

Positive-Unlabeled Learning for Control Group Construction in Observational Causal Inference

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Abstract

In causal inference, whether through randomized controlled trials or observational studies, access to both treated and control units is essential for estimating the effect of a treatment on an outcome of interest. When treatment assignment is random, the average treatment effect (ATE) can be estimated directly by comparing outcomes between groups. In non-randomized settings, various techniques are employed to adjust for confounding and approximate the counterfactual scenario to recover an unbiased ATE. A common challenge, especially in observational studies, is the absence of units clearly labeled as controls—that is, units known not to have received the treatment. To address this, we propose positive-unlabeled (PU) learning as a framework for identifying, with high confidence, control units from a pool of unlabeled ones, using only the available treated (positive) units. We evaluate this approach using both simulated and real-world data. We construct a causal graph with diverse relationships and use it to generate synthetic data under various scenarios, assessing how reliably the method recovers control groups that allow estimates of true ATE. We also apply our approach to real-world data on optimal sowing and fertilizer treatments in sustainable agriculture. Our findings show that PU learning can successfully identify control (negative) units from unlabeled data based only on treated units and, through the resulting control group, estimate an ATE that closely approximates the

true value. This work has important implications for observational causal inference, especially in fields where randomized experiments are difficult or costly. In domains such as earth, environmental, and agricultural sciences, it enables a plethora of quasi-experiments by leveraging available earth observation and climate data, particularly when treated units are available but control units are lacking.

Keywords

Causality, Machine Learning, Propensity Score, Treatment

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1 Introduction

In modern science, when a randomized controlled trial is not a feasible option, we turn to observational studies to answer causal questions. The most common type of these questions is of the form “What is the effect of intervention T on outcome Y ?”. The average treatment effect (ATE) is a popular quantity that we estimate to answer these types of questions. Inferring causal ATE estimates of an intervention on any outcome formally requires access to control and treated units. Equally important for observational causal inference is the capability to adjust for other variables that are involved as confounders in the intervention-outcome system of interest, so that any difference in outcome between control and treated groups to be attributed only to the intervention.

The absence of treated or control group data is a critical concern. Molinari [10] presents how we can realize estimation of ATE if we do not know the treatment status of a part of the units. Kuzmanovic

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et al. propose how to estimate conditional average treatment effects (CATE) [7] with missing treatment information. Beyond effect estimation under settings with partial absence of treatment information, Lancaster & Imbens [8], building on [17], show that even when some control units are mistakenly classified and may have actually received the treatment—what they refer to as "contaminated controls"—it is still possible to recover unbiased estimates, as long as this misclassification is properly modeled in the analysis. Additionally, Rosenbaum & Rubin exploit the availability of a pool of potential controls on building a balanced control group using multivariate matching methods that incorporate the propensity score, ensuring similarity between treated and control units based on observed covariates [13].

In this work, we focus on the case of the absolute absence of units that are clearly labeled as controls — that is, units known not to have received the treatment. To address this issue, we propose the use of positive-unlabeled (PU) learning [1] as a formal framework for causal effect estimation in the absence of control units. Specifically, we identify, with high confidence, control units from a pool of unlabeled ones, using only the available treated (positive) units. Quite recently, PU learning has been proposed as a methodological solution to identify reliable control units from a pool of unlabeled one [20]. In parallel Kato et al. [5] propose a novel end-to-end PU learning method to estimate ATE in settings with a lack of control units. Complementary, with this work we especially contribute to this conceptual proposition through the following: i. Use PU learning to construct a reliable control group from unlabeled data delinked from the effect estimation step. In this way, we facilitate the use of any causal model and adjustment set in the effect estimation part instead of the end-to-end solution of [5]. ii. We compare the use of an adjustment set defined by the back-door criterion for training the PU learner with a more exhaustive feature set that also includes *bad controls*—such as mediators, colliders, and even the outcome variable itself, and show that the latter yields superior performance. iii. We perform experiments with simulated and real-world data around sustainable agriculture to showcase the usefulness of our approach. These contributions aim to showcase the PU learning as a useful addition to the observational causal inference toolbox, specifically when real-world interventions have taken place, but we lack of labeled control units to realise an experiment. Especially, it applies in the domains of earth, environmental and agricultural sciences, where given the availability of earth observation and meteorological data it can unlock a plethora of quasi-experiments, as we showcase in our real-world examples.

2 Preliminaries & Problem Formulation

2.1 Observational Causal Inference

For each of the experimental setups that follow, simulated or real-world, we employ the relevant causal directed acyclic graph $G = (V, A)$ which includes all involved variables as vertices V connected through directed edges E and represent the causal relationships within the relevant treatment T - outcome Y system, e.g., the fertilizer - yield system. We limited all setups to binary treatments $T \in \{1, 0\}$ and we aim to estimate their unbiased effects on an outcome of interest Y . We choose the exact adjustment set $Z \subseteq V$,

if any, that satisfies the back-door criterion relative to (T, Y) , blocking every path from T to Y that contains an arrow into T , and no descendant nodes from Z to T are allowed. Then, we retrieve ATE as shown in Eq. 1 based only on observational quantities.

$$\begin{aligned} ATE &= \mathbb{E}[Y \mid do(T = 1)] - \mathbb{E}[Y \mid do(T = 0)] \\ &= \sum_z (\mathbb{E}[Y \mid T = 1, Z = z] - \mathbb{E}[Y \mid T = 0, Z = z]) \cdot P(Z = z) \end{aligned} \quad (1)$$

The capability to retrieve the ATE , whether we express it in Equation 1 through as a structural causal model [11], or we express it via potential outcomes framework [14], rests on some fundamental assumptions that both frameworks directly or indirectly rely on:

$$\text{Unconfoundedness: } Y(t) \perp\!\!\!\perp T \mid Z \quad \forall t \in \{0, 1\} \quad (2)$$

$$\text{Positivity: } 0 < P(T = t \mid Z = z) < 1 \quad \forall t \in \{0, 1\}, \forall z \in Z \quad (3)$$

$$\text{Consistency: } Y = Y(t) \quad \text{if } T = t \quad (4)$$

Firstly, it is the stable unit treatment value assumption (SUTVA) that requires there are (i) no interference between units, i.e., one unit's outcome is unaffected by other units' treatment, and (ii) well-defined treatment with no different forms of each treatment level. The unconfoundedness assumption (Eq. 2) requires all confounders are measured, and conditioning on them to removes bias. The positivity assumption (Eq. 3) requires every unit has a positive probability of receiving each treatment level given adjustment set Z . The consistency assumption (Eq. 4) requires that when we observe $T = t$, the observed outcome Y is equal to the outcome that would result from an intervention setting T to t through $do(\cdot)$ operator.

2.2 PU learning for control group construction

In this causal inference context, we should properly define the notation and slightly reformulate the assumptions of PU learning for the case of control group identification. In general, the typical target of PU learning is to learn a binary classifier using only a set of labeled positive instances and a set of unlabeled instances which include both positive and negative instances. In this work, we instrumentalize the PU learning framework as the means to recover from unlabeled units using only positive-treated units a subset of reliable negative-control units, for the downstream task of effect estimation.

Thus, the target variable is the true class label, which in our case is the treatment $T \in \{1, 0\}$ that indicates the real state of unit, where $T = 1$ indicates a real treated/positive and $T = 0$ indicates a real control/negative. X represents the feature vector that describes all units and will be used to estimate T . A critical innovation we propose and explore in this work is that X does not need to be limited to the aforementioned adjustment set Z ; instead, in our formulation X may contain any covariate included in V (from causal graph G that will be beneficial for a robust estimator of T) and even variables exogenous of G system that will be useful. So we state that $Z \subseteq V \subseteq X$. The variable that differentiates the notation from typical supervised learning is a third variable $S \in \{1, 0\}$, which differs from T that represents the real state of unit in terms of whether it has received or not treatment, S is a label indicator. The $S = 1$ indicates that the unit is observed/annotated

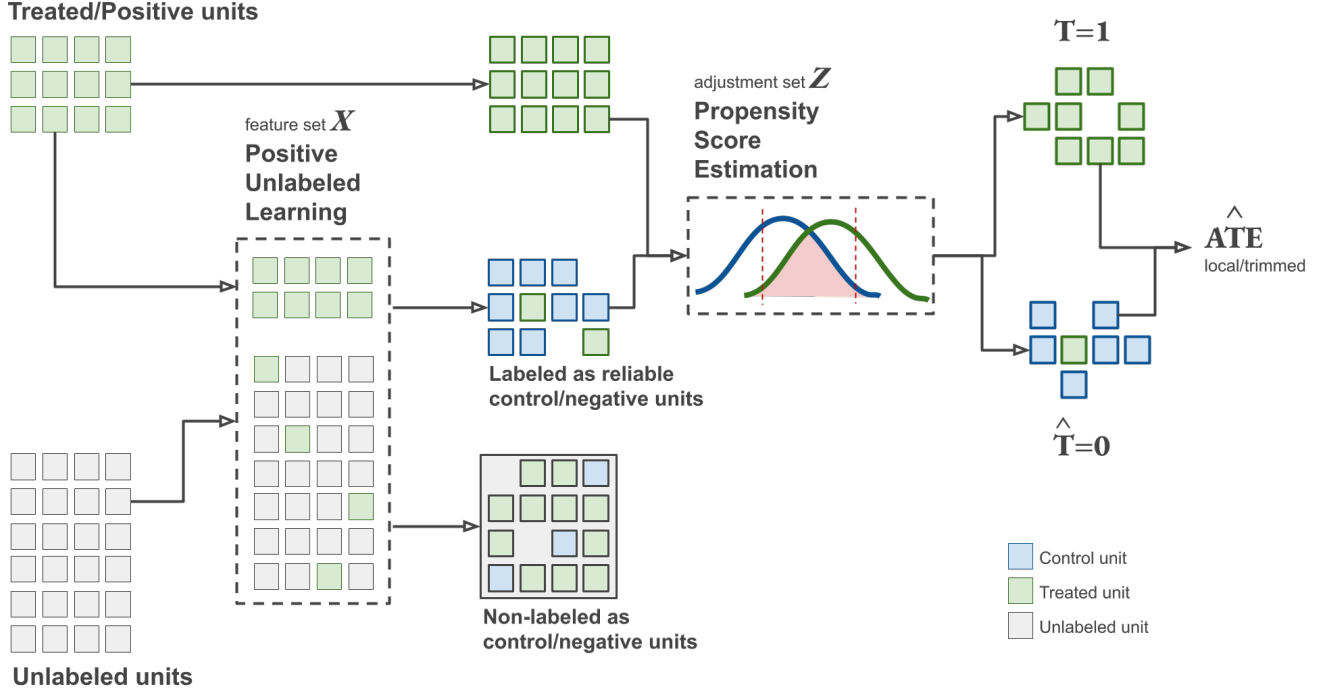


Figure 1: Overview of the use of PU learning as a preparatory step for causal estimation tasks that lack control groups.

as treated/positive and $S = 0$ indicates that unit is unlabeled, so it can be either a control/negative or a treated/positive.

$$\text{SCAR: } P(S = 1 \mid T = 1, X) = P(S = 1 \mid T = 1) = c \quad c \in (0, 1) \quad (5)$$

$$\text{No Label Noise in Treated: } P(T = 0 \mid S = 1) = 0 \quad (6)$$

$$\text{Controls in Unlabeled Set: } P(T = 0 \mid S = 0) > 0 \quad (7)$$

Separability:

$$\begin{aligned} P(t = 1 \mid x) &= \sigma(f(x)) \gg 0.5 \quad \text{for most } x \in \text{Treated} \\ P(t = 0 \mid x) &= \sigma(f(x)) \ll 0.5 \quad \text{for most } x \in \text{Controls} \end{aligned} \quad (8)$$

Smoothness:

$$\begin{aligned} \|x - x'\| < \epsilon, \text{ for small } \epsilon > 0 \\ \Rightarrow P(y = 1 \mid x) \approx P(y = 1 \mid x') \end{aligned} \quad (9)$$

The selected completely at random (SCAR) assumption (Eq. 5) states that labeled positives are selected uniformly at random from all treated units, and selection for labeling is independent of features. The Eq. 6 implies that there is no possibility of mislabeling, e.g. a unit labeled as treated to be truly control. The Eq. 7 requires at least a control unit to be included in the unlabeled dataset. The separability assumption (Eq. 8) states that there exists a decision function $f(x)$ that reliably separates the two classes among unlabeled units via score thresholding (ie $\sigma(\cdot)$ denotes the sigmoid function). The smoothness assumption (Eq. 9) states that two units with nearby feature vectors x, x' shared the same treatment status, which forces us to allow post-treatment and exogenous features to be included in X . Finally, the proposed end target of PU learner is to estimate the treatment assignment probability $P(T = 1 \mid X)$ which allows to

derive units that strongly looks truly untreated given its features (Eq. 10) that can be used as controls in causal effect estimation.

$$P(T = 0 \mid X) = 1 - P(T = 1 \mid X) \gg 0.5 \quad (10)$$

3 Methodology & Experimentation

In this section, we describe in more detail: i. how we employ PU learning as a preparatory step to construct a reliable control group in the case of its absence to enable causal effect estimation and ii. the four experimental setups - two simulated and two real-world datasets - where we test our idea.

3.1 Framework for control group construction

As Fig. 1 illustrates, we emphasize cases where treated and unlabeled units are available, in single-training-set scenarios either with simulated or real-world datasets, because we focus mainly in earth, environmental and agriculture cases where dominantly the units are pieces of land (e.g. agricultural parcels) that belong on the same population/dataset and either they receive an intervention/event or we do not know if they receive it or not. Specifically, we use a 2-step technique. In the first step we leverage the SPY method [9] where some of the real treated units are turned into spies, which we "hide" in the unlabeled dataset. A Naive Bayes classifier is trained, considering the unlabeled units as controls. Then, we label as "reliable" control units those for which the posterior probability is lower than the lowest of spies. In the second step, we employ iterative SVM (iSVM) [21]. In each iteration, an SVM classifier is trained using the real treated units and the reliable controls from the first step. The unlabeled units that are classified as controls by this classifier are

then added to the set of reliable controls for the next iteration till no class change occurs between two iterations. Thus, we categorize the unlabeled units into two groups: the reliable control units, in which the PU learning assigned the control label with a tunable confidence; and the group with units that were left unlabeled because they do not differ enough from the real treated given features X . We do not consider the latter as treated because we already have a group with confirmed real treated units, so there is no reason to risk to add bias with some possible false labeled units as treated. Naturally, these two new groups will probably contain some false labeled units.

Afterwards, we train a propensity score estimator (i.e. a logistic regression) with the real treated units and the labeled from PU learning as reliable controls. However, we have already chosen the adjustment set Z that satisfies the backdoor criterion based on the relevant causal graph G that represents the system relationships for the estimation of the effect of T on Y and we train the propensity score estimator only using this subset of X , the adjustment set Z . We plot the propensity scores per group and we trim the scores of the two groups to ensure sufficient overlap between them. This trimming ensures that we avoid an extrapolation in regions with little comparability between groups, and we focus on ATE estimation on the region of common support. Given that we have recovered as reliable controls the units that, intuitively speaking, significantly differ from the real treated for the PU learning estimator, which is trained on X and in parallel we estimate propensity scores training an estimator on Z , it is clear that we risk drastic shrinkage of units in the area of overlap between the two groups due to the significant overlap of feature sets $Z \subseteq X$. This area of overlap is prone to be the area of the smallest propensity scores, given that reliable controls are units that are based on X place in a conceptually similar area from the PU learning estimator. Consequently, an issue arises about how strong the positivity assumption holds each time and what exactly this strong 'trimmed' or 'local' ATE quantity represents. Finally, we estimate the ATE with several estimators using the trimmed, based on propensity scores, treated and reliable control groups for reasons of completeness and framework assessment. We use linear regression and distance matching as baseline estimation methods, and Inverse Propensity Score Weighing (IPW) [18] and the causal machine learning method T-learner [6].

3.2 Experimental setups & data

We simulate data under two different assumptions (generating $n = 1000$ samples for each), one with linear and one with non-linear causal relationships, to test our ideas in a fully controllable environment. For this purpose, we construct the causal graph G_{sim} of Fig. 2 where we employ the Cinelli et al. work [2] in order to introduce G_{sim} a wide palette of different relationships 'confounders', 'mediators', 'colliders'. Specifically, vertices $V_{good} = \{X_{1.1}, X_{1.2}, X_{2.1}, X_{2.2}, U_3\}$ are 'good controls' reducing bias by blocking back-door paths if we control for them. The $V_{bad} = \{X_3, X_5, X_7, X_9, M\}$ are 'bad controls', with addition of X_3 as control would lead to 'bias amplification'. The X_5 are known as 'M-bias' that induce bias through U_1, U_2 . M mediates the effect we want to estimate, so we keep this path untouched without controlling for this variable, similarly to X_7 , where a control for it is equivalent to a partial

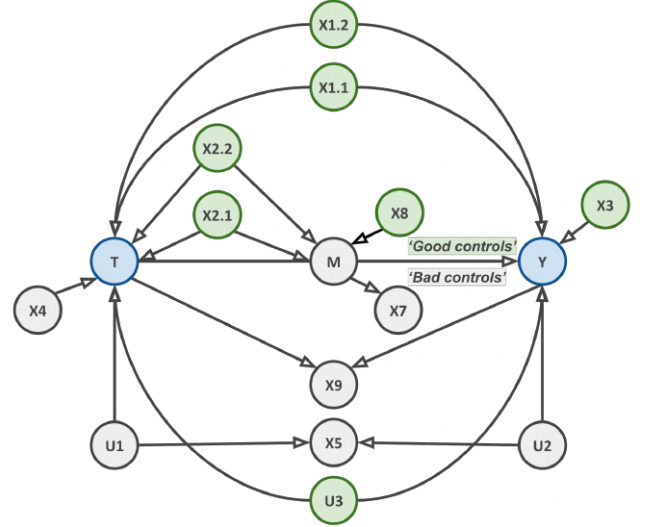


Figure 2: The causal graph G_{sim} serves as the data-generating process for both linear and non-linear simulations.

control for mediator M . X_9 is a typical 'bad control' because controlling for it opens a colliding path and induces 'selection bias'. Finally, vertices $V_{neutral} = \{X_3, X_8\}$ are neutral in terms of inserting or removing bias but can be useful controls in terms of ATE precision. Thus, as expected from graph construction, the minimum adjustment set Z_{sim} that satisfies the back-door criterion contains the 'good controls' so $Z_{sim} = V_{good} = \{X_{1.1}, X_{1.2}, X_{2.1}, X_{2.2}, U_3\}$ for an unbiased estimation of ATE of treatment T on outcome Y of causal system G_{sim} . The Sec. B of the Appendix present the data-generating process in detail.

Also, we investigate the applicability of our ideas in two real-world scenarios from the domain of sustainable agriculture. First, we use the causal graph, data and causal effect estimation setup from Tsoumas et al. work [19]. They estimate the ATE of treatment T : whether the cotton field is sown on an annotated date as favorable or not, on the outcome Y , which is the final yield of cotton. We use the adjustment set $Z_{sowing} = \{Weather\ on\ sowing\ date, Soil\ moisture\ on\ sowing\ date, Topsoil\ properties, Topsoil\ organic\ carbon, Seed\ variety, Geometry\ of\ field\}$ that satisfies the back-door criterion of their proposed causal graph, and also we use the additional available variables $V_{extra} = \{Crop\ growth, Location\ \&\ area\ of\ field, Harvest\ date\ \&\ cultivation\ period, Yield\}$ that are not used for effect estimation in order to test the use of an expanded feature set $X_{sowing} = Z_{sowing} + V_{extra}$ over the adjustment set Z_{sowing} to construct a group of reliable control units and the hold of the positivity assumption. As a second real-world scenario, we introduce a new dataset about the impact of a digestate fertilizer (i.e., a sustainable alternative to chemical fertilizers) on wheat biomass in fields cultivated with durum wheat. For this paper, we adopt the popular example of fertilization-yield causal graph from Pearl's book [12], incorporate it with the richer ground truth causal graph in [16] regarding soil processes. In this dataset, the adjustment set and the feature set are composed as follows: $Z_{fertilizer} = \{Topsoil\ organic\ carbon, Accumulated\ precipitation, Growing\ degree\ days, Accumulated\ vegetation\ moisture\ content, Soil\ moisture, Soil\ type\ Seed$

Dataset	PU method	Feature Set	# Positives (true treated)	# Spies	# Unlabeled		Evaluation Metrics							
					controls	treated	# Selected		# Non-selected		Control Recall	Control Precision	Contamination Rate	Treated Leakage
							# Controls	# Treated	# Controls	# Treated				
Linear	SPY	Z	346	103 (30%)	505	149	334	31	171	118	0.661	0.915	0.085	0.208
		X					505	28	0	121	1.000	0.947	0.053	0.188
		Z					143	4	362	145	0.283	0.973	0.027	0.027
Non-linear	SPY+iSVM	X	365	109 (30%)	478	157	505	0	0	149	1.000	1.000	0	0
		Z					186	28	292	129	0.389	0.870	0.131	0.178
		X					476	15	2	142	0.996	0.969	0.031	0.095
Sowing	SPY	Z	35	5 (15%)	121	15	121	16	357	141	0.253	0.883	0.117	0.102
		X					474	0	4	157	0.992	1.000	0	0
		Z					92	3	29	12	0.760	0.968	0.032	0.200
Fertilization	SPY+iSVM	X	23	3 (15%)	99	11	72	4	49	11	0.595	0.947	0.053	0.267
		Z					97	5	24	10	0.802	0.951	0.049	0.333
		X					101	5	20	10	0.835	0.953	0.047	0.333
Fertilization	SPY	Z	23	3 (15%)	99	11	64	3	35	8	0.646	0.955	0.045	0.273
		X					71	5	28	6	0.717	0.934	0.066	0.455
		Z					89	7	10	4	0.899	0.927	0.073	0.636
Fertilization	SPY+iSVM	X					87	8	12	3	0.878	0.916	0.084	0.727

Table 1: Summary of control group selection using SPY and SPY+iSVM across four datasets (Linear, Non-linear, Sowing, Fertilization), evaluated with feature sets Z (adjustment set) and X (the most informative variables set about treatment).

variety} and $X_{sowing} = Z_{sowing} + \{Exogenous\ organic\ matter\ indexes, Produced\ biomass\ proxy\}$. More details about the effect estimation and the data in the Table 3 on Sec. A of Appendix.

4 Results

In this section we present & discuss the results of our experiments regarding the proposed utilization of PU learning as an enabler of any causal effect estimation task when a confirmed control group is completely absent, but a source of unlabeled units is available.

For the evaluation of the framework, we emulate PU conditions through the popular ‘hide and seek’ approach [15]. Specifically, we engineer positive-unlabeled datasets from the aforementioned simulated and real-world positive-negative datasets. We do this simply by hiding a percentage of positive/treated units within the negative/control units, something that allows us to consider this mixed group with units from both treatment classes as an unlabelled set to test our ideas. This satisfies the SCAR assumption (Eq. 5) and facilitates the assessment of the PU learner using common binary classification evaluation metrics. However, we have to clarify some slight conceptual changes from typical classification metrics that better align with and reflect a causal inference context. While throughout the paper we refer to treated units as positives and controls as negatives in the PU learning setup, during evaluation, we treat true controls as the positive class to assess how well the method recovers clean / reliable control units. Thus, for clarity, under this evaluation perspective, True Positives (TP) correspond to true control units correctly recovered as controls, False Positives (FP) correspond to treated units wrongly selected as controls, False Negatives (FN) to true control units that were not recovered and True Negatives (TN) to treated units correctly not selected (held out as no control units). Thus, we use: the Control Recall equation (Eq. 11) to assess how many of the true controls were recovered (it measures the coverage of the control group); the Control Precision equation (Eq. 12), which summarizes how many were actual controls out of selected as ‘reliable controls’; the Contamination Rate (Eq. 13), which refers to the proportion of selected as ‘reliable controls’ that were actually treated; and we introduce the Treated Leakage metrics (Eq. 14) that measures how many units mistakenly ended up in ‘reliable controls’ among true treated units.

$$\text{Control Recall} = \frac{TP}{TP + FN} \quad (11)$$

$$\text{Control Precision} = \frac{TP}{TP + FP} \quad (12)$$

$$\text{Contamination Rate} = \frac{FP}{TP + FP} \quad (13)$$

$$\text{Treated Leakage} = \frac{FP}{FP + TN} \quad (14)$$

In Table 1, the evaluation metrics of PU learning for retrieving real control units from an unlabeled pool of mixed control and treated units are presented in detail for the four different datasets. In the two simulated, linear and non-linear, datasets our results show that the combination of SPY with iSVM returns the best results in all metrics with the use of X feature set instead of Z adjustment set. The use of X extremely outperforms in any metric, with more significant gains in the almost elimination of any leakage of treated in the ‘reliable controls’ and the increase of recall. Even SPY method alone using X outperforms the combined solution of SPY and iSVM when they are trained on Z. In the sowing and fertilization datasets, recall and precision follow almost the same fluctuations as in the simulated data. However, leakage of treated units presents a slight increase with the use of the feature set X in comparison with the adjustment set Z. Furthermore, the fertilization dataset, when SPY and iSVM are trained on X presents very high treated leakage, with 8 out of 11 hidden treated units classified as controls, which risks significantly biasing the results of the following effect estimation task. A likely explanation is the very small sample size of spies and hidden treated units for the machine learning task.

In all datasets, the number of retrieved ‘reliable controls’ tend to be more if the larger X feature set is used for PU learning - column ‘# Selected’ in Table 1. After the trimming of both groups’ units based on propensity scores to secure treated and control units have overlapped propensities, it appears (in the column ‘(treated, control)’ of Table 2) that bigger overlap between groups emerges in the more complex 2-steps setup (SPY plus iSVM with the use of X feature set). This is also visualized in Sec. C of the Appendix, where the propensity scores overlap for all datasets are depicted. Due to the skewed propensity scores distribution of inferred reliable controls even for the best case (i.s. SPY plus iSVM with X) of

Dataset	Control Units	(treated, control)	true effect	PU Feature Set	Causal Effect Estimation Methods											
					Linear Regression			IPS weighting			Matching			T-Learner(RF)		
					ATE	CI	p-value	ATE	CI	p-value	ATE	CI	p-value	ATE	CI	p-value
Linear	real controls	(495, 505) - no trim	3.000	-	3.664	(3.447, 3.895)	0.000	3.848	(3.451, 4.237)	0.001	3.927	(3.601, 4.192)	0.001	4.029	(3.939, 4.119)	-
	SPY	(36, 232)		Z	2.718	(2.250, 3.143)	0.000	3.081	(1.927, 4.121)	0.001	3.261	(2.648, 3.620)	0.001	3.520	(3.211, 3.828)	-
	(450, 414)			X	2.800	(2.631, 2.997)	0.000	2.818	(2.337, 3.376)	0.001	3.282	(2.989, 3.392)	0.001	3.529	(3.428, 3.630)	-
	SPY+iSVM	(22, 147)		Z	2.757	(2.109, 3.338)	0.000	3.231	(1.817, 4.500)	0.001	3.667	(2.906, 4.250)	0.001	3.771	(3.331, 4.212)	-
	(414, 424)			X	3.021	(2.861, 3.185)	0.000	3.188	(2.765, 3.559)	0.001	3.574	(3.320, 3.726)	0.001	3.814	(3.720, 3.909)	-
Non-linear	real controls	(522, 478) - no trim	9.525	-	9.717	(9.367, 10.094)	0.000	9.799	(9.296, 10.229)	0.001	9.597	(9.155, 9.869)	0.001	9.829	(9.646, 10.011)	-
	SPY	(17, 77)		Z	8.057	(5.989, 10.452)	0.000	7.775	(4.819, 10.827)	0.001	7.209	(4.660, 8.793)	0.001	7.261	(6.322, 8.201)	-
	(513, 487)			X	9.480	(9.100, 9.886)	0.000	9.570	(9.040, 10.035)	0.001	9.321	(8.900, 9.607)	0.001	9.324	(9.132, 9.516)	-
	SPY+iSVM	(86, 137)		Z	7.962	(6.762, 8.993)	0.000	7.884	(6.269, 9.466)	0.001	7.556	(6.318, 8.178)	0.001	7.877	(7.384, 8.371)	-
	(513, 470)			X	9.719	(9.378, 10.0953)	0.000	9.820	(9.369, 10.254)	0.001	9.805	(9.446, 10.092)	0.001	9.887	(9.701, 10.073)	-
Sowing	real controls	(50, 121)	expected positive	-	546	(211, 880)	0.002	471	(138, 816)	0.001	448	(186, 760)	0.006	372	(215, 528)	0.024
	SPY	(13, 92)		Z	211	(-479, 902)	0.544	315	(-487, 1024)	0.138	244	(-733, 1099)	0.226	259	(-134, 653)	-
	(14, 14)			X	664	(-267, 1596)	0.147	811	(122, 1660)	0.030	689	(-54, 1369)	0.063	777	(376, 1178)	-
	SPY+iSVM	(25, 43)		Z	156	(-463, 776)	0.615	322	(-25, 724)	0.087	293	(-145, 723)	0.128	306	(82, 530)	-
	(39, 47)			X	466	(-61, 993)	0.082	524	(170, 992)	0.029	480	(132, 857)	0.015	390	(159, 586)	-
Fertilization	real controls	(34, 99) - no trim	expected positive	-	1.188	(-0.386, 2.762)	0.138	1.160	(-0.094, 2.649)	0.055	0.708	(-0.834, 2.266)	0.200	1.104	(0.484, 1.725)	-
	SPY	(8, 38)		Z	3.000	(-0.600, 6.599)	0.097	1.866	(-0.173, 4.351)	0.094	1.111	(-1.188, 2.842)	0.219	0.903	(-0.141, 1.947)	-
	(20, 47)			X	2.342	(-0.168, 4.851)	0.067	0.805	(-0.711, 2.604)	0.167	0.425	(-1.173, 2.268)	0.345	0.464	(-0.363, 1.292)	-
	SPY+iSVM	(24, 67)		Z	1.302	(-0.566, 3.170)	0.168	1.190	(-0.391, 2.843)	0.076	0.981	(-0.426, 3.142)	0.162	0.542	(-0.228, 1.312)	-
	(31, 67)			X	1.750	(0.003, 3.498)	0.049	1.322	(-0.347, 3.122)	0.047	0.742	(-0.555, 2.265)	0.192	0.823	(0.158, 1.488)	-

Table 2: Effect estimation using treated units and (i) real control, (ii) retrieved reliable controls under various PU learning methods, feature sets, and ATE estimation techniques.

sowing and fertilization datasets, we apply asymmetric trimming to retain units with estimated propensity scores in the range $[0.1, 0.6]$. This decision ensures that we operate within a region of the covariate space where there is reasonable overlap between positively labeled treated units and inferred control candidates. However, this approach limits our estimand to an *ATE* within this low- to moderate-propensity subpopulation. Consequently, our *ATE* estimates are not directly generalizable to the full population or to high-propensity treated units, which are trimmed out due to lack of comparable control analogs. While this trimming reduces the risks of extrapolation and positivity violation, it introduces a form of selection bias and may underestimate the true heterogeneity of treatment effects across the broader covariate space. So, in terms of proper classification/reliable controls identification, the full 2-step PU learning method outperforms the use of SPY alone in most cases and the superiority of use of *X* feature set instead of *Z* adjustment set for the PU learning is profound. In the Sec. D of the Appendix we included a slope chart per dataset that compares the top-15 features in terms of influence and their change between the iSVM trained on *Z* and *X*, using model coefficients as feature importance.

However, as a final evaluation step given in reality we have control units for each dataset, we leverage various methods from different methodological backgrounds to estimate the causal *ATE* of each treatment on the outcome of interest before and after the retrieval of control units through our proposed solution. Observing the results in Table 2, we easily summarize for the two simulated and the sowing datasets that the setup with SPY and iSVM model trained on the feature set *X* succeeds in retrieving a statistically significant *ATE* very close to that is retrieved by the confirmed treated & control groups with all different causal estimators. Also, we observe that in the cases where *Z* is used in PU learning, we have an underestimate of *ATE* and lacking of statistical significance, probably due to extremely large trimming $[0.1, 0.3]$ that isolate our estimation to a limited subpopulation and also leads to a very small number of units left in both groups.

For the fertilization dataset, the results are less stable (Table 2). Using the real control units, we observe a positive *ATE*, though not statistically significant. After applying the PU learning method –

specifically the more robust SPY plus iSVM plus *X* scenario – we observe a slight increase in *ATE* estimates, with linear regression and IPW yielding statistically significant results (p -value < 0.05), and matching and T-Learner producing similar outcomes. However, these results should be interpreted with caution due to high treated leakage in this scenario. Additionally, we applied our method to a real unlabeled dataset, enriched with available confirmed controls, to identify reliable units and estimate the *ATE* using only these controls (ignoring their actual treatment status) and the treated group. This dataset includes 616 unlabeled units and 99 confirmed controls. Using the SPY plus iSVM plus *X* method and trimming the propensity scores to the range $[0.05, 0.6]$ to ensure overlap, we identified 67 reliable controls, 55 of which are confirmed controls. Once again, the results align with those obtained using only real controls or engineered pseudo-unlabeled data (Table 2). Specifically, for the real unlabeled dataset: linear regression estimated an *ATE* of 1.641 ($CI : [-0.393, 3.675]$, $p = 0.112$); IPW estimated an *ATE* of 1.255 ($CI : [-0.613, 3.002]$, $p = 0.113$); matching yielded an *ATE* of 1.207 ($CI : [-0.709, 2.528]$, $p = 0.133$); and the T-Learner produced an *ATE* of 0.877 ($CI : [0.075, 1.679]$). Overall, even in this less reliable setting of the fertilization dataset, the results suggest that our PU learning approach can effectively recover the true *ATE* in the absence of a known control group.

5 Conclusions

In this work, we proposed, implemented, and evaluated the use of PU learning as a reliable approach for identifying control units from unlabeled data, addressing the challenge of missing confirmed controls. Our experiments demonstrate that, under appropriate configurations—such as avoiding restrictions on effect estimation covariates when training the PU learner—this approach can be effective. Further work should examine the trimming–extrapolation trade-off, explore using $P(T = 1|X)$ to enrich the treated group, apply more advanced PU methods, and test on causal effect benchmarks. Ultimately, we provide a simple, practical, and realistic solution that can unlock a wide range of quasi-experiments in earth, environmental, and agricultural sciences, especially given the growing availability of large-scale earth observation data.

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A Real-World Datasets

For the sowing case, we follow the causal graph construction presented in Tsoumas et al. [19], which guides the selection of relevant variables. In the fertilization case, we model the effect of fertilizer application on biomass production during the final phenological stages, incorporating both decisional and biological confounders. These confounders are selected based on a merged causal graph that combines the canonical fertilization–yield graph from Pearl’s book [12] with a more detailed soil-process causal graph from [16]. Additionally, exogenous organic matter indexes, included as X variables, are retrieved from the literature as features indicative of fertilization activity detectable by Sentinel-2 [3, 4]. As detailed in Table 3, adjustment variables (Z) cover the cultivation period up to 01/05/2023, the treatment variable (T) indicates whether fertilizer was applied at least once between 01/09/2022 and 01/05/2023, and the outcome (Y) corresponds to NDVI-derived trapezoidal area between 01/05/2023 and 30/06/2023, capturing the produced biomass at the end of the season.

B Simulation Datasets

We simulate data under two different structural assumptions. A **linear** setup and a **nonlinear** setup. In both cases, we generate $n = 1000$ samples.

Observed, Unobserved and Latent Variables

$$\begin{aligned} X_1, X_2, X_{11}, X_{22}, X_3, X_4, X_8 &\sim \mathcal{N}(0, 1) \\ U_1, U_2, U_3 &\sim \mathcal{N}(0, 1) \\ X_5 &= 0.6U_1 + 0.6U_2 + \varepsilon_5, \quad \varepsilon_5 \sim \mathcal{N}(0, 0.1^2) \end{aligned}$$

Linear Setup

Treatment Assignment.

$$\text{logit}(P(T = 1)) = 1.2X_1 + 0.8X_2 + 1.4X_{11} + 0.6X_{22} + 0.7X_4 + 1.0U_1 + 1.0U_3$$

$$T \sim \text{Bernoulli}(\sigma(\cdot)), \quad \sigma(z) = \frac{1}{1 + e^{-z}}$$

Mediator.

$$M = 1.5T + 0.7X_8 + 0.5X_2 + 0.3X_{22} + \varepsilon_M, \quad \varepsilon_M \sim \mathcal{N}(0, 0.1^2)$$

Outcome.

$$Y = 2.0M + 0.7X_1 + 0.5X_{11} + 0.6X_3 + 1.0U_2 + 1.0U_3 + \varepsilon_Y, \quad \varepsilon_Y \sim \mathcal{N}(0, 0.1^2)$$

Proxy Variables.

$$\begin{aligned} X_7 &= 1.2M + \varepsilon_{X_7}, \quad \varepsilon_{X_7} \sim \mathcal{N}(0, 0.1^2) \\ X_9 &= 1.0T + 1.0Y + \varepsilon_{X_9}, \quad \varepsilon_{X_9} \sim \mathcal{N}(0, 0.1^2) \end{aligned}$$

Nonlinear Setup

Treatment Assignment.

$$\begin{aligned} \text{logit}(P(T = 1)) &= 1.2 \tanh(X_1) + 0.8 \sin(X_2) + 1.4 \tanh(X_{11}) + 0.6 \sin(X_{22}) \\ &\quad + 0.7 \tanh(X_4) + 1.0U_1 + 0.8U_3X_1 \\ T &\sim \text{Bernoulli}(\sigma(\cdot)) \end{aligned}$$

Mediator.

$$M = 1.5T + 0.7\sqrt{|X_8|} + 0.5 \log(1 + |X_2|) + 0.3X_{22} + 0.1X_2X_8 + \varepsilon_M$$

Outcome.

$$Y = 2.0M^2 + 0.7X_1 + 0.5X_{11} + 0.6 \sin(X_3) + 0.2X_3^2 + 1.0U_2 + 1.0U_3 + \varepsilon_Y$$

Proxy Variables.

$$\begin{aligned} X_7 &= 1.2M + \varepsilon_{X_7} \\ X_9 &= 1.0T + 1.0Y + \varepsilon_{X_9} \end{aligned}$$

In both setups, the variables X_7 and X_9 serve as proxies. X_7 for the mediator M , and X_9 as a collider involving both T and Y .

C Propensity scores

Following the figures for each experimental dataset with an overview of how propensity score overlap varies in the current experimental dataset when using different predictor sets (i.e X , Z) and methods (i.e. SPY, SPY + iSVM). This highlights how the choice of predictor variables and estimation approach affects the positivity assumption and common support.

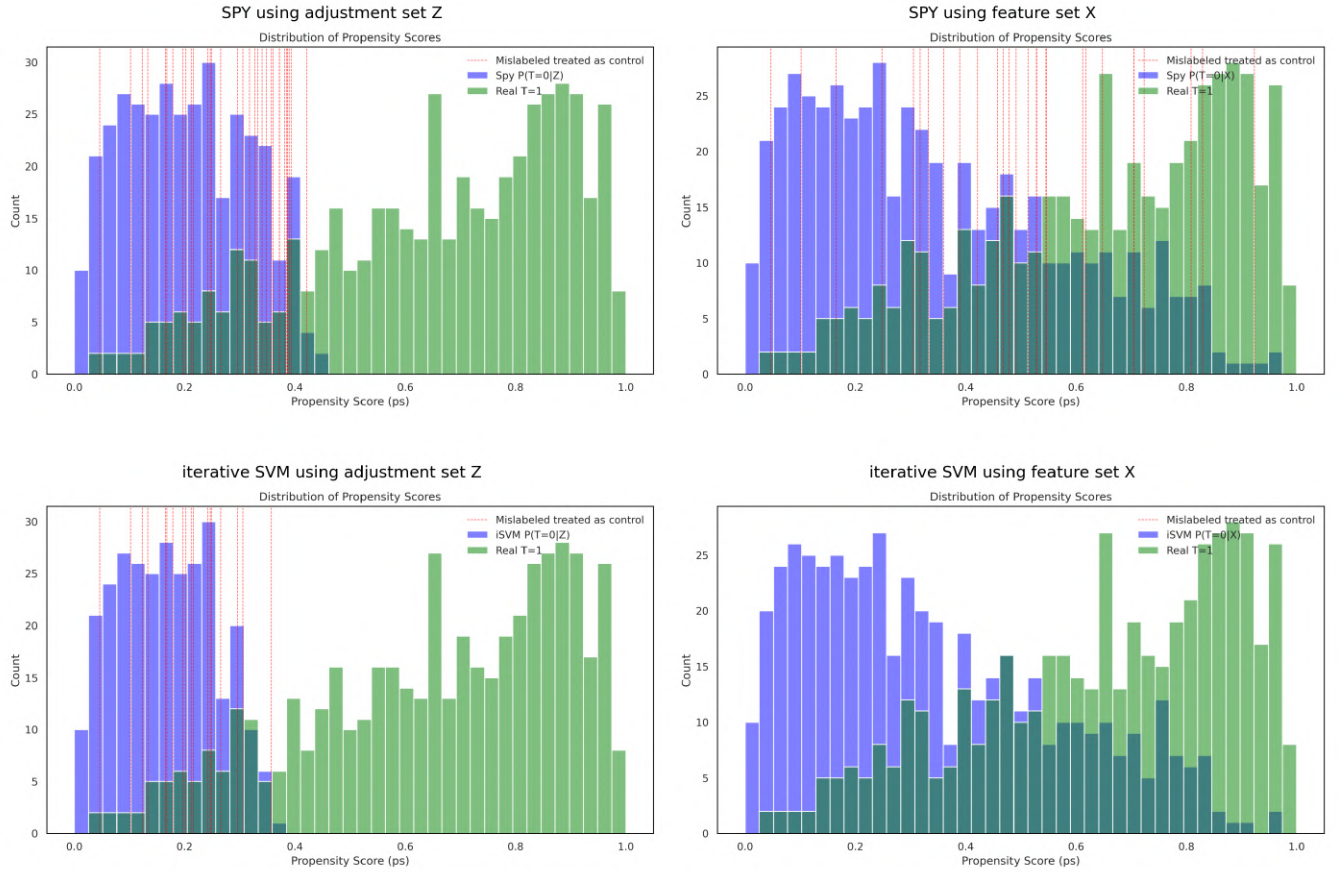


Figure 3: Propensity scores of 4 different combinations on linear experimental dataset

Sowing				Fertilization			
Feature(s) name	Variable/Vertex	Source	Set	Feature(s) name	Variable/Vertex	Source	Set
LOW, HIGH	Weather on sowing date	Nearest weather station	Z	SOC_prediction	Topsoil organic carbon (2022)	NOA ML model	Z
peak_ndvi, trapezoidal_ndvi_sow2harvest	Crop growth	NDVI via Sentinel-2	X	accum_precip_total_m	Accumulated precipitation (2022-09-01 - 2023-05-01)	ERA5-land	Z
ndwi_sowingday	Soil moisture on sowing date	NDWI via Sentinel-2	Z	gdd_base_0	Growing degree days (2022-09-01 - 2023-05-01)	ERA5-land	Z
clay_mean, silt_mean, sand_mean	Topsoil properties	Map by ESDAC	Z	ndmi_trapezoidal_area	Accumulated vegetation moisture content (2022-12-01 - 2023-05-01)	NDMI via Sentinel-2	Z
occont_mean	Topsoil organic carbon	Map by ESDAC	Z	sum_soil_moisture_mean	Soil moisture (2022-09-01 - 2023-05-01)	ERA5-land	Z
var_ST_402, ..., ELPIDA}	Seed variety	Farmers' Cooperative	Z	st_[Cambisols, ..., st_Luvisols]	Soil type	SoilGrids World Reference Base(2006) Soil Groups	Z
ratio	Geometry of field	Farmers' Cooperative	Z	POL_[7807, ..., 10486]	Seed variety	LPIS from NPA	Z
lat, lon, perimeter, field_area	Location & area of field	Farmers' Cooperative	X	eomi_[1-4], nbr2 - stats: max, min, mean, std, skew	Exogenous organic matter indexes	via Sentinel-2	X
hday_sin, hday_cos, len_season	Harvest date & cultivation period	Farmers' Cooperative	X				
prediction	Treatment (sown on recommended or not date)	Farmers' Cooperative, RS	T	TREATMENT	Treatment (apply or not fertilizer)	Fertilizer company	T
yield21	Outcome (Yield)	Farmers' Cooperative	X	ndvi_trapezoidal_area	Outcome (produced biomass proxy for 2023-05-01 - 2023-06-30)	NDVI via Sentinel-2	X

Table 3: Variables used for causal modeling in the sowing and fertilization case studies, categorized by their role (Z: adjustment set, X: features set, T: treatment, Y: outcome) and source.

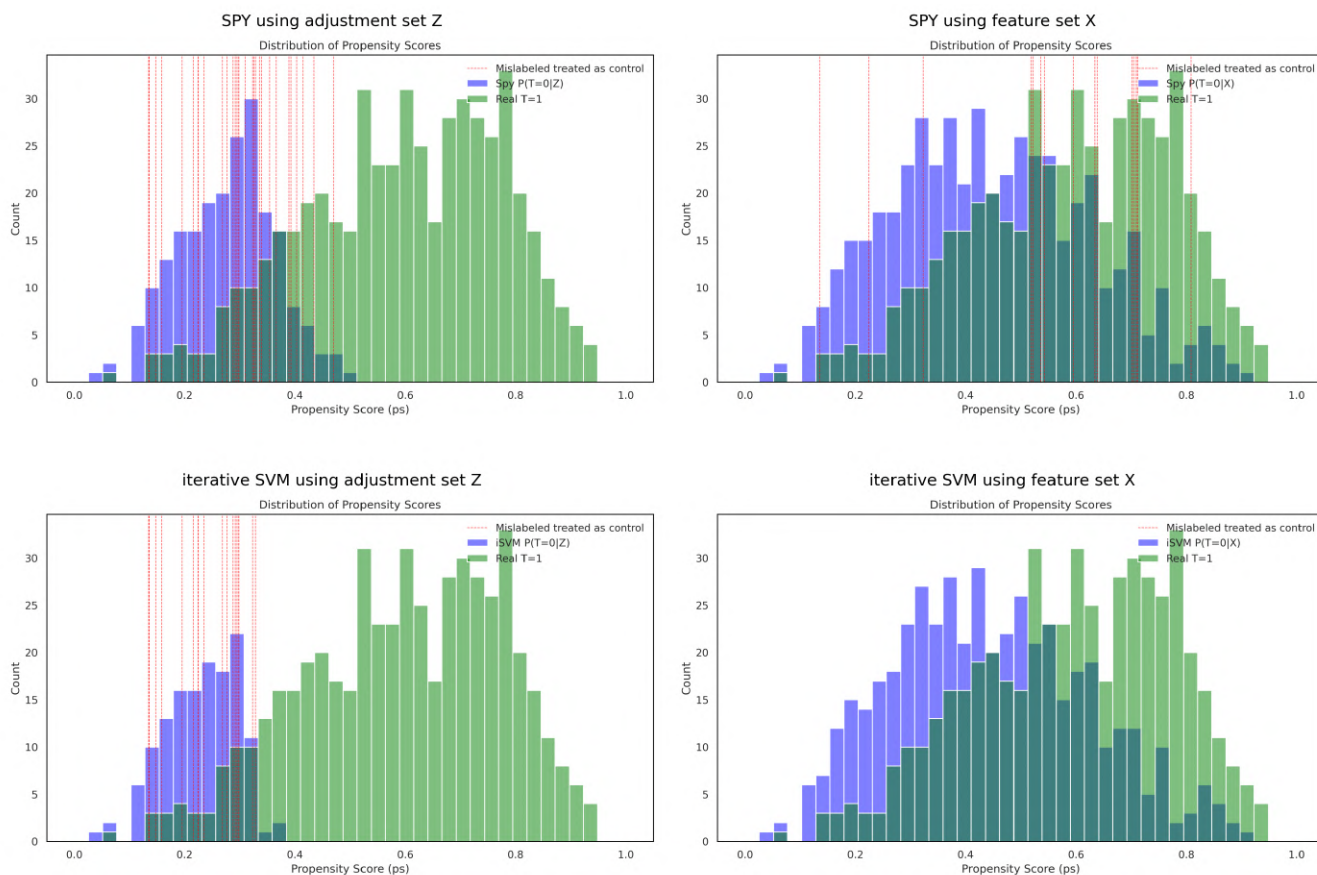


Figure 4: Propensity scores of 4 different combinations on non-linear experimental dataset

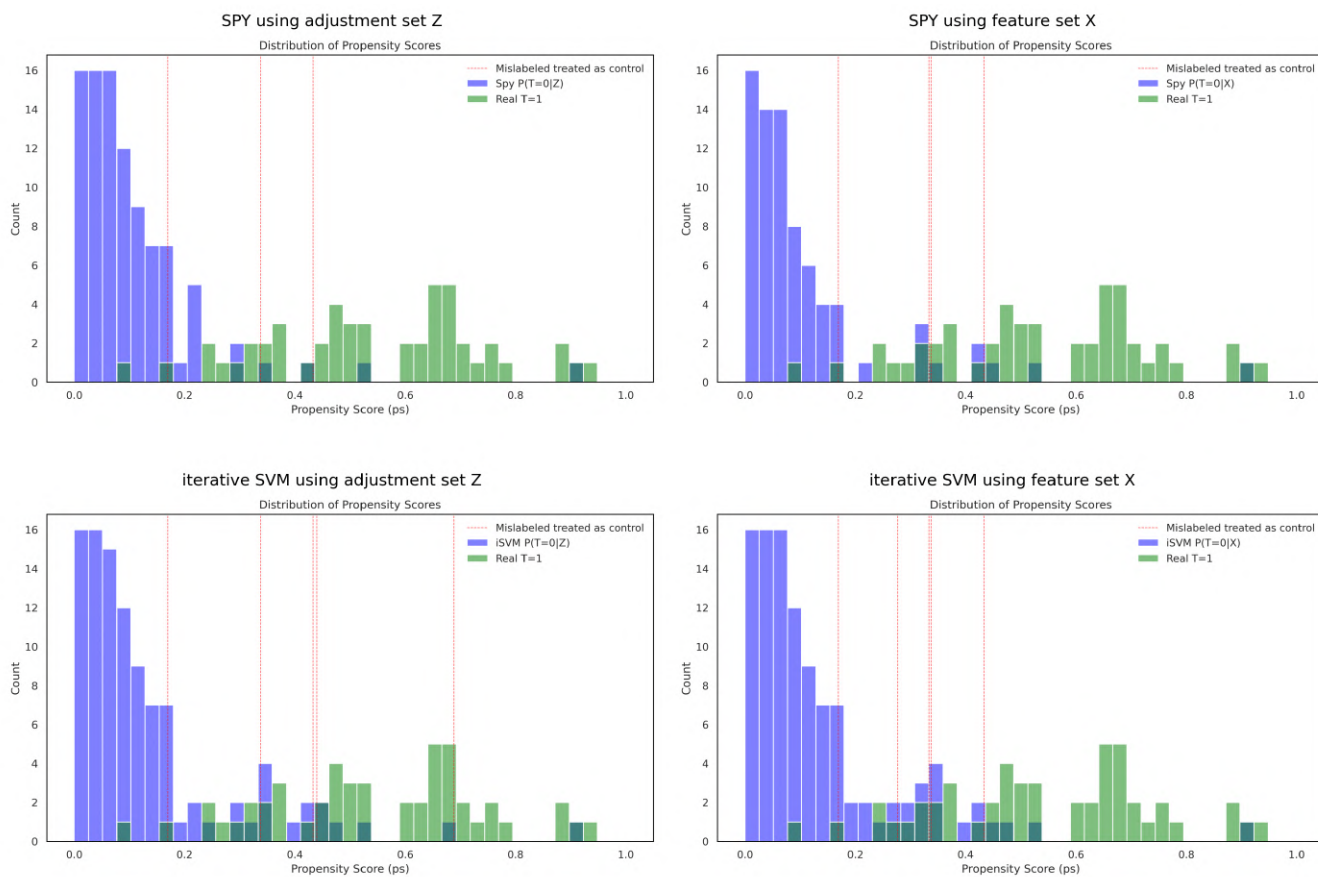


Figure 5: Propensity scores of 4 different combinations on experimental dataset regarding optimal sowing

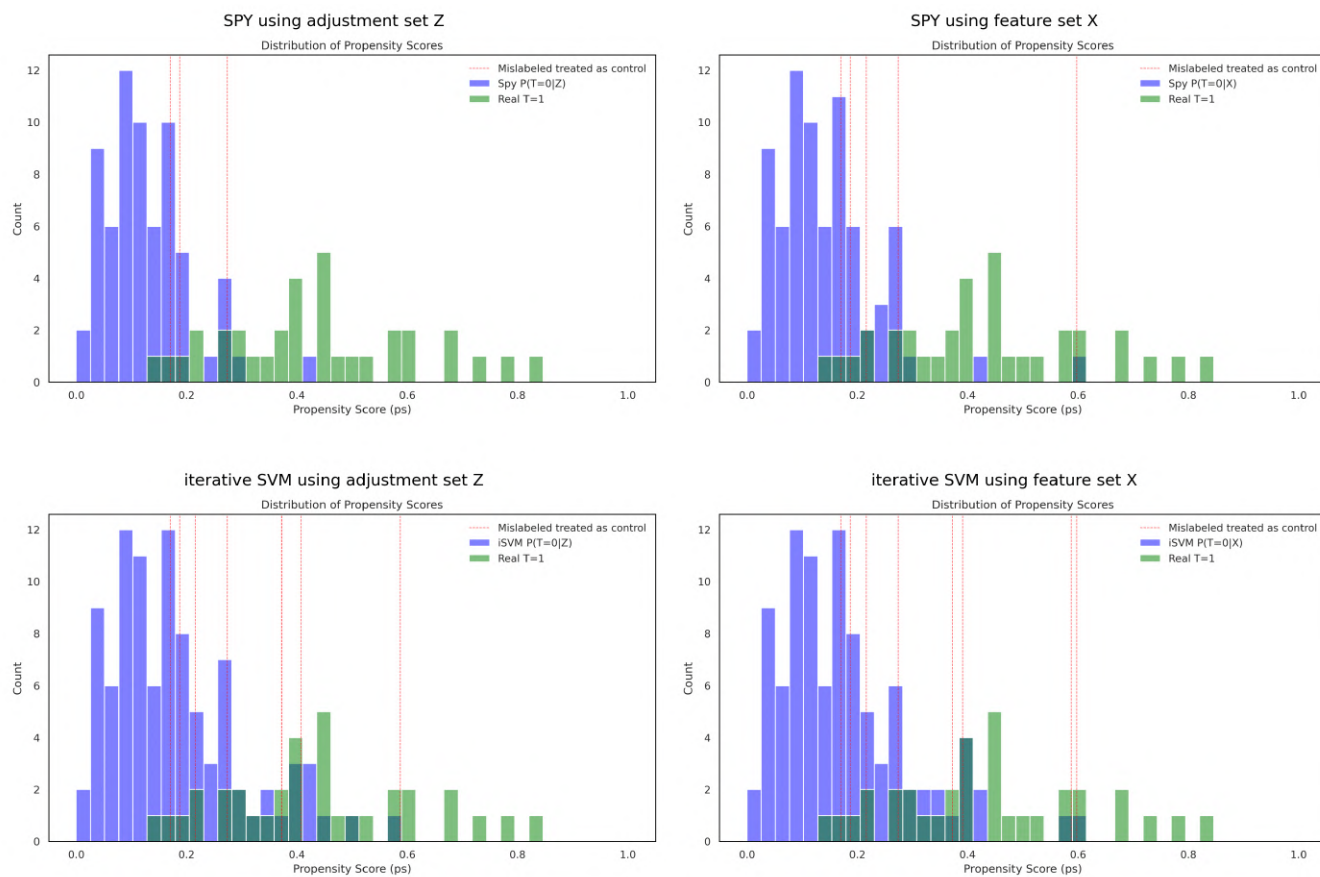


Figure 6: Propensity scores of 4 different combinations on experimental dataset regarding digestate fertilization application

D Interpretability and Model Comparison

To investigate and compare the internal decision mechanisms of two Support Vector Machine (SVM) classifiers, we examine the learned feature coefficients from each model. Both classifiers share a common architecture but differ in the feature sets used for training. We leverage the linear nature of the SVM (with a linear kernel) to extract and interpret feature importance directly from the model coefficients. These coefficients represent the influence of each feature on the decision boundary—positive values contribute toward predicting the positive class (e.g., sowing on a good day), and negative values contribute toward the negative class.

To visually communicate how feature importance shifts between the two models, we use a slope chart. Each line in the chart corresponds to a feature, connecting its normalized coefficient in the model trained on adjustment set Z (left axis) to its corresponding value in the model trained of the superset of it, the feature set X (right axis). Features that are newly introduced in the superset X appear at zero on the left and are highlighted to emphasize their emergence in the decision function. Such comparative interpretability enhances our understanding of how additional information reshapes the model’s decision boundary..

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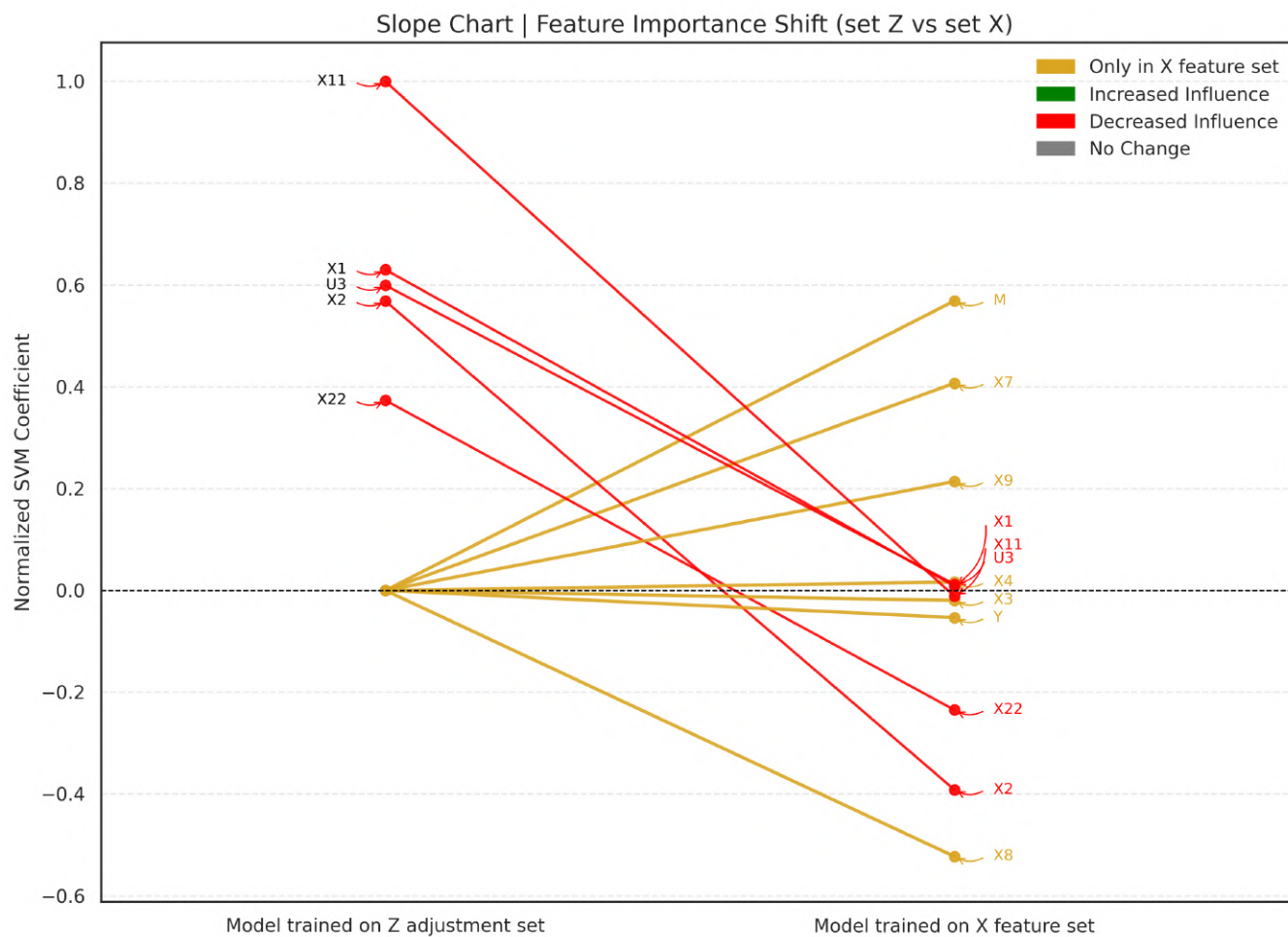


Figure 7: Interpretability and Model Comparison via SVM Coefficient Slope Chart for linear dataset

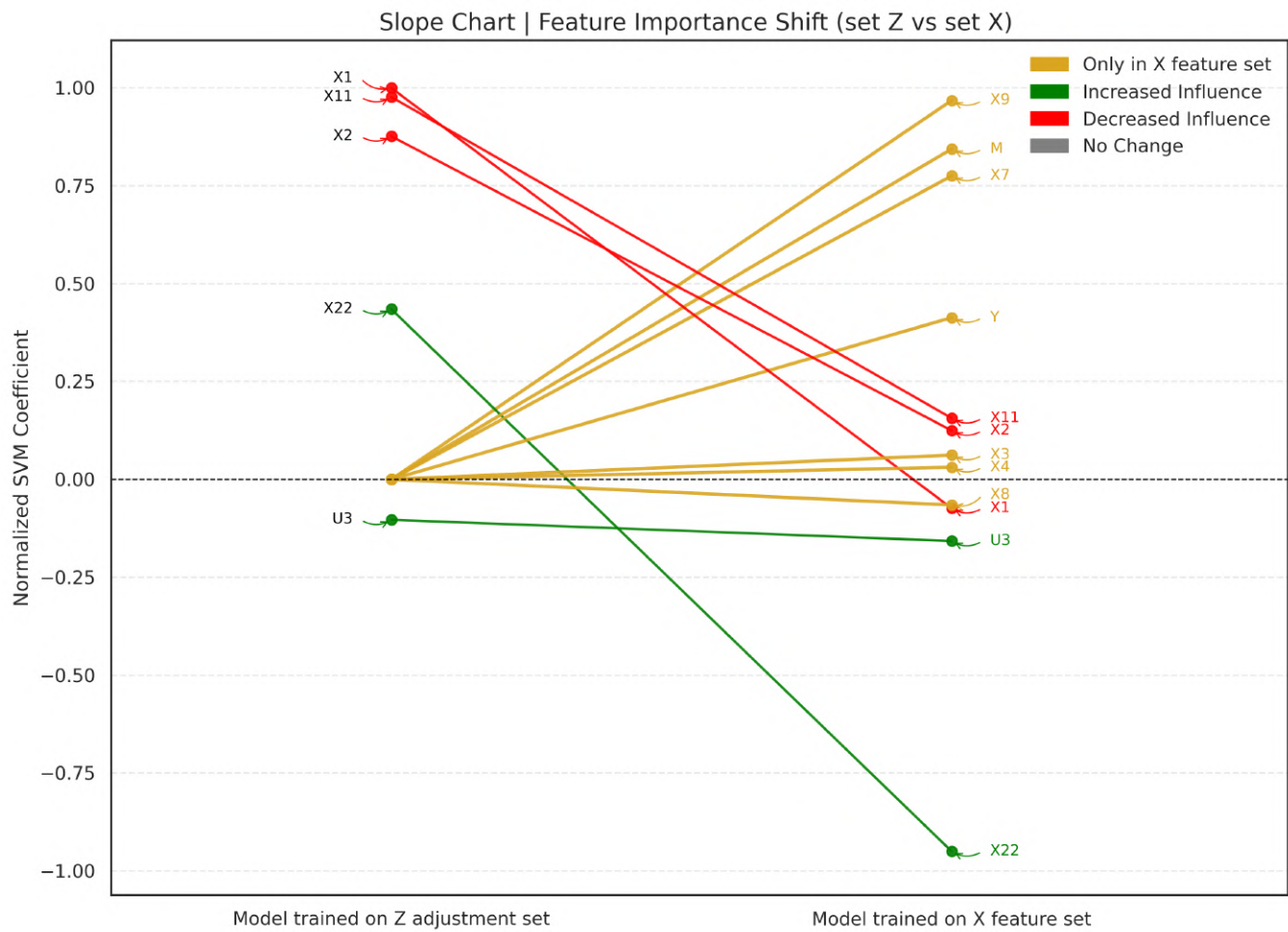


Figure 8: Interpretability and Model Comparison via SVM Coefficient Slope Chart for non-linear dataset

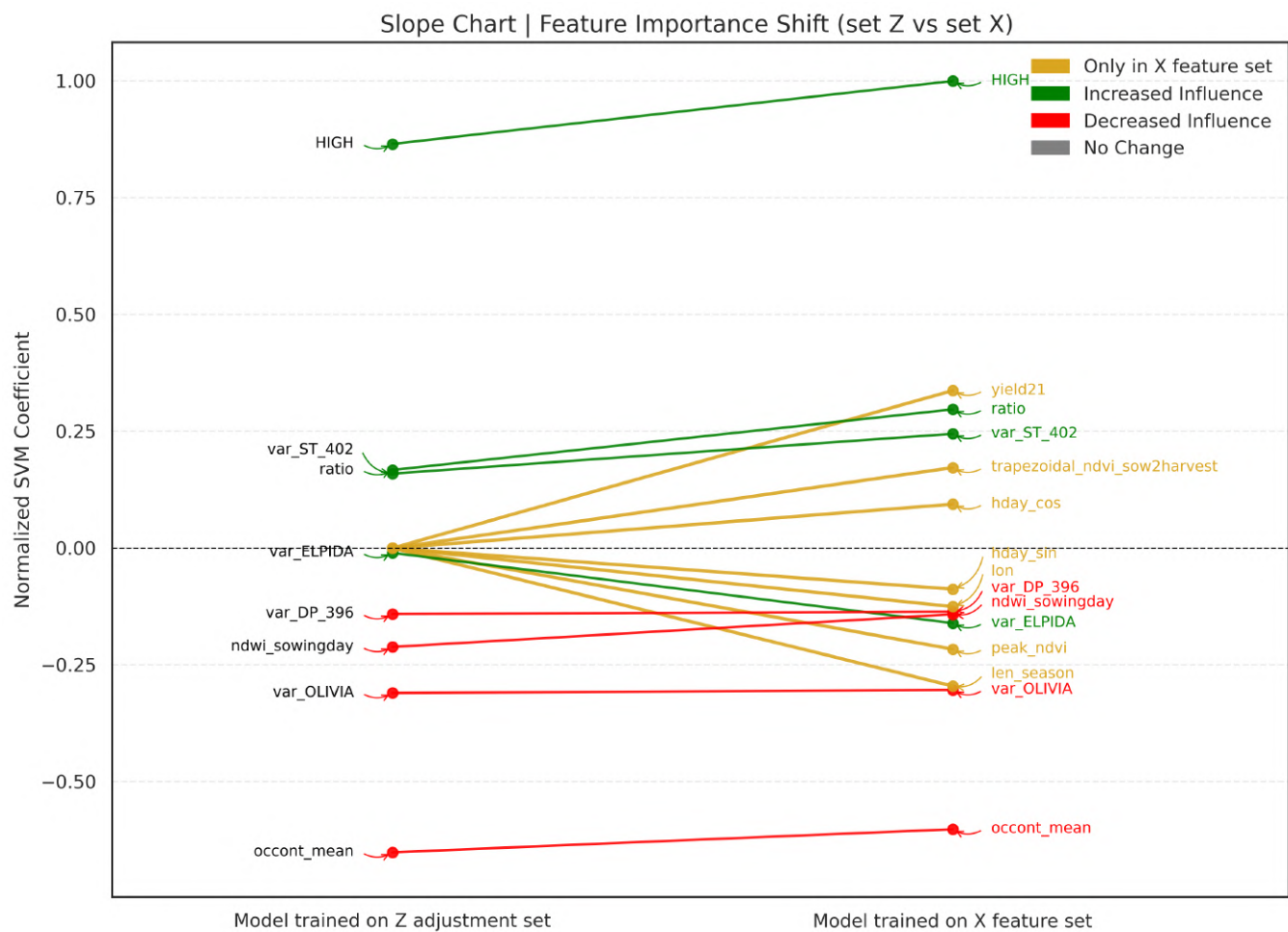


Figure 9: Interpretability and Model Comparison via SVM Coefficient Slope Chart for dataset regarding optimal sowing

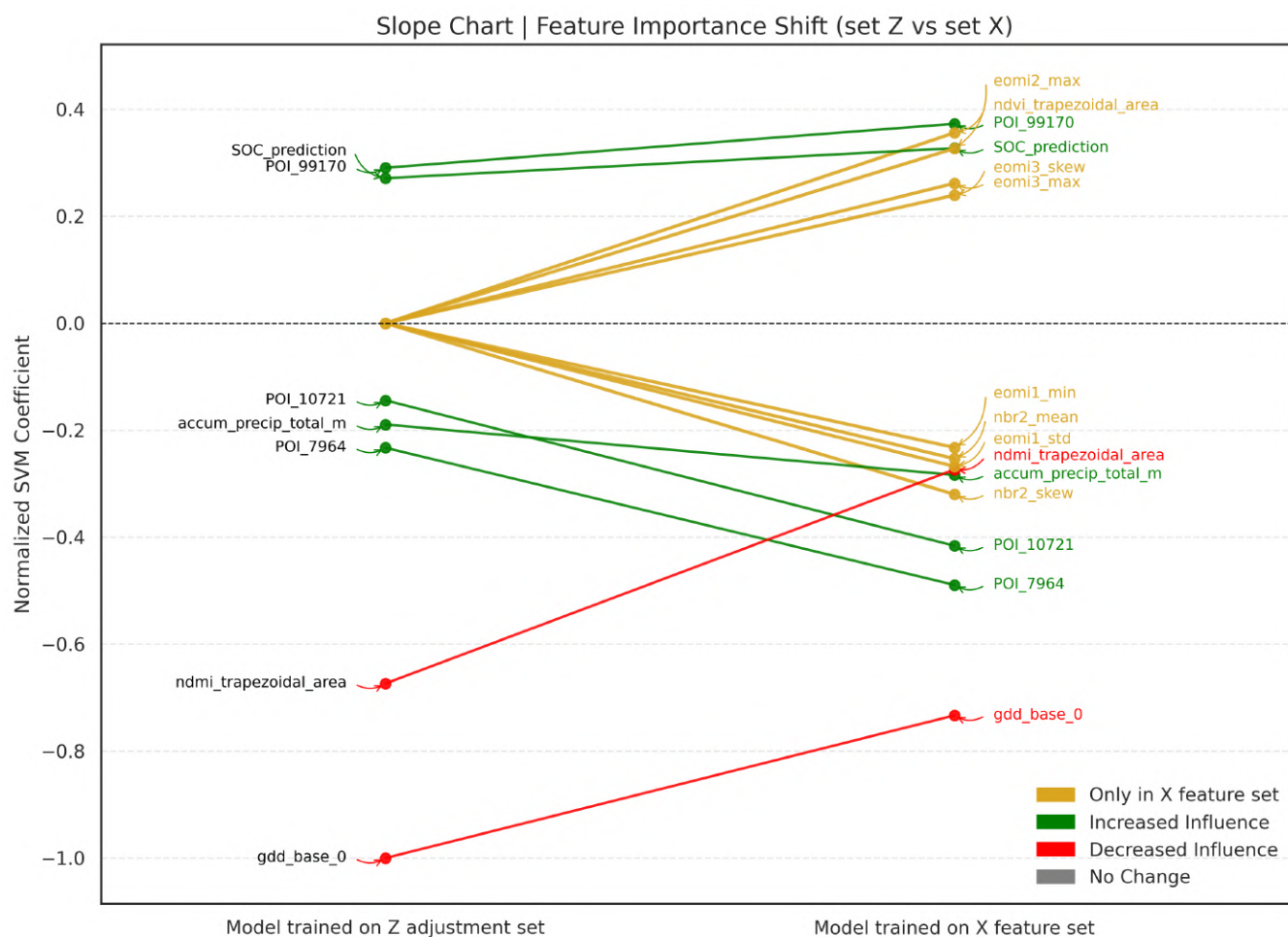


Figure 10: Interpretability and Model Comparison via SVM Coefficient Slope Chart for dataset regarding digestate fertilization application