the DDML model. Allows to run multiple DDML models simul-
    taneously. Defaults to *m0*.

kfolds(*integer*) number of cross-fitting folds. The default is 5.

fcluster(*varname*) cluster identifiers for cluster randomization of folds.

foldvar(*varlist*) integer variables to specify custom folds (one per cross-fitting repeti-
    tion).

reps(*integer*) number of cross-fitting repetitions, i.e., how often the cross-fitting pro-
    cedure is repeated on randomly generated folds.

tabfold prints a table with frequency of observations by fold.

Step 2 options: Adding learners.

vname(*varname*) name of the dependent variable in the reduced form estimation. This
    is usually inferred from the *command* line but is mandatory for the fiv model.

learner(*varname*) optional name of the variable to be created.

vtype(*string*) optional variable type of the variable to be created. Defaults to *double*.
    none can be used to leave the type field blank. (Setting vtype(*none*) is required
    when using ddml with rforest.)

predopt(*varname*) predict option to be used to get predicted values. Typical values
    could be xb or pr. Default is blank.

Step 3 options: Cross-fitting.

shortstack asks for short-stacking to be used. Short-stacking uses the cross-fitted
    predicted values to obtain a weighted average of several base learners.

poolstack asks for pooled stacking to be used. This is available only if pystacked has been used for standard stacking in all equations.

nostdstack is used in conjunction with pystacked and short-stacking; it tells pystacked to generate the base learner predictions without the computationally-expensive additional step of obtaining the stacking weights.

finalest(*name*) sets the final estimator for all stacking methods; the default *nnls1* is least squares without a constant and with the constraints that weights are non-negative and sum to one. Alternative final estimators include *singlebest* (use the minimum MSE base learner), *ols* (ordinary least squares) and *avg* (unweighted average of all base learners).

Step 4 options: Estimation.

spec(*string*) select specification. This can either be the specification number, *mse* for minimum-MSE specification (the default) or *ss* for short-stacking.

rep(*string*) select cross-fitting repetitions. This can either be the cross-fit repetition number, *mn* for mean aggregation or *md* for median aggregation (the default). See Remark 2 for more information.

robust report SEs that are robust to the presence of arbitrary heteroskedasticity.

cluster(*varname*) select cluster-robust variance-covariance estimator.

vce(*type*) select variance-covariance estimator, e.g. vce(hc3) or vce(cluster id). See help regress##vcetype for available options.

trim(*real*) trimming of propensity scores for the Interactive and Interactive IV models. The default is 0.01 (that is, values below 0.01 and above 0.99 are set to 0.01 and 0.99, respectively).

atet report average treatment effect of the treated (default is ATE).

noconstant suppress constant term in the estimation stage (only relevant for partially linear models).

shortstack, poolstack, finalest(*name*) see above under ddml crossfit.

Re-fitting the final learner using ddml estimate with stacking options is generally very fast because it does not require re-cross-fitting.

5.3   Short syntax: qddml

The ddml package includes the wrapper program qddml which provides a one-line syntax for estimating a ddml model. The one-line syntax follows the syntax of pdslasso and ivlasso (Ahrens et al. 2018). The main restriction of qddml compared to the more

flexible multi-line syntax is that `qddml` only allows for one user-specified machine learner (in addition to `regress`, which is added by default).

   `qddml` has integrated support for `pystacked`, and `pystacked`, is the default learner in all equations. The syntax for `qddml` options differs depending on whether `pystacked` is used as the learner in each equation.

Syntax when used with `pystacked`

`qddml` *depvar treatment_vars* (*controls*) (*treatment_vars=excluded_instruments*) $\lceil$

   `pystacked(string) pystacked_y(string) pystacked_d(string)`

   `pystacked_z(string) shortstack stdstack poolstack finalest(name)`

   `mname(name)` *options* $\rceil$

The `pystacked` option sets the options for all the conditional expectations estimated by `pystacked`; the `_y`, `_d` and `_z` variants control the options sent to the corresponding conditional expectation estimations. Other options are as in `ddml`.

Syntax when used with other learners

`qddml` *depvar treatment_vars* (*controls*) (*treatment_vars=excluded_instruments*) $\lceil$

   `cmd(string) ycmd(string) dcmd(string) zcmd(string) *cmdopt(string)`

   `*vtype(name) *predopt(name)` *options* $\rceil$

The `cmd` option sets the options for all the conditional expectations estimated by `pystacked`; the `ycmd`, `dcmd` and `zcmd` variants control the options sent to the corresponding conditional expectation estimations. The `cmdopt` option can be used either to set the options for all equations, or, by replacing the asterisk with y, d or z, set the options for the corresponding conditional expectation estimation. Other options are as in `ddml`.

5.4   Supported machine learning programs

`ddml` is compatible with any supervised ML program in Stata that supports the typical "`reg y x`" syntax, comes with a post-estimation `predict` and supports `if` statements. We have tested `ddml` with the following programs:

- `pystacked` facilitates the stacking of a wide range of machine learners including regularized regression, random forests, support vector machines, gradient boosted trees and feed-forward neural nets using Python's *scikit-learn* (Ahrens et al. 2022; Pedregosa et al. 2011; Buitinck et al. 2013). In addition, `pystacked` can also be used as a front-end to fit individual machine learners. `ddml` has integrated support for `pystacked` and is the recommended default learner.

- `lassopack` implements regularized regression, e.g. lasso, ridge, elastic net (Ahrens et al. 2020).
- `rforest` is a random forest wrapper for WEKA (Schonlau and Zou 2020; Frank et al. 2009).
- `svmachines` allows for the estimation of support vector machines using `libsvm` (Chang and Lin 2011; Guenther and Schonlau 2018).
- The program `parsnip` of the package `mlrtime` provides access to R's *parsnip* machine learning library through `rcall` (Huntington-Klein 2021; Haghish 2019). Using `parsnip` requires the installation of the supplementary wrapper program `parsnip2`.[19]

Stata programs that are currently not supported can be added relatively easily using wrapper programs (see `parsnip2` for an example).

5.5   Inspecting results and replication

In this section we discuss how to ensure replicability when using `ddml`. We also discuss some tools available for tracing replication failures. First, however, we briefly describe how `ddml` stores results.

`ddml` stores estimated conditional expectations in Stata's memory as Stata variables. These variables can be inspected, graphed and summarized in the usual way. Fold ID variables are also stored as Stata variables (by default named `m0_fid_`r, where `m0` is the default model name and r is the cross-fitting repetition). `ddml` models are stored on Mata `struct`s and using Mata's associative arrays. Specifically, the `ddml` model created by `ddml init` is an `mStruct`, and information relating to the estimation of conditional expectations are stored in `eStruct`s. Results relating to the overall model estimation are stored in associative arrays that live in the `mStruct`, and results relating to the estimation of conditional expectations are stored in associative arrays that live in the corresponding `eStruct`s.

Replication tips:

- Set the Stata seed before `ddml init`. This ensures that the same random fold variable is used for a given data set.

- Using the same fold variable alone is usually not sufficient to ensure replication, since many machine learning algorithms involve randomization. That said, note that the fold variable is stored in memory and can be reused for subsequent estimations via the `foldvar(`*varlist*`)` option.

- Replication of `ddml` results may require additional steps with some programs that rely on randomization in other software environments, e.g., R or Python. `pystacked` uses a Python seed generated in Stata. Thus, when `ddml` is used with `pystacked`, setting the seed before `ddml init` also guarantees that the same

---

19. Available from `https://github.com/aahrens1/parsnip2`.

Python seed underlies the stacking estimation. Other programs relying on randomization outside of Stata might not behave in the same way. Thus, when using other programs, check the help files for options to set external random seeds. Try estimating each of the individual learners on the entire sample to see what settings need to be passed to them for their results to replicate.

- Beware of changing samples. Fold splits or learner idiosyncracies may mean that sample sizes vary slightly across learners, estimation samples and/or cross-fitting repetitions.

- The `ddml export` utility can be used to export the estimated conditional expectations, fold variables and sample indicators to a CSV format file for examination and comparison in other software environments.

6 Applications

We demonstrate the `ddml` workflow using two applications. In Section 6.1, we apply the DDML estimator to estimate the effect of 401(k) eligibility on financial wealth following Poterba et al. (1995). We focus on the Partially Linear Model for the sake of brevity, but provide code that demonstrates the use of `ddml` with the Interactive Model, Partially Linear IV Model and Interactive IV Model using the same application in Appendix C. Additional examples can also be found in the help file. Based on Berry et al. (1995), we show in Section 6.2 how to employ `ddml` for the estimation of the Flexible Partially Linear IV Model which allows both for flexibly controlling for confounding factors using high-dimensional function approximation of confounding factors and for estimation of optimal instrumental variables.

6.1 401(k) and financial wealth

The data consists of $n = 9915$ households from the 1991 SIPP. The application is originally due to Poterba et al. (1995), but has been revisited by Belloni et al. (2017), Chernozhukov et al. (2018), and Wüthrich and Zhu (2021), among others. Following previous studies, we include the control variables age, income, years of education, family size, as well as indicators for martial status, two-earner status, benefit pension status, IRA participation, and home ownership. The outcome is net financial assets and the treatment is eligibility to enroll for the 401(k) pension plan.

We load the data and define three globals for outcome, treatment and control variables. We then proceed in the four steps outlined in Section 5.1.

```
. use "sipp1991.dta", clear
. global Y net_tfa
. global X age inc educ fsize marr twoearn db pira hown
. global D e401
```

Step 1: Initialize `ddml` **model.**

We initialize the `ddml` model and select the Partially Linear Model in (2). Before initialization, we set the seed to ensure replication. This should always be done before `ddml init`, which executes the random fold assignment. In this example, we opt for four folds to ensure the readability of some of the output shown below, although we recommend considering a larger number of folds in practice.

```
. set seed 123
. ddml init partial, kfolds(4)
```

Step 2: Add supervised machine learners for estimating conditional expectations.

In this step, we specify which machine learning programs should be used for the estimation of the conditional expectations $E[Y|\mathbf{X}]$ and $E[D|\mathbf{X}]$. For each conditional expectation, at least one learner is required. For illustrative purposes, we consider `regress` for linear regression, `pystacked` with the `m(lassocv)` option for cross-validated lasso (as an example of how to use `pystacked` to estimate a single learner) and `rforest` for random forests. When using `rforest`, we need to add the option `vtype(none)` since the post-estimation `predict` command of `rforest` does not support variable types.

```
. *** add learners for E[Y|X]
. ddml E[Y|X]: reg $Y $X
Learner Y1_reg added successfully.
. ddml E[Y|X]: pystacked $Y c.($X)##c.($X), type(reg) m(lassocv)
Learner Y2_pystacked added successfully.
. ddml E[Y|X], vtype(none): rforest $Y $X, type(reg)
Learner Y3_rforest added successfully.
. *** add learners for E[D|X]
. ddml E[D|X]: reg $D $X
Learner D1_reg added successfully.
. ddml E[D|X]: pystacked $D c.($X)##c.($X), type(reg) m(lassocv)
Learner D2_pystacked added successfully.
. ddml E[D|X], vtype(none): rforest $D $X, type(reg)
Learner D3_rforest added successfully.
```

The flexible `ddml` syntax allows specification of different sets of covariates for different learners. This flexibility can be useful as, for example, linear learners such as the lasso might perform better if interactions are provided as inputs, whereas tree-based methods such as random forests may detect certain interactions in a data-driven way. Here, we use interactions and second-order polynomials for the cross-validated lasso, but not for the other learners.

This application has only one treatment variable, but `ddml` does support multiple treatment variables. To add a second treatment variable, we would simply add a statement such as `ddml E[D|X]: reg D2 $X` where D2 would be the name of the second treatment variable. An example with two treatments is provided in the help file.

The auxiliary `ddml` sub-command `describe` allows us to verify that the learners were correctly registered:

```
. ddml describe
Model:                  partial, crossfit folds k=4, resamples r=1
Mata global (mname):    m0
Dependent variable (Y): net_tfa
 net_tfa learners:      Y1_reg Y2_pystacked Y3_rforest
D equations (1):        e401
 e401 learners:         D1_reg D2_pystacked D3_rforest
```

Step 3: Perform cross-fitting.

The third step performs cross-fitting, which is the most time-intensive process. The `shortstack` option enables the short-stacking algorithm of Section 4.1.

```
. ddml crossfit, shortstack
Cross-fitting E[y|X] equation: net_tfa
Cross-fitting fold 1 2 3 4 ...completed cross-fitting...completed short-stacking
Cross-fitting E[D|X] equation: e401
Cross-fitting fold 1 2 3 4 ...completed cross-fitting...completed short-stacking
```

Six variables are created and stored in memory which correspond to the six learners specified in the previous step. These variables are called `Y1_reg_1`, `Y2_pystacked_1_1`, `Y3_rforest_1`, `D1_reg_1`, `D2_pystacked_1_1` and `D3_rforest_1`. Y and D indicate outcome and treatment variable. The index 1 to 3 is a learner counter. `reg`, `pystacked` and `rforest` correspond to the names of the commands used. The `_1` suffix indicates the cross-fitting repetition. The additional `_1` in the case of `D2_pystacked_1_1` indicates the learner number (there is only a single `pystacked` learner).

After cross-fitting, we can inspect the mean-squared prediction errors by fold and learner:

```
. ddml desc, crossfit
Model:                  partial, crossfit folds k=4, resamples r=1
Mata global (mname):    m0
Dependent variable (Y): net_tfa
 net_tfa learners:      Y1_reg Y2_pystacked Y3_rforest
D equations (1):        e401
 e401 learners:         D1_reg D2_pystacked D3_rforest
Crossfit results (detail):
                                    All     By fold:
Cond. exp.  Learner     rep         MSE       1        2        3        4
net_tfa     shortstack   1        1.5e+09  1.8e+09  1.4e+09  1.4e+09  1.5e+09
e401        shortstack   1          0.18     0.17     0.17     0.18     0.18
```

Step 4: Estimate causal effects.

In this final step, we obtain the causal effect estimates. Since we requested short-stacking in Step 3, `ddml` shows the short-stacking result which relies on the cross-fitted values of each base learner. In addition, the specification that corresponds to the minimum-MSE learners is listed at the beginning of the output.

```
. ddml estimate, robust

Model:                   partial, crossfit folds k=4, resamples r=1
Mata global (mname):     m0
Dependent variable (Y):  net_tfa
 net_tfa learners:       Y1_reg Y2_pystacked Y3_rforest
D equations (1):         e401
 e401 learners:          D1_reg D2_pystacked D3_rforest

DDML estimation results:
spec  r       Y learner     D learner          b          SE
 mse  1   Y2_pystacked  D2_pystacked   9788.291 (1339.797)
  ss  1   [shortstack]          [ss]   9748.788 (1331.364)
mse = minimum MSE specification for that resample.

Shortstack DDML model
y-E[y|X]  = y-Y_net_tfa_ss_1                     Number of obs    =       9915
D-E[D|X]  = D-D_e401_ss_1
```

	Coefficient	Robust std. err.	z	P>|z|	[95% conf. interval]	
e401	9748.788	1331.364	7.32	0.000	7139.362	12358.21
_cons	92.48199	534.8262	0.17	0.863	-955.7581	1140.722

```
Stacking final estimator: nnls1
```

Since we have specified three learners per conditional expectation, there are in total 9 specifications relying on the base learners (since we can combine `Y1_reg_1`, `Y2_pystacked_1` and `Y3_rforest_1` with `D1_reg_1`, `D2_pystacked_1` and `D3_rforest_1`). To get all results, we add the `allcombos` option:

```
. ddml estimate, robust allcombos

Model:                   partial, crossfit folds k=4, resamples r=1
Mata global (mname):     m0
Dependent variable (Y):  net_tfa
 net_tfa learners:       Y1_reg Y2_pystacked Y3_rforest
D equations (1):         e401
 e401 learners:          D1_reg D2_pystacked D3_rforest

DDML estimation results:
spec  r       Y learner     D learner          b          SE
   1  1          Y1_reg         D1_reg   5986.657 (1523.694)
   2  1          Y1_reg   D2_pystacked   9563.875 (1389.172)
   3  1          Y1_reg     D3_rforest   8659.141 (1258.982)
   4  1    Y2_pystacked        D1_reg   9175.519 (1371.065)
*  5  1    Y2_pystacked  D2_pystacked   9788.291 (1339.797)
   6  1    Y2_pystacked    D3_rforest   8497.214 (1200.268)
   7  1      Y3_rforest        D1_reg   9044.071 (1485.073)
   8  1      Y3_rforest  D2_pystacked  10103.630 (1426.134)
```

```
    9  1    Y3_rforest    D3_rforest  9528.449 (1293.485)
   ss  1  [shortstack]          [ss]  9748.788 (1331.364)
* = minimum MSE specification for that resample.

Shortstack DDML model
y-E[y|X]  = y-Y_net_tfa_ss_1                    Number of obs   =      9915
D-E[D|X]  = D-D_e401_ss_1
```

		Robust				
net_tfa	Coefficient	std. err.	z	P>|z|	[95% conf. interval]
e401	9748.788	1331.364	7.32	0.000	7139.362	12358.21
_cons	92.48199	534.8262	0.17	0.863	-955.7581	1140.722

```
Stacking final estimator: nnls1
```

We can use the spec(*string*) option to select among the listed specifications. *string* is either the specification number, ss, st or ps, to get the short-stacking, standard stacking or pooled stacking specification, respectively, or mse for the specification corresponding to the minimal MSPE. In the example above, spec(1) reports in full the specification using regress for estimating both $E[Y|\boldsymbol{X}]$ and $E[D|\boldsymbol{X}]$. The spec(*string*) option can be provided either in combination with allcombos, or after estimation in combination with the replay option, for example:

```
. ddml estimate, spec(1) replay

Model:                 partial, crossfit folds k=4, resamples r=1
Mata global (mname):   m0
Dependent variable (Y): net_tfa
 net_tfa learners:      Y1_reg Y2_pystacked Y3_rforest
D equations (1):        e401
 e401 learners:         D1_reg D2_pystacked D3_rforest

DDML estimation results:
spec  r    Y learner      D learner       b         SE
   1  1  Y2_pystacked  D2_pystacked  5986.657 (1523.694)
  ss  1  [shortstack]          [ss]  9748.788 (1331.364)
mse = minimum MSE specification for that resample.

DDML model, specification 1
y-E[y|X]  = y-Y1_reg_1                          Number of obs   =      9915
D-E[D|X]  = D-D1_reg_1
```

		Robust				
net_tfa	Coefficient	std. err.	z	P>|z|	[95% conf. interval]
e401	5986.657	1523.694	3.93	0.000	3000.271	8973.042
_cons	10.74705	561.2911	0.02	0.985	-1089.363	1110.857

Manual final estimation.

In the background, ddml estimate regresses Y1_reg_1 against D1_reg_1 with a constant. We can verify this manually:

```
. gen double Y1_resid = $Y - Y1_reg
. gen double D1_resid = $D - D1_reg
. reg Y1_resid D1_resid,  robust
Linear regression                           Number of obs   =      9,915
                                            F(1, 9913)      =      15.44
                                            Prob > F        =     0.0001
                                            R-squared       =     0.0023
                                            Root MSE        =      55891
```

Y1_resid	Coefficient	Robust std. err.	t	P>|t|	[95% conf. interval]	
D1_resid	5986.657	1523.694	3.93	0.000	2999.906	8973.407
_cons	10.74705	561.2911	0.02	0.985	−1089.498	1110.992

Manual estimation using `regress` allows the use of `regress`'s postestimation tools.

Stacking

We next demonstrate DDML with stacking. To this end, we exploit the stacking regressor implemented in `pystacked`. `pystacked` allows combining multiple base learners with learner-specific settings and covariates into a final meta learner. The learners are separated by `||`. `method(name)` selects the learner, `xvars(varlist)` specifies learner-specific covariates (overwritting the default covariates `$X`) and `opt(string)` passes options to the learners. In this example, we use OLS, cross-validated lasso and ridge, random forests and gradient boosting. We furthermore use parallelization with 5 cores. A detailed explanation of the `pystacked` syntax can be found in Ahrens et al. (2022).

```
. *** add learners for E[Y|X]
. ddml E[Y|X]: pystacked $Y $X                                    || ///
>     method(ols)                                                 || ///
>     m(lassocv) xvars(c.($X)##c.($X))                            || ///
>     m(ridgecv) xvars(c.($X)##c.($X))                            || ///
>     m(rf) pipe(sparse) opt(max_features(5))                     || ///
>     m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>     njobs(5)
Learner Y1_pystacked added successfully.
. *** add learners for E[D|X]
. ddml E[D|X]: pystacked $D $X                                    || ///
>     method(ols)                                                 || ///
>     m(lassocv) xvars(c.($X)##c.($X))                            || ///
>     m(ridgecv) xvars(c.($X)##c.($X))                            || ///
>     m(rf) pipe(sparse) opt(max_features(5))                     || ///
>     m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>     njobs(5)
Learner D1_pystacked added successfully.
```

After cross-fitting, we retrieve the cross-fitted MSPE using `ddml extract` with `show(mse)` or examine the stacking weights using `stweights`:

```
. qui ddml crossfit
```

```
. ddml extract, show(stweights)
mean stacking weights across folds/resamples for D1_pystacked (e401)
final stacking estimator: nnls1
              learner  mean_weight       rep_1
       ols        1    .01557419    .01557419
   lassocv        2    .10077907    .10077907
    ridgecv       3    .43674242    .43674242
        rf        4    .02946916    .02946916
 gradboost        5    .41743516    .41743516
mean stacking weights across folds/resamples for Y1_pystacked (net_tfa)
final stacking estimator: nnls1
              learner  mean_weight       rep_1
       ols        1    .09662631    .09662631
   lassocv        2    .46475744    .46475744
    ridgecv       3    .32388159    .32388159
        rf        4    .09392877    .09392877
 gradboost        5     .0145518     .0145518
```

Finally, in the estimation stage, we retrieve the results of DDML with stacking:

```
. ddml estimate, robust

Model:                   partial, crossfit folds k=4, resamples r=1
Mata global (mname):     m0
Dependent variable (Y): net_tfa
 net_tfa learners:       Y1_pystacked
D equations (1):         e401
 e401 learners:          D1_pystacked

DDML estimation results:
spec  r     Y learner     D learner         b          SE
  st  1  Y1_pystacked  D1_pystacked   9406.385 (1300.170)

Stacking DDML model
y-E[y|X]  = y-Y1_pystacked_1                      Number of obs   =      9915
D-E[D|X]  = D-D1_pystacked_1
```

net_tfa	Coefficient	Robust std. err.	z	P>|z|	[95% conf. interval]	
e401	9406.385	1300.17	7.23	0.000	6858.099	11954.67
_cons	199.9921	535.7477	0.37	0.709	-850.0541	1250.038

```
Stacking final estimator: nnls1
```

The DDML-specific stacking approaches of short-stacking and pooled stacking can be requested at either the cross-fitting or estimation steps. Re-fitting the final learner at the estimation step allows us to avoid repeating the computationally-intensive cross-fitting. Here, we request short-stacking and pooled stacking but using the single-best base learner.

```
. ddml estimate, robust shortstack poolstack finalest(singlebest)

Model:                   partial, crossfit folds k=4, resamples r=1
Mata global (mname):     m0
Dependent variable (Y): net_tfa
 net_tfa learners:       Y1_pystacked
```

```
D equations (1):          e401
 e401 learners:           D1_pystacked
DDML estimation results:
spec  r      Y learner       D learner       b           SE
  st  1  Y1_pystacked  D1_pystacked  9406.385  (1300.170)
  ss  1  [shortstack]          [ss]  9847.256  (1339.419)
  ps  1  [poolstack]           [ps]  9788.291  (1339.797)
Shortstack DDML model
y-E[y|X]  = y-Y_net_tfa_ss_1                 Number of obs   =      9915
D-E[D|X]  = D-D_e401_ss_1
```

net_tfa	Coefficient	Robust std. err.	z	P>|z|	[95% conf. interval]	
e401	9847.256	1339.419	7.35	0.000	7222.044	12472.47
_cons	78.69447	534.6452	0.15	0.883	−969.1909	1126.58

```
Stacking final estimator: singlebest
```

Short-stacking is computationally substantially faster than regular stacking (or pooled stacking) because it avoids the cross-validation within cross-fit folds. Below, we disable regular stacking with the `nostdstack` option in the cross-fitting stage. In this example, where we use parallelization with 5 cores, the run time is only 50.7 seconds DDML with short-stakcing compared to 93.0 seconds for DDML with regular stacking.

```
. qui ddml crossfit, shortstack nostdstack

. ddml estimate, robust

Model:                 partial, crossfit folds k=4, resamples r=1
Mata global (mname):   m0
Dependent variable (Y): net_tfa
 net_tfa learners:      Y1_pystacked
D equations (1):       e401
 e401 learners:        D1_pystacked
DDML estimation results:
spec  r      Y learner       D learner       b           SE
  ss  1  [shortstack]          [ss]  9602.257  (1300.825)
Shortstack DDML model
y-E[y|X]  = y-Y_net_tfa_ss_1                 Number of obs   =      9915
D-E[D|X]  = D-D_e401_ss_1
```

net_tfa	Coefficient	Robust std. err.	z	P>|z|	[95% conf. interval]	
e401	9602.257	1300.825	7.38	0.000	7052.686	12151.83
_cons	83.96648	533.9871	0.16	0.875	−962.6289	1130.562

```
Stacking final estimator:
```

One-line syntax.

`qddml` provides a simplified and convenient one-line syntax. The main constraint of `qddml` is that it only allows for one user-specified learner. The default learner is `pystacked`, which by default uses OLS, cross-validated lasso and gradient boosting as default learners. The `pystacked` base learners as well as non-`pystacked` commands can be be modified via various options. Below we use `qddml` with `pystacked`'s default base learners. We omit the output for the sake of brevity.

```
. qui qddml $Y $D (c.($X)##c.($X)), model(partial) kfolds(4) robust
```

6.2   The market for automobiles

For this demonstration, we follow Chernozhukov et al. (2015b) who estimate a stylized demand model using instrumental variables based on the data from Berry et al. (1995). The authors of the original study estimate the effect of prices on the market share of automobile models in a given year ($n = 2217$). The controls are product characteristics (a constant, air conditioning dummy, horsepower divided by weight, miles per dollar, vehicle size). To account for endogenous prices, Berry et al. (1995) suggest exploiting other products' characteristics as instruments. Following Chernozhukov et al. (2015b), we define the baseline set of instruments as the sum over all other products' characteristics, calculated separately for own-firm and other-firm products, which yields 10 baseline instruments. Chernozhukov et al. (2015b) also construct an augmented set of instruments, including first-order interactions, squared and cubic terms. In the analysis below, we extend Chernozhukov et al. (2015b) by applying DDML with stacking and a diverse set of learners including OLS, lasso, ridge, random forest and gradient boosted trees. We use the augmented set of controls for all base learners and OLS, which we include for reference.

We load and prepare the data:

```
. use BLP_CHS.dta, clear
. global Y y
. global D price
. global Xbase hpwt air mpd space
. global Xaug augX*
. global Zbase Zbase*
. global Zaug Zaug*
```

Step 1: Initialize `ddml` model.

```
. set seed 123
. ddml init fiv, kfolds(4) reps(5)
```

Note that in the `ddml init` step, we include the option `reps(5)` which will result

in running the full cross-fitting procedure five times, each with a different random split of the data. Replicating the procedure multiple times allows us to gauge the impact of randomness due to the random splitting of the data into subsamples.

Step 2: Add supervised machine learners for estimating conditional expectations.
Estimation of a `fiv` model requires us to add learners for $E[Y|\boldsymbol{X}]$, $E[D|\boldsymbol{X}, \boldsymbol{Z}]$ and $E[D|\boldsymbol{X}]$. Compared to the other models supported by `ddml`, there is one complication that arises because, in order to estimate $E[D|\boldsymbol{X}]$, we exploit fitted values of $E[D|\boldsymbol{X}, \boldsymbol{Z}]$ to impose LIE-compliance. Since these fitted values have not yet been generated, we use the placeholder `{D}` that in the cross-fitting stage will be internally replaced with estimates of $E[D|\boldsymbol{X}, \boldsymbol{Z}]$. We use the `learner(string)` option to match one learner for $E[D|\boldsymbol{X}]$ with a learner for $E[D|\boldsymbol{X}, \boldsymbol{Z}]$, and `vname(varname)` to indicate the name of the treatment variable.

```
. *** add learners for E[Y|X]
. ddml E[Y|X], learner(Ypystacked): pystacked $Y $Xaug            || ///
>     method(ols) xvars($Xbase)                                   || ///
>     m(lassocv)                                                  || ///
>     m(ridgecv)                                                  || ///
>     m(rf) opt(n_estimators(200) max_features(None))             || ///
>     m(rf) opt(n_estimators(200) max_features(10))               || ///
>     m(rf) opt(n_estimators(200) max_features(5))                || ///
>     m(gradboost) opt(n_estimators(800) learning_rate(0.01))     || ///
>     m(gradboost) opt(n_estimators(800) learning_rate(0.1))      || ///
>     m(gradboost) opt(n_estimators(800) learning_rate(0.3))      ,  ///
>     njobs(4)
Learner Ypystacked added successfully.
. ddml E[D|X,Z], learner(Dpystacked): pystacked $D $Xaug $Zaug    || ///
>     method(ols) xvars($Xbase $Zbase)                            || ///
>     m(lassocv)                                                  || ///
>     m(ridgecv)                                                  || ///
>     m(rf) opt(n_estimators(200) max_features(None))             || ///
>     m(rf) opt(n_estimators(200) max_features(10))               || ///
>     m(rf) opt(n_estimators(200) max_features(5))                || ///
>     m(gradboost) opt(n_estimators(800) learning_rate(0.01))     || ///
>     m(gradboost) opt(n_estimators(800) learning_rate(0.1))      || ///
>     m(gradboost) opt(n_estimators(800) learning_rate(0.3))      ,  ///
>     njobs(4)
Learner Dpystacked added successfully.
. ddml E[D|X], mname(m0) learner(Dpystacked) vname($D):               ///
>                                              pystacked {D} $Xaug || ///
>     method(ols) xvars($Xaug)                                    || ///
>     m(lassocv)                                                  || ///
>     m(ridgecv)                                                  || ///
>     m(rf) opt(n_estimators(200) max_features(None))             || ///
>     m(rf) opt(n_estimators(200) max_features(10))               || ///
>     m(rf) opt(n_estimators(200) max_features(5))                || ///
>     m(gradboost) opt(n_estimators(800) learning_rate(0.01))     || ///
>     m(gradboost) opt(n_estimators(800) learning_rate(0.1))      || ///
>     m(gradboost) opt(n_estimators(800) learning_rate(0.3))      ,  ///
>     njobs(4)
Learner Dpystacked_h added successfully.
```

Steps 3-4: Perform cross-fitting (output omitted) and estimate causal effects.

```
. qui ddml crossfit

. ddml estimate, robust

Model:                   fiv, crossfit folds k=4, resamples r=5
Mata global (mname):    m0
Dependent variable (Y): y
 y learners:            Ypystacked
D equations (1):        price
 price learners:        Dpystacked

DDML estimation results:
spec  r      Y learner     D learner        b        SE      DH learner
  st  1    Ypystacked    Dpystacked    -0.108   (0.010)   Dpystacked_h
  st  2    Ypystacked    Dpystacked    -0.123   (0.010)   Dpystacked_h
  st  3    Ypystacked    Dpystacked    -0.110   (0.011)   Dpystacked_h
  st  4    Ypystacked    Dpystacked    -0.127   (0.011)   Dpystacked_h
  st  5    Ypystacked    Dpystacked    -0.132   (0.012)   Dpystacked_h

Mean/med     Y learner     D learner        b        SE      DH learner
  st mn    Ypystacked    Dpystacked    -0.120   (0.014)   Dpystacked_h
  st md    Ypystacked    Dpystacked    -0.123   (0.015)   Dpystacked_h

Median over 5 stacking resamples
y-E[y|X]  = y-Ypystacked                          Number of obs   =      2217
E[D|X,Z]  = D-Dpystacked
E[D^|X]   = Dpystacked_h
Orthogonalized D = D - E[D^|X]; optimal IV = E[D|X,Z] - E[D^|X].
```

	Coefficient	Robust std. err.	z	P>|z|	[95% conf. interval]
price	-.1230112	.0152603	-8.06	0.000	-.1529209 -.0931016

```
Stacking final estimator: nnls1

Summary over 5 resamples:
      D eqn      mean       min       p25       p50       p75       max
      price    -0.1199   -0.1318   -0.1271   -0.1230   -0.1101   -0.1075
```

Manual final estimation. We can obtain the final estimate manually. To this end, we construct the instrument as $\hat{E}[D|X,Z] - \hat{E}[D|X]$ and the residualized endogenous regressor as $D - \hat{E}[D|X]$. The residualized dependent variable is saved in memory. Here we obtain the estimate from the first cross-fitting replication. We could obtain the estimate for replication r by changing the "_1" to "_r".

```
. gen double Y1_resid = $Y - Ypystacked_1

. gen double dtilde = $D - Dpystacked_h_1

. gen double optiv = Dpystacked_1 - Dpystacked_h_1

. ivreg Y1_resid (dtilde=optiv), robust

Instrumental variables 2SLS regression        Number of obs   =       2,217
                                               F(1, 2215)      =      110.49
                                               Prob > F        =      0.0000
                                               R-squared       =      0.0888
                                               Root MSE        =        .965
```

```
                        Robust
     Y1_resid │ Coefficient  std. err.       t    P>|t|     [95% conf. interval]

       dtilde │  -.1075272   .0102295   -10.51   0.000    -.1275875   -.0874668
        _cons │   .0064207   .0205008     0.31   0.754    -.0337821    .0466235
```

```
Instrumented: dtilde
 Instruments: optiv
```

7 Acknowledgments

8 References

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A Algorithms

❏ **Algorithm A.1. DDML for the Interactive Model.**

Split the sample $\{(Y_i, D_i, \boldsymbol{X}_i)\}_{i \in I}$ with $I = \{1, \dots, n\}$ in K folds of approximately equal size. Denote I_k the set of observations included in fold k and $I_k^c = I \setminus I_k$ its complement.

1. Estimate conditional expectations. For each k:

    a. Fit the CEF estimator to observations in the sub-sample I_k^c for which $D_i = 1$ using Y_i as the outcome and $\boldsymbol{X}_i$ as predictors to estimate the conditional expectation $g_0(1, \boldsymbol{X}) = E[Y | \boldsymbol{X}, D = 1]$. Obtain the out-of-sample predicted values $\hat{g}_{I_{k_i}^c}(1, \boldsymbol{X}_i)$ for $i \in I_k$. Proceed in the same way to obtain $\hat{g}(0, \boldsymbol{X})$.

    b. For each k, fit the CEF estimator to the sub-sample I_k^c using D_i as outcome and $\boldsymbol{X}_i$ as predictors to estimate the conditional expectation $m(\boldsymbol{X}) = E[D | \boldsymbol{X}]$. Obtain the out-of-sample predicted values $\hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)$ for $i \in I_k$.

2. Compute the ATE and ATET using (7) and (8).

                                                                                    ❏

❏ **Algorithm A.2. DDML for the Partially Linear IV Model.**

Split the sample $\{(Y_i, D_i, \boldsymbol{X}_i)\}_{i \in I}$ with $I = \{1, \dots, n\}$ in K folds of approximately equal size. Denote I_k the set of observations included in fold k and $I_k^c = I \setminus I_k$ its complement.

1. Estimate conditional expectations. For each k:

    a. Fit the CEF estimator to the sub-sample I_k^c using Y_i as outcome and $\boldsymbol{X}_i$ as predictors to estimate the conditional expectation $\ell_0(\boldsymbol{X}) = E[Y | \boldsymbol{X}]$. Obtain the out-of-sample predicted values $\hat{\ell}_{I_{k_i}^c}(\boldsymbol{X}_i)$ for $i \in I_k$.

    b. Fit the CEF estimator to the sub-sample I_k^c using D_i as outcome and $\boldsymbol{X}_i$ as predictors to estimate the conditional expectation $m_0(\boldsymbol{X}) = E[D | \boldsymbol{X}]$. Obtain the out-of-sample predicted values $\hat{m}_{I_{k_i}^c}(\boldsymbol{X}_i)$ for $i \in I_k$.

    c. Fit the CEF estimator to the sub-sample I_k^c using Z_i as outcome and $\boldsymbol{X}_i$ as predictors to estimate the conditional expectation $r_0(\boldsymbol{X}) = E[Z | \boldsymbol{X}]$. Obtain the out-of-sample predicted values $\hat{r}_{I_{k_i}^c}(\boldsymbol{X}_i)$ for $i \in I_k$.

2. Compute (10).

                                                                                    ❏

❏ **Algorithm A.3. DDML for the Interactive IV Model.**

Split the sample $\{(Y_i, D_i, \boldsymbol{X}_i)\}_{i \in I}$ with $I = \{1, \dots, n\}$ in K folds of approximately equal size. Denote I_k the set of observations included in fold k and $I_k^c = I \setminus I_k$ its complement.

1. Estimate conditional expectations. For each k:

a. Fit the CEF estimator to observations in the sub-sample I_k^c for which $Z_i = 1$ using Y_i as outcome and $\boldsymbol{X}_i$ as predictors to estimate the conditional expectation $\ell_0(1, \boldsymbol{X}) = E[Y|\boldsymbol{X}, Z = 1]$. Obtain the out-of-sample predicted values $\hat{\ell}_{I_{k_i}^c}(1, \boldsymbol{X}_i)$ for $i \in I_k$. Proceed in the same way for the estimation of $\ell_0(0, \boldsymbol{X})$.

b. Fit the CEF estimator to observations in the sub-sample I_k^c for which $Z_i = 1$ using D_i as outcome and $\boldsymbol{X}_i$ as predictors to estimate the conditional expectation $p_0(1, \boldsymbol{X}) = \Pr(D = 1|\boldsymbol{X}, Z = 1)$. Obtain the out-of-sample predicted values $\hat{p}_{I_{k_i}^c}(1, \boldsymbol{X}_i)$ for $i \in I_k$. Proceed in the same way for the estimation of $p_0(0, \boldsymbol{X})$.

c. Fit the CEF estimator to the sub-sample I_k^c using D_i as outcome and $\boldsymbol{X}_i$ as predictors to estimate the conditional expectation $r(\boldsymbol{X}) = E[Z|\boldsymbol{X}]$. Obtain the out-of-sample predicted values $\hat{r}_{I_{k_i}^c}(\boldsymbol{X}_i)$ for $i \in I_k$.

2. Compute (17).

❏

❏ **Algorithm A.4. DDML with short-stacking for the Partially Linear Model.**

Split the sample $\{(Y_i, D_i, \boldsymbol{X}_i)\}_{i \in I}$ with $I = \{1, \ldots, n\}$ in K folds of approximately equal size. Denote I_k the set of observations included in fold k and $I_k^c = I \setminus I_k$ its complement. Select a set of J base learners with $J \geq 2$.

1. Estimate conditional expectations. For each k and base learner j:
   a. Fit a CEF estimator j to the sub-sample I_k^c using Y_i as the outcome and $\boldsymbol{X}_i$ as predictors. Obtain the out-of-sample predicted values $\hat{\ell}_{I_k^c}^{(j)}(\boldsymbol{X}_i)$ for $i \in I_k$.
   b. Fit a CEF estimator j to the sub-sample I_k^c using D_i as the outcome and $\boldsymbol{X}_i$ as predictors. Obtain the out-of-sample predicted values $\hat{m}_{I_k^c}^{(j)}(\boldsymbol{X}_i)$ for $i \in I_k$.

2. Short-stacking:
   a. Apply constrained regression of Y_i against $\hat{\ell}_{I_k^c}^{(1)}(\boldsymbol{X}_i), \ldots, \hat{\ell}_{I_k^c}^{(J)}(\boldsymbol{X}_i)$ using the full sample I, which yields the short-stacked predicted values $\hat{\ell}^*(\boldsymbol{X}_i)$.
   b. Apply constrained regression of D_i against $\hat{m}_{I_k^c}^{(1)}(\boldsymbol{X}_i), \ldots, \hat{m}_{I_k^c}^{(J)}(\boldsymbol{X}_i)$ using the full sample I, which yields the short-stacked predicted values $\hat{m}^*(\boldsymbol{X}_i)$.

3. Compute the short-stacked DDML esitmator using

$$\hat{\theta}_n = \frac{\frac{1}{n} \sum_{i=1}^n \left(Y_i - \hat{\ell}^*(\boldsymbol{X}_i)\right)\left(D_i - \hat{m}^*(\boldsymbol{X}_i)\right)}{\frac{1}{n} \sum_{i=i}^n \left(D_i - \hat{m}^*(\boldsymbol{X}_i)\right)^2}.$$

❏

❏ **Algorithm A.5. DDML with short-stacking for the Flexible IV Model.**

Split the sample $\{(Y_i, D_i, \boldsymbol{X}_i)\}_{i \in I}$ with $I = \{1, \ldots, n\}$ in K folds of approximately equal size. Denote I_k the set of observations included in fold k and $I_k^c = I \setminus I_k$ its complement. Select a set of J base learners with $J \geq 2$.

1. Estimating conditional expectations $\ell_0(\boldsymbol{X}) = E[Y|\boldsymbol{X}]$:

   a. For each k and base learner j, fit the CEF estimator to the sub-sample I_k^c using Y_i as outcome and $\boldsymbol{X}_i$ as predictors. Obtain the out-of-sample predicted values $\hat{\ell}_{I_k^c}^{(j)}(\boldsymbol{X}_i)$ for $i \in I_k$.

   b. Fit a constrained regression of Y_i against $\hat{\ell}_{I_k^c}^{(j)}(\boldsymbol{X}_i), \ldots, \hat{\ell}_{I_k^c}^{(J)}(\boldsymbol{X}_i)$ over the full sample I. The fitted values are the short-stacking estimates $\hat{\ell}^\star(\boldsymbol{X}_i)$.

2. Estimating conditional expectations $p_0(\boldsymbol{X}, \boldsymbol{Z}) = E[D|\boldsymbol{X}, \boldsymbol{Z}]$:

   a. For each k and base learner j, fit the CEF estimator to the sub-sample I_k^c using D_i as outcome and $(\boldsymbol{X}_i, \boldsymbol{Z}_i)$ as predictors. Obtain the out-of-sample predicted values $\hat{p}_{I_k^c}^{(j)}(\boldsymbol{X}_i, \boldsymbol{Z}_i)$ for $i \in I_k$, and the in-sample predicted values $\tilde{p}_k^{(j)}(\boldsymbol{X}_i, \boldsymbol{Z}_i) \equiv \hat{p}_{I_k^c}^{(j)}(\boldsymbol{X}_i, \boldsymbol{Z}_i)$ for $i \in I_k^c$.

   b. For each k, fit a constrained regression of D_i against in-sample predicted values $\tilde{p}_k^{(1)}(\boldsymbol{X}_i, \boldsymbol{Z}_i), \ldots, \tilde{p}_k^{(J)}(\boldsymbol{X}_i, \boldsymbol{Z}_i)$ over the sample I_k^c to obtain the out-of-sample short-stack predicted values $\hat{p}_{I_k^c}^\star(\boldsymbol{X}_i, \boldsymbol{Z}_i)$ for $i \in I_k$.

   c. Fit a constrained regression of D_i against $\hat{p}_{I_k^c}^{(1)}(\boldsymbol{X}_i, \boldsymbol{Z}_i), \ldots, \hat{p}_{I_k^c}^{(J)}(\boldsymbol{X}_i, \boldsymbol{Z}_i)$ over the full sample I. The fitted values are the short-stacking estimates $\hat{p}^\star(\boldsymbol{Z}_i, \boldsymbol{X}_i)$.

3. Estimating conditional expectations $m_0(\boldsymbol{X}) = E[D|\boldsymbol{X}]$:

   a. For each k and base learner j, fit the CEF estimator to the sub-sample I_k^c using in-sample fitted values $\tilde{p}_k^{(j)}(\boldsymbol{X}_i, \boldsymbol{Z}_i)$ as the outcome and $\boldsymbol{X}_i$ as predictors. Obtain the out-of-sample predicted values $\hat{m}_{I_k^c}^{(j)}(\boldsymbol{X}_i)$ for $i \in I_k$.

   b. Apply a constrained regression of $\hat{p}_{I_k^c}^\star(\boldsymbol{X}_i, \boldsymbol{Z}_i)$ against $\hat{m}_{I_k^c}^{(1)}(\boldsymbol{X}_i), \ldots, \hat{m}_{I_k^c}^{(J)}(\boldsymbol{X}_i)$ over the full sample I. The fitted values are the short-stacking estimates $\hat{m}^\star(\boldsymbol{X}_i)$.

4. Compute

$$\hat{\theta}_n = \frac{\frac{1}{n} \sum_{i=1}^n \left(Y_i - \hat{\ell}^\star(\boldsymbol{X}_i)\right)\left(\hat{p}^\star(\boldsymbol{Z}_i, \boldsymbol{X}_i) - \hat{m}^\star(\boldsymbol{X}_i)\right)}{\frac{1}{n} \sum_{i=i}^n \left(D_i - \hat{m}^\star(\boldsymbol{X}_i)\right)\left(\hat{p}^\star(\boldsymbol{Z}_i, \boldsymbol{X}_i) - \hat{m}^\star(\boldsymbol{X}_i)\right)}. \tag{21}$$

❏

B Additional simulation results

We briefly summarize the results for DGPs 4 and 5 shown in Table B.1. The stacking weights and MSPEs of the individual learners are reported in Tables B.2 and B.3, respectively.

The bias of DDML with stacking is relatively robust to the inclusion of additional noisy covariates. For $n = 100$, DDML with stacking performs at least as well as feasible full-sample estimators. For $n = 1000$, DDML with stacking outperforms OLS and PDS-Lasso, and exhibits a bias that is only slightly above the infeasible oracle estimator.

Table B.1: Bias and Coverage Rates in the Linear and Nonlinear DGPs

| | DGP 4 | | | | DGP 5 | | | |
| | $n = 100$ | | $n = 1000$ | | $n = 100$ | | $n = 1000$ | |
	MAB	Cov.	MAB	Cov.	MAB	Cov.	MAB	Cov.
Full sample:								
Oracle	0.100	0.928	0.032	0.944	0.100	0.912	0.031	0.956
OLS (Base)	0.127	0.855	0.078	0.613	0.113	0.858	0.077	0.615
PDS-Lasso (Base)	0.119	0.833	0.078	0.611	0.115	0.852	0.077	0.611
PDS-Lasso (Poly 5)	0.128	0.808	0.050	0.843	0.113	0.839	0.041	0.884
DDML methods:								
Base learners								
PDS-Lasso (Poly 2 + Inter.)	0.132	0.802	0.050	0.828	0.113	0.859	0.036	0.918
OLS	0.133	0.678	0.078	0.582	0.117	0.839	0.077	0.608
Lasso with CV (Base)	0.121	0.851	0.081	0.605	0.115	0.853	0.077	0.614
Ridge with CV (Base)	0.161	0.712	0.078	0.583	0.115	0.850	0.077	0.608
Lasso with CV (Poly 5)	0.121	0.852	0.040	0.916	0.125	0.853	0.035	0.928
Ridge with CV (Poly 5)	0.171	0.687	0.104	0.376	0.141	0.795	0.047	0.898
Lasso with CV (Poly 2 + Inter.)	0.130	0.818	0.043	0.900	0.110	0.877	0.036	0.926
Ridge with CV (Poly 2 + Inter.)	0.143	0.736	0.148	0.107	0.133	0.818	0.035	0.914
Random forest (Low)	0.201	0.618	0.117	0.294	0.121	0.842	0.046	0.845
Random forest (Medium)	0.203	0.609	0.141	0.151	0.125	0.838	0.066	0.701
Random forest (High)	0.244	0.477	0.226	0.001	0.174	0.727	0.171	0.038
Gradient boosting (Low)	0.098	0.905	0.033	0.941	0.101	0.899	0.033	0.936
Gradient boosting (Medium)	0.121	0.842	0.049	0.844	0.105	0.888	0.041	0.896
Gradient boosting (High)	0.218	0.552	0.127	0.234	0.171	0.718	0.114	0.311
Neural net	0.094	0.893	0.127	0.186	0.108	0.875	0.034	0.927
Meta learners								
Stacking: CLS	0.114	0.864	0.040	0.915	0.106	0.879	0.035	0.935
Stacking: Single best	0.114	0.875	0.038	0.925	0.107	0.888	0.034	0.940
Short-stacking: CLS	0.114	0.869	0.040	0.914	0.105	0.887	0.033	0.945
Short-stacking: Single best	0.114	0.869	0.039	0.923	0.103	0.898	0.034	0.938

Notes: The table reports median absolute bias (MAB) and coverage rate of a 95% confidence interval (CR). We employ standard errors robust to heteroskedasticity. For comparison, we report the following full sample estimators: infeasible Oracle, OLS, PDS-Lasso with base and two different expanded sets of covariates. DDML estimators use 20 folds for cross-fitting if $n = 100$, and 5 folds if $n = 1000$. Meta-learning approaches rely on all listed base learners. Results are based on 1,000 replications. Results for DGPs 1-3 can be found in Table 1 in the main text.

Table B.2: Stacking weights for the estimation of conditional expectation functions

Observations n	DGP 1		DGP 2		DGP 3		DGP 4		DGP 5	
	100	1000	100	1000	100	1000	100	1000	100	1000
Estimation of $E[Y|\mathbf{X}]$:										
OLS	0.027	0.113	0.016	0.	0.034	0.002	0.041	0.017	0.156	0.005
Lasso with CV (Base)	0.182	0.642	0.017	0.	0.206	0.	0.414	0.016	0.120	0.012
Ridge with CV (Base)	0.350	0.041	0.003	0.	0.021	0.	0.033	0.014	0.053	0.018
Lasso with CV (Poly 5)	0.058	0.057	0.205	0.045	0.058	0.	0.149	0.544	0.099	0.272
Ridge with CV (Poly 5)	0.050	0.042	0.121	0.009	0.014	0.	0.023	0.001	0.079	0.050
Lasso with CV (Poly 2 + Inter.)	0.037	0.024	0.222	0.939	0.070	0.008	0.074	0.311	0.092	0.343
Ridge with CV (Poly 2 + Inter.)	0.097	0.011	0.071	0.001	0.039	0.	0.054	0.001	0.043	0.090
Random forest (Low regularization)	0.031	0.004	0.097	0.	0.083	0.064	0.029	0.	0.071	0.054
Random forest (Medium regularization)	0.018	0.	0.066	0.	0.079	0.	0.022	0.	0.041	0.003
Random forest (High regularization)	0.002	0.	0.021	0.	0.018	0.	0.002	0.	0.012	0.
Gradient boosting (Low regularization)	0.055	0.023	0.058	0.002	0.183	0.156	0.077	0.046	0.054	0.033
Gradient boosting (Medium regularization)	0.021	0.013	0.038	0.	0.124	0.687	0.033	0.023	0.021	0.013
Gradient boosting (High regularization)	0.003	0.	0.022	0.	0.025	0.071	0.003	0.	0.006	0.
Neural net	0.069	0.029	0.045	0.004	0.047	0.012	0.045	0.026	0.154	0.105
Estimation of $E[D|\mathbf{X}]$:										
OLS	0.029	0.119	0.017	0.	0.034	0.002	0.044	0.016	0.161	0.006
Lasso with CV (Base)	0.171	0.637	0.016	0.	0.182	0.	0.405	0.014	0.123	0.012
Ridge with CV (Base)	0.350	0.034	0.003	0.	0.020	0.	0.031	0.013	0.053	0.018
Lasso with CV (Poly 5)	0.059	0.058	0.218	0.045	0.057	0.	0.151	0.561	0.103	0.272
Ridge with CV (Poly 5)	0.048	0.047	0.116	0.006	0.014	0.	0.026	0.001	0.074	0.049
Lasso with CV (Poly 2 + Inter.)	0.038	0.024	0.237	0.943	0.068	0.007	0.076	0.301	0.099	0.340
Ridge with CV (Poly 2 + Inter.)	0.094	0.011	0.067	0.001	0.039	0.	0.054	0.001	0.044	0.096
Random forest (Low regularization)	0.036	0.005	0.085	0.	0.083	0.047	0.030	0.	0.066	0.055
Random forest (Medium regularization)	0.022	0.	0.063	0.	0.079	0.	0.022	0.	0.036	0.003
Random forest (High regularization)	0.002	0.	0.021	0.	0.024	0.	0.003	0.	0.015	0.
Gradient boosting (Low regularization)	0.055	0.024	0.055	0.001	0.190	0.171	0.079	0.050	0.054	0.034
Gradient boosting (Medium regularization)	0.022	0.012	0.036	0.	0.139	0.731	0.032	0.020	0.022	0.012
Gradient boosting (High regularization)	0.004	0.	0.021	0.	0.024	0.030	0.003	0.	0.006	0.
Neural net	0.069	0.029	0.046	0.003	0.045	0.011	0.045	0.023	0.146	0.103

Notes: This table shows the stacking weights averaged over bootstrap and cross-fitting iterations for each base learner. We report the stacking weights for the estimation of $E[Y|\mathbf{X}]$ and $E[D|\mathbf{X}]$, and for sample sizes of $n = 100$ and $n = 1000$.

Table B.3: Mean-squared prediction error the estimation of conditional expectation functions

Observations n	DGP 1		DGP 2		DGP 3		DGP 4		DGP 5	
	100	1000	100	1000	100	1000	100	1000	100	1000
Estimation of $E[Y|\mathbf{X}]$:										
OLS	2.753	1.372	4.625	2.085	3.292	1.165	3.364	1.766	1.811	1.687
Lasso with CV (Base)	0.941	1.148	1.900	1.882	0.801	0.909	1.299	1.492	1.572	1.611
Ridge with CV (Base)	0.760	1.258	1.887	1.875	0.761	0.752	1.147	1.765	1.661	1.687
Lasso with CV (Poly 5)	1.254	1.030	2.783	2.608	0.988	0.951	1.575	1.575	1.926	1.742
Ridge with CV (Poly 5)	1.176	0.940	2.445	2.471	0.777	0.849	1.468	1.304	1.591	1.764
Lasso with CV (Poly 2 + Inter.)	0.545	0.872	2.119	2.614	0.728	0.916	1.096	1.450	1.534	1.677
Ridge with CV (Poly 2 + Inter.)	3.299	0.787	2.888	2.520	1.392	0.562	2.629	1.247	1.203	1.904
Random forest (Low regularization)	0.288	0.492	2.016	2.026	0.771	0.985	0.927	1.113	1.327	1.512
Random forest (Medium regularization)	0.272	0.378	1.991	1.922	0.752	0.816	0.907	0.975	1.290	1.350
Random forest (High regularization)	0.128	0.110	1.866	1.840	0.567	0.529	0.725	0.698	0.925	0.852
Gradient boosting (Low regularization)	0.959	1.040	2.458	2.478	1.568	1.440	1.600	1.623	1.806	1.729
Gradient boosting (Medium regularization)	0.581	0.778	2.118	2.226	1.121	1.260	1.220	1.407	1.392	1.498
Gradient boosting (High regularization)	0.183	0.317	1.898	1.890	0.699	0.962	0.818	0.995	0.928	1.037
Neural net	1.614	2.116	2.925	3.469	1.856	2.326	2.035	2.612	1.983	1.944
Estimation of $E[D|\mathbf{X}]$:										
OLS	2.166	1.063	3.801	1.737	2.615	0.925	2.673	1.422	1.458	1.364
Lasso with CV (Base)	0.733	0.886	1.584	1.571	0.641	0.721	1.043	1.201	1.266	1.303
Ridge with CV (Base)	0.590	0.950	1.573	1.565	0.609	0.595	0.915	1.421	1.342	1.364
Lasso with CV (Poly 5)	1.008	0.793	2.274	2.182	0.966	0.751	1.404	1.271	1.497	1.407
Ridge with CV (Poly 5)	0.953	0.729	2.077	2.061	0.629	0.674	1.220	1.050	1.248	1.423
Lasso with CV (Poly 2 + Inter.)	0.420	0.671	1.776	2.192	0.586	0.726	0.880	1.170	1.232	1.357
Ridge with CV (Poly 2 + Inter.)	2.541	0.615	2.415	2.114	1.110	0.443	2.100	1.002	0.967	1.540
Random forest (Low regularization)	0.221	0.376	1.659	1.680	0.596	0.763	0.725	0.881	1.056	1.209
Random forest (Medium regularization)	0.210	0.295	1.642	1.600	0.583	0.642	0.712	0.780	1.027	1.087
Random forest (High regularization)	0.100	0.087	1.549	1.536	0.445	0.420	0.576	0.563	0.742	0.690
Gradient boosting (Low regularization)	0.732	0.791	2.005	2.041	1.220	1.137	1.250	1.291	1.424	1.378
Gradient boosting (Medium regularization)	0.440	0.583	1.739	1.841	0.884	0.997	0.951	1.118	1.101	1.191
Gradient boosting (High regularization)	0.129	0.205	1.573	1.569	0.554	0.733	0.635	0.767	0.723	0.796
Neural net	1.290	1.673	2.428	2.886	1.491	1.867	1.637	2.111	1.608	1.578

Notes: This table shows the cross-fitted mean-squared prediction error averaged over bootstrap iterations for the listed conditional expectation function estimators. We report the mean-squared predictor error for the estimation of $E[Y|\mathbf{X}]$ and $E[D|\mathbf{X}]$, and for sample sizes of $n = 100$ and $n = 1000$.

C   Applications

Here we continue the 401(k) application from the main text to illustrate estimation of the interactive model and IV models. We use the same data and variables as outlined in the main text. For the IV models, we use eligibility to enroll for the 401(k) pension plan as the instrument and treat participation in a 401(k) as the endogenous variable.

C.1   Interactive Model (`interactive`)

We allow for heterogenous treatment effects using the `interactive` model. To this end, the conditional expectation of Y given X is fit separately for $D = 1$ and $D = 0$. We also use `reps(5)`. This will execute the `ddml` estimation three times using different random folds. This reduces dependence on a specific fold.

```
. *** initialize
. set seed 123
. ddml init interactive, kfolds(5) reps(5)


. *** add learners for E[Y|X,D=0] and E[Y|X,D=0]
. ddml E[Y|X,D]: pystacked $Y $X                                    || ///
>       method(ols)                                                 || ///
>       m(lassocv) xvars(c.($X)##c.($X))                            || ///
>       m(ridgecv) xvars(c.($X)##c.($X))                            || ///
>       m(rf) pipe(sparse) opt(max_features(5))                     || ///
>       m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>       njobs(5)
Learner Y1_pystacked added successfully.
. *** add learners for E[D|X]
. ddml E[D|X]: pystacked $D $X                                      || ///
>       method(ols)                                                 || ///
>       m(lassocv) xvars(c.($X)##c.($X))                            || ///
>       m(ridgecv) xvars(c.($X)##c.($X))                            || ///
>       m(rf) pipe(sparse) opt(max_features(5))                     || ///
>       m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>       njobs(5)
Learner D1_pystacked added successfully.


. ddml estimate

Model:                   interactive, crossfit folds k=5, resamples r=5
Mata global (mname):     m0
Dependent variable (Y): net_tfa
 net_tfa learners:       Y1_pystacked
D equations (1):         e401
 e401 learners:          D1_pystacked

DDML estimation results (ATE):
spec  r  Y(0) learner  Y(1) learner    D learner        b        SE
  st  1  Y1_pystacked  Y1_pystacked  D1_pystacked  8026.894 (1126.459)
  st  2  Y1_pystacked  Y1_pystacked  D1_pystacked  7879.717 (1122.815)
  st  3  Y1_pystacked  Y1_pystacked  D1_pystacked  8050.997 (1119.537)
  st  4  Y1_pystacked  Y1_pystacked  D1_pystacked  8157.737 (1113.299)
  st  5  Y1_pystacked  Y1_pystacked  D1_pystacked  7753.948 (1138.377)
```

```
Mean/med Y(0) learner  Y(1) learner    D learner          b          SE
  st mn  Y1_pystacked  Y1_pystacked  D1_pystacked  7973.859 (1132.658)
  st md  Y1_pystacked  Y1_pystacked  D1_pystacked  8026.894 (1126.459)
Median over 5 stacking resamples (ATE)
E[y|X,D=0]   = Y1_pystacked0                        Number of obs   =      9915
E[y|X,D=1]   = Y1_pystacked1
E[D|X]       = D1_pystacked
```

		Robust					
net_tfa	Coefficient	std. err.	z	P>|z|	[95% conf. interval]	
e401	8026.894	1126.459	7.13	0.000	5819.075	10234.71

```
Stacking final estimator: nnls1
Warning: 5 resamples had propensity scores trimmed to lower limit .01.

Summary over 5 resamples:
       D eqn       mean       min       p25       p50       p75       max
       e401   7973.8585  7753.9478  7879.7173  8026.8940  8050.9966  8157.7368
```

One-line syntax (output omitted).

```
. qui qddml $Y $D ($X), model(interactive)
```

C.2   IV model (iv)

```
. use "sipp1991.dta", clear
. global Y net_tfa
. global X age inc educ fsize marr twoearn db pira hown
. global Z e401
. global D p401
```

Step 1: Initialize `ddml` **model.**

```
. set seed 123
. ddml init iv
```

Step 2: Add supervised machine learners for estimating conditional expectations.

```
. *** E[Y|X]
. ddml E[Y|X]: pystacked $Y $X                                      || ///
>      method(ols)                                                  || ///
>      m(lassocv) xvars(c.($X)##c.($X))                             || ///
>      m(ridgecv) xvars(c.($X)##c.($X))                             || ///
>      m(rf) pipe(sparse) opt(max_features(5))                      || ///
>      m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>      njobs(4)
Learner Y1_pystacked added successfully.
```

```
. *** E[D|X]
. ddml E[D|X]: pystacked $D $X                                           || ///
>     method(ols)                                                        || ///
>     m(lassocv) xvars(c.($X)##c.($X))                                   || ///
>     m(ridgecv) xvars(c.($X)##c.($X))                                   || ///
>     m(rf) pipe(sparse) opt(max_features(5))                            || ///
>     m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>     njobs(4)
Learner D1_pystacked added successfully.
. *** E[Z|X]
. ddml E[Z|X]: pystacked $Z $X                                           || ///
>     method(ols)                                                        || ///
>     m(lassocv) xvars(c.($X)##c.($X))                                   || ///
>     m(ridgecv) xvars(c.($X)##c.($X))                                   || ///
>     m(rf) pipe(sparse) opt(max_features(5))                            || ///
>     m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>     njobs(4)
Learner Z1_pystacked added successfully.
```

Step 3: Perform cross-fitting.

```
. ddml crossfit
Cross-fitting E[y|X] equation: net_tfa
Cross-fitting fold 1 2 3 4 5 ...completed cross-fitting
Cross-fitting E[D|X] equation: p401
Cross-fitting fold 1 2 3 4 5 ...completed cross-fitting
Cross-fitting E[Z|X]: e401
Cross-fitting fold 1 2 3 4 5 ...completed cross-fitting
. ddml extract, show(pystacked)
pystacked weights for Z1_pystacked (e401)
            learner   resample     fold_1      fold_2      fold_3      fold_4      fold_5
        ols         1          1          0           0   1.577e-17           0   .04870791
    lassocv         2          1          0   .36068464   .19641246   .23065829           0
    ridgecv         3          1  .50644273   .32367528   .36796975   .30346779   .45676698
         rf         4          1  .04990979   .03383132   8.761e-18   .04246409   .02379444
  gradboost         5          1  .44364749   .28180876   .43561779   .42340983   .47073066
mean stacking weights across folds/resamples for Z1_pystacked (e401)
final stacking estimator: nnls1
            learner   mean_weight       rep_1
        ols         1   .00974158    .00974158
    lassocv         2   .15755108    .15755108
    ridgecv         3    .3916645     .3916645
         rf         4   .02999993    .02999993
  gradboost         5    .4110429     .4110429
pystacked MSEs for Z1_pystacked (e401)
            learner   resample     fold_1      fold_2      fold_3      fold_4      fold_5
        ols         1          1  .19946988   .20137585   .20302906   .20030431    .2013705
    lassocv         2          1  .19523544   .19689361   .19807185   .19569792   .19799156
    ridgecv         3          1  .19512701   .19728582   .19849531   .19614749    .1981114
         rf         4          1  .21307726     .215616   .21841171   .21446185   .21691469
  gradboost         5          1  .19529958   .19797459   .19862763   .19615183   .19795431
mean stacking MSEs across folds/resamples for Z1_pystacked (e401)
final stacking estimator: nnls1
            learner    mean_MSE       rep_1
        ols         1   .20110992    .20110992
```

```
      lassocv          2   .19677808   .19677808
       ridgecv          3   .19703341   .19703341
            rf          4    .2156963    .2156963
     gradboost          5   .19720159   .19720159
```
pystacked weights for Y1_pystacked (net_tfa)
```
            learner   resample      fold_1      fold_2      fold_3      fold_4      fold_5
         ols          1          1   .15175107   .01201745   .14501553   .07072362   .03857199
     lassocv          2          1           0   .86668516           0           0   .26575544
     ridgecv          3          1   .76036209   .10111911   .80863601   .75672014   .61229963
          rf          4          1    .0802917           0   .0208563           0   .06587322
   gradboost          5          1           0   .01161239   .02847589   .19812117   .01749972
```
mean stacking weights across folds/resamples for Y1_pystacked (net_tfa)
final stacking estimator: nnls1
```
            learner   mean_weight       rep_1
         ols          1    .08361593   .08361593
     lassocv          2    .22648812   .22648812
     ridgecv          3    .60782739   .60782739
          rf          4    .03340424   .03340424
   gradboost          5    .05114183   .05114183
```
pystacked MSEs for Y1_pystacked (net_tfa)
```
            learner   resample      fold_1      fold_2      fold_3      fold_4      fold_5
         ols          1          1   3.135e+09   3.040e+09   2.674e+09   3.438e+09   3.378e+09
     lassocv          2          1   2.958e+09   2.843e+09   2.463e+09   3.107e+09   3.025e+09
     ridgecv          3          1   2.952e+09   2.857e+09   2.434e+09   3.099e+09   3.024e+09
          rf          4          1   3.344e+09   3.213e+09   2.765e+09   3.541e+09   3.493e+09
   gradboost          5          1   3.217e+09   2.990e+09   2.656e+09   3.317e+09   3.344e+09
```
mean stacking MSEs across folds/resamples for Y1_pystacked (net_tfa)
final stacking estimator: nnls1
```
            learner   mean_MSE       rep_1
         ols          1   3.133e+09   3.133e+09
     lassocv          2   2.879e+09   2.879e+09
     ridgecv          3   2.873e+09   2.873e+09
          rf          4   3.271e+09   3.271e+09
   gradboost          5   3.105e+09   3.105e+09
```
pystacked weights for D1_pystacked (p401)
```
            learner   resample      fold_1      fold_2      fold_3      fold_4      fold_5
         ols          1          1   .05947061   8.397e-18   .06447698   .06941268   .06619485
     lassocv          2          1   .05876314   .32796901   .20842013   .39455972   .21484529
     ridgecv          3          1   .41441662    .2760156   .36272642   .22474909   .47123129
          rf          4          1   .03741096   .05709511   .02323724    .0711886   .08544984
   gradboost          5          1   .42993867   .33892028   .34113922   .24008991   .16227873
```
mean stacking weights across folds/resamples for D1_pystacked (p401)
final stacking estimator: nnls1
```
            learner   mean_weight       rep_1
         ols          1    .05191103   .05191103
     lassocv          2    .24091146   .24091146
     ridgecv          3    .34982781   .34982781
          rf          4    .05487635   .05487635
   gradboost          5    .30247336   .30247336
```
pystacked MSEs for D1_pystacked (p401)
```
            learner   resample      fold_1      fold_2      fold_3      fold_4      fold_5
         ols          1          1   .17102922   .17168453   .17532105   .17229367   .17290828
     lassocv          2          1   .16965393   .17005015   .17383906   .17092387   .17131014
     ridgecv          3          1   .16988454   .17045619   .17415227   .17155958   .17134841
          rf          4          1    .1850616    .1848705   .19065443   .18625053    .1863959
   gradboost          5          1   .16981445   .17040097   .17420905   .17155253   .17207733
```
mean stacking MSEs across folds/resamples for D1_pystacked (p401)

```
final stacking estimator: nnls1
              learner    mean_MSE        rep_1
       ols          1   .17264735    .17264735
   lassocv          2   .17115543    .17115543
   ridgecv          3    .1714802     .1714802
        rf          4   .18664659    .18664659
 gradboost          5   .17161087    .17161087
```

Step 4: Estimate causal effects.

```
. ddml estimate

Model:                   iv, crossfit folds k=5, resamples r=1
Mata global (mname):    m0
Dependent variable (Y): net_tfa
 net_tfa learners:      Y1_pystacked
D equations (1):        p401
 p401 learners:         D1_pystacked
Z equations (1):        e401
 e401 learners:         Z1_pystacked

DDML estimation results:
spec  r     Y learner     D learner          b          SE      Z learner
  st  1  Y1_pystacked  D1_pystacked  13528.537  (1726.023)  Z1_pystacked

Stacking DDML model
y-E[y|X]  = y-Y1_pystacked_1                    Number of obs   =      9915
D-E[D|X]  = D-D1_pystacked_1
Z-E[Z|X]  = Z-Z1_pystacked_1
```

net_tfa	Coefficient	Std. err.	z	P>|z|	[95% conf. interval]	
p401	13528.54	1726.023	7.84	0.000	10145.59	16911.48
_cons	-42.83654	531.1319	-0.08	0.936	-1083.836	998.1628

```
Stacking final estimator: nnls1
```

One-line syntax.

```
. qui qddml $Y ($X) ($D = $Z), model(iv)
```

C.3   Interactive IV Model interactiveiv

```
. use "sipp1991.dta", clear
. global Y net_tfa
. global X age inc educ fsize marr twoearn db pira hown
. global Z e401
. global D p401
```

Step 1: Initialize `ddml` **model.**

```
. set seed 123
. ddml init interactiveiv
```

Step 2: Add supervised machine learners for estimating conditional expectations.

```
. * add learners for E[Y|X,Z=0] and E[Y|X,Z=0]
. ddml E[Y|X,Z]: pystacked $Y $X                                      || ///
>     method(ols)                                                     || ///
>     m(lassocv) xvars(c.($X)##c.($X))                                || ///
>     m(ridgecv) xvars(c.($X)##c.($X))                                || ///
>     m(rf) pipe(sparse) opt(max_features(5))                         || ///
>     m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>     njobs(4)
Learner Y1_pystacked added successfully.
. * add learners for E[D|X,Z=0] and E[D|X,Z=1]
. ddml E[D|X,Z]: pystacked $D $X                                      || ///
>     method(ols)                                                     || ///
>     m(lassocv) xvars(c.($X)##c.($X))                                || ///
>     m(ridgecv) xvars(c.($X)##c.($X))                                || ///
>     m(rf) pipe(sparse) opt(max_features(5))                         || ///
>     m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>     njobs(4)
Learner D1_pystacked added successfully.
. * add learners for E[Z|X]
. ddml E[Z|X]: pystacked $Z $X                                        || ///
>     method(ols)                                                     || ///
>     m(lassocv) xvars(c.($X)##c.($X))                                || ///
>     m(ridgecv) xvars(c.($X)##c.($X))                                || ///
>     m(rf) pipe(sparse) opt(max_features(5))                         || ///
>     m(gradboost) pipe(sparse) opt(n_estimators(250) learning_rate(0.01)) , ///
>     njobs(4)
Learner Z1_pystacked added successfully.
```

Step 3: Perform cross-fitting.

```
. ddml crossfit
Cross-fitting E[y|X,Z] equation: net_tfa
Cross-fitting fold 1 2 3 4 5 ...completed cross-fitting
Cross-fitting E[D|X,Z] equation: p401
Cross-fitting fold 1 2 3 4 5 ...completed cross-fitting
Cross-fitting E[Z|X]: e401
Cross-fitting fold 1 2 3 4 5 ...completed cross-fitting
```

Step 4: Estimate causal effects.

```
. ddml estimate

Model:                 interactiveiv, crossfit folds k=5, resamples r=1
Mata global (mname):   m0
Dependent variable (Y): net_tfa
 net_tfa learners:     Y1_pystacked
D equations (1):       p401
 p401 learners:        D1_pystacked
```

```
Z equations (1):         e401
 e401 learners:          Z1_pystacked
DDML estimation results (LATE):
spec  r  Y(0) learner  Y(1) learner  D(0) learner  D(1) learner         b         SE      Z learner
  st  1  Y1_pystacked  Y1_pystacked  D1_pystacked  D1_pystacked 11579.166 (1613.058)  Z1_pystacked
Stacking DDML model (LATE)
E[y|X,Z=0]   = Y1_pystacked0_1                      Number of obs   =      9915
E[y|X,Z=1]   = Y1_pystacked1_1
E[D|X,Z=0]   = D1_pystacked0_1
E[D|X,Z=1]   = D1_pystacked1_1
E[Z|X]       = Z1_pystacked_1
```

	Coefficient	Robust std. err.	z	P>|z|	[95% conf. interval]	
net_tfa						
p401	11579.17	1613.058	7.18	0.000	8417.631	14740.7

```
Stacking final estimator: nnls1
Warning: 13 propensity scores trimmed to lower limit .01.
```

One-line syntax.

```
. qui qddml $Y ($X) ($D=$Z), model(interactiveiv)
```