Almost-Exact Matching with Replacement for Causal Inference

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Abstract

We aim to create the highest possible quality of treatment-control matches for categorical data in the potential outcomes framework. Matching methods are heavily used in the social sciences due to their interpretability, but most matching methods do not pass basic sanity checks: they fail when irrelevant variables are introduced, and tend to be either computationally slow or produce low-quality matches. The method proposed in this work aims to match units on a weighted Hamming distance, taking into account the relative importance of the covariates; the algorithm aims to match units on as many relevant variables as possible. To do this, the algorithm creates a hierarchy of covariate combinations on which to match (similar to downward closure), in the process solving an optimization problem for each unit in order to construct the optimal matches. The algorithm uses a single dynamic program to solve all of the optimization problems simultaneously. Notable advantages of our method over existing matching procedures are its high-quality matches, versatility in handling different data distributions that may have irrelevant variables, and ability to handle missing data by matching on as many available covariates as possible.

1 Introduction

In observational causal inference where the scientist does not control the randomization of individuals into treatment, an ideal approach matches each treatment unit to a control unit with identical covariates. However, in high dimensions, few such “identical twins” exist, since it becomes unlikely that any two units have identical covariates in high dimensions. In that case, how might we construct a match assignment that would lead to accurate estimates of conditional average treatment effects (CATEs)?

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For categorical variables, we might choose a Hamming distance to measure similarity between covariates. Then, the goal is to find control units that are similar to the treatment units on as many covariates as possible. This leads to two challenges, the first being computational (how does one compute optimal matches on Hamming distance?), and the second being that not all covariates are equally relevant, which can impact the Hamming distance.

This second issue, that not all covariates are equally important, has serious implications for CATE estimation. Matching methods generally suffer in the presence of many irrelevant covariates (covariates that are not related to either treatment or outcome): the irrelevant variables would dominate the Hamming distance calculation, so that the treatment units would mainly be matched to the control units on the irrelevant variables. This means that matching methods do not always pass an important sanity check in that irrelevant variables should be irrelevant. As our experiments show, the participation of irrelevant variables can overwhelm many state of the art matching methods, including Propensity Score Matching [13], Nearest Neighbor matching [14], as well as methods not explicitly designed for matching such as Causal Forest.

We propose a method in this work that aims to mitigate the problems listed above. The algorithm uses a hold-out training set to determine which variables are the most important to match on. It then determines matches by optimizing a weighted Hamming distance, where the weights on each variable are determined from the analysis of the hold-out set. Finding a matched group for a given unit then becomes a constrained discrete optimization problem, and we solve all of these optimization problems efficiently with a single dynamic program. This algorithm has the same basic monotonicity property (downwards closure) and structure as that of the Apriori algorithm [1] used in data mining for finding frequent itemsets. However, frequency of itemsets is irrelevant here, instead the goal is to find a largest (weighted) number of covariates that both a treatment and control unit have in common. The algorithm fully optimizes the weighted Hamming distance of each treatment unit to the nearest control unit (and vice versa). It is efficient, owing to the use of database programming and bit-vector computations, and does not require an integer programming solver. The method adaptively chooses subsets of features to consider, based on the other subsets of features that have already been considered. The method is named D-AEMR: Dynamic Almost-Exact Matching with Replacement.

2 Related work

Randomized experiments are a gold standard for causal inference [18]; however, much of the available data for causal inference is observational, where the experimenter does not control the randomization mechanism. Observational datasets can be much larger and easier to obtain than randomized trial data, and matching techniques provide ways to approximate the covariate balance that would have come from a randomized trial.

Exact matching is not possible in high dimensions, as “identical twins” in treatment and control samples are not likely to exist. Early on, this led to techniques that reduce dimension using propensity score matching [15] [14] [16] [5], which extend to penalized regression approaches [19] [11] [4] [6]. Propensity score matching methods project the entire dataset to one dimension and thus cannot be
used for estimating CATE (conditional average treatment effect), since the matched groups often do not agree on important covariates. In “optimal matching,” \[12\], an optimization problem is formed to choose matches according to a pre-defined distance measure, with balance constraints, though as discussed above, this distance measure can be dominated by irrelevant covariates, often leading to poor matched groups and biased estimates of treatment effect. Coarsened exact matching \([9][10]\) has the same problem.

A recent alternative framework is that of almost-exact matching, where each matched group contains units that are close on covariates that are important for predicting outcomes. For example, Coarsened Exact Matching \([9][10]\) is almost-exact, if one were to use an oracle (should one ever become available) that bins covariates according to importance for estimating causal effects. The FLAME algorithm \([3]\) is an almost-exact matching method that adapts the distance metric to the data using machine learning. It starts by matching “identical twins,” and proceeds by eliminating less important covariates one by one, attempting to match individuals on the largest set of covariates available. FLAME has a balance constraint to ensure that it does not remove too many treatment or control units as it eliminates covariates. It uses a hold-out training set to determine importance of covariates. The combination of balance and importance of covariates is called “match quality” (MQ). FLAME can handle datasets too large to fit in memory, and scales well with the number of covariates, but removing covariates in exactly one order (rather than all possible orders as in the present work) means that many high-quality matches will be missed.

\(D\text{-AEMR}'s\) matched groups tend to match on more covariates than FLAME; the distances between matched units in \(D\text{-AEMR}\) are smaller within each matched group, thus its matches are distinctly higher quality. This has implications for missing data, where \(D\text{-AEMR}\) can find matched groups that FLAME cannot.

### 3 Almost-Exact Matching Framework

Consider a dataframe \(D = [X, Y, T]\) where \(X \in \mathbb{R}^{n \times p}\), \(Y \in \mathbb{R}^n\), \(T \in \{0, 1\}^n\) respectively denote the covariates for all units, the outcome vector and the treatment indicator (1 for treated, 0 for control). Unit \(i\)'s \(j\)th covariate \(X\) is denoted \(x_{ij} \in \{0, 1\}\). Notation \(x_i \in \mathbb{R}^p\) indicates covariates for the \(i\)th unit, and \(T(i) \in \{0, 1\}\) is an indicator for whether or not unit \(i\) is treated.

Throughout we make SUTVA and ignorability assumptions \([17]\). The goal is to match treatment and control units on as many relevant covariates as possible. Relevance of covariate \(j\) is denoted by \(w_j \geq 0\) and it is determined using a hold-out training set. Either \(w_j\)'s can be fixed beforehand or adjusted dynamically using a for-loop inside the algorithm.

Assuming that we have a fixed weight \(w_j\) for each covariate \(j\), we would like to find a match for each treatment unit \(t\) that matches at least one control unit on as many relevant covariates as possible. Thus we consider the following matching problem:

**Almost-Exact Matching with Replacement (AEMR):** For each treatment unit \(t\),

\[
\mathbf{v}^* \in \arg\max_{\mathbf{v} \in \{0, 1\}^p} \mathbf{v}^T \mathbf{w} \text{ such that } \exists \ell \text{ with } T(\ell) = 0 \text{ and } x_\ell \circ \mathbf{v} = x_t \circ \mathbf{v},
\]

where \(\circ\) denotes Hadamard product.
The solution to the AEMR problem is an indicator of the optimal set of covariates for treatment unit \( t \)'s matched group. The constraint says that the optimal matched group contains at least one control unit. The solution of the AEMR problem can be the same for multiple treatment units, in which case they would form a single matched group. Formally, we define the matched group for treatment unit \( t \).

**Main Matched Group** corresponding to treatment unit \( t \) contains all units \( \ell \) such that

\[
x_t \odot v^{t*} = x_\ell \odot v^{t*}.
\]

That is, the main matched group contains all treatment and control units that have identical covariate values to \( t \) on the covariates for which \( v^{t*} \) is 1.

The formulation of the AEMR and main matched group formulation is symmetric for control units.

### 3.1 Straightforward AEMR solutions do not suffice

There are two straightforward (but inefficient) approaches to solving the AEMR problem for all units.

**AEMR Solution 1 (quadratic in \( n \), linear in \( p \)):** Brute force pairwise comparison of treatment points to control points. For all treatment units \( t \), we (i) iterate over all control units \( c \), (ii) find the vector \( v_{tc} \in \{0, 1\}^p \) with value 1 if there is a match on the values of the corresponding covariates, and 0 otherwise, (iii) find the control unit(s) with the highest value of \( v_{tc}^T w \), and (iv) return them as the main matched group for the treatment unit \( t \) (and compute the auxiliary group). Whenever a previously matched unit \( \alpha \) is matched to a previously unmatched unit \( \eta \), record the \( \eta \)'s main matched group as an auxiliary group for the previously matched unit \( \alpha \). When all units are ‘done’ (all units are either matched already or cannot be matched) then stop, and compute the CATE for each treatment and control unit using its main matched group. If a unit belongs to auxiliary matched groups then its outcome is used for computing both its own CATE (in its own main matched group) and the CATEs of units for whom it is in an auxiliary group (e.g., \( \alpha \) will be used to compute \( \eta \)'s estimated CATE). This algorithm is polynomial in both \( n \) and \( p \), however, the quadratic time complexity in \( n \) also makes this approach impractical for large datasets (for instance, when we have more than a million units with half being treatment units).

**AEMR Solution 2 (order \( n \log n \), exponential in \( p \))**: Brute force iteration over all \( 2^p \) subsets of the \( p \) covariates. This approach solves the AEMR problem simultaneously for all treatment and control units for a fixed weight vector \( w \). First, (i) enumerate every \( v \in \{0, 1\}^p \) (which serves as an indicator for a subset of covariates), (ii) order the \( v \)'s according to \( v^T w \), (iii) form all valid main matched groups having at least one treated and one control unit (iv) the first time each unit is matched, mark that unit with a ‘done’ flag, and record its corresponding main matched group and, to facilitate matching with replacement, (v) whenever a previously matched unit is matched to a previously unmatched unit, record this main matched group as an auxiliary group. When all units are ‘done’ (all units are either matched already or cannot be matched) then stop, and compute the CATE for each treatment and control unit using its main matched group. Each unit’s outcome will be used to estimate CATEs for every auxiliary group that it is a member of, as before. Although this approach exploits the efficient ‘group by’ function (e.g., provided in database (SQL) queries), which can be implemented in \( O(n \log n) \) time by sorting the units, iterating over all possible vectors \( v \in \{0, 1\}^p \) makes this approach unsuitable for practical purposes (exponential in \( p \)).
3.2 Key to D–AEMR: Downward closure will help solve AEMR more efficiently

If \( n \) is in the millions, the first solution, or any simple variation of it, is practically infeasible. A straightforward implementation of the second solution is also inefficient. However, a monotonicity property (downward closure) stated below will allow us to prune the search space so that the second solution can be modified to be completely practical, as we will demonstrate in the D–AEMR algorithm in the next section, which does not enumerate all \( v \)'s, it uses the monotonicity to reduce the number of \( v \)'s it considers.

**Proposition 3.1.** (Monotonicity of \( v^* \) in AEMR solutions) Fix treatment unit \( t \). Consider feasible \( v \), meaning \( \exists \ell \) with \( T(\ell) = 0 \) and \( x_\ell \circ v = x_t \circ v \). Then,

- Any feasible \( v' \) such that \( v' < v \) elementwise will have \( v'^T w \leq v^T w \).
- Consequently, consider feasible vectors \( v \) and \( v' \). Define \( \tilde{v} \) as the elementwise \( \min(v, v') \). Then \( \tilde{v}^T w < v^T w \), and \( \tilde{v}^T w < v'^T w \).

These follow from the fact that the elements of \( v \) are binary and the elements of \( w \) are non-negative. The first property means that if we have found a feasible \( v \), we need not consider any \( v' \) with fewer 1’s as a possible solution of the AEMR for unit \( t \). Thus, D–AEMR starts from \( v \) being all 1’s (consider all covariates). It systematically drops one element of \( v \) to zero at a time, then two, then three, ordered according to values of \( v^T w \). The second property implies that we must evaluate both \( v \) and \( v' \) as possible AEMR solutions before evaluating \( \tilde{v} \). Conversely, a new subset of variables defined by \( \tilde{v} \) cannot be considered unless all of its supersets have been considered.

These two properties form the basis of the D–AEMR algorithm.

4 The Dynamic AEMR (D–AEMR) Algorithm

AEMR has two computations: the weights and the actual matching mechanism. The weights correspond to the importance of the covariates and are computed by running regression on a hold-out training set prior to running the algorithm, or are computed adaptively as the algorithm executes (the computation of the weights is discussed in the supplement). The matching mechanism is designed to solve the AEMR.

We call a covariate-set any set of covariates. We denote by \( J \) the original set of all covariates from the input dataset, where \( p = |J| \). When we drop a set of covariates \( s \), it means we will match on \( J \setminus s \). For any covariate-set \( s \), we associate an indicator-vector \( v_s \in \{0, 1\}^p \) defined as follows:

\[
v_{s,i} = 1_{\{i \in s\}} \quad \forall \, i \in \{1, \ldots, p\}
\]

i.e. the value is 1 if the covariate is not in \( s \) implying that it is being used for matching.
Algorithm 2 gives the pseudocode of the D-AEMR algorithm. Instead of looping over all possible $2^p$ vectors to solve the AEMR, it considers a covariate-set $s$ for dropping only if satisfies the monotonicity property of Proposition 3.1. For example, if $\{1\}$ has been considered for dropping to form matched groups, it would not process $\{1, 2, 3\}$ next because the monotonicity property requires $\{1, 2\}$, $\{1, 3\}$ and $\{2, 3\}$ to have been considered previously for dropping.

The D-AEMR algorithm uses the GroupedMR (Grouped Matching with Replacement) subroutine given in Algorithm 1 to form all valid main matched groups having at least one treated and one control unit. GroupedMR takes a given subset of covariates and finds all subsets of treatment and control units that have identical values of those covariates. We use an efficient implementation of the group-by operation used in the algorithm using bit-vectors, which is discussed in the supplement.

To keep track of main and auxiliary matched groups, GroupedMR takes the entire set of units $D$ as well as the set of unmatched units from the previous iteration $D_{(i-1)}$ as input along with the covariate-set $J \setminus s^*_i$, to match on in this iteration. Instead of matching only the unmatched units in $D_{(i-1)}$ using the group-by operator, it matches all units in $D$ to allow for matching with replacement as in the AEMR objective. It keeps track of the main matched groups for the unmatched units $D_{(i-1)}$ that are matched for the first time, and auxiliary groups (see previous section) for the other matched units.

**Algorithm 1: Procedure GroupedMR**

Input : Unmatched data $D_{um} = (X,Y,T)$, subset of indexes of covariates $J^s \subseteq \{1, ..., p\}$.
Output : Newly matched units $D_m$ using covariates indexed by $J^s$ where groups have at least one treatment and one control unit, the remaining data as $D_{um} \setminus D_m$ and the matched groups

- $M_{raw} =$ group-by ($D_{um}, J^s$) (form groups by exact matching on $J^s$)
- $M =$ prune($M_{raw}$) (remove groups without at least one treatment and control unit)
- $D_m =$ Get subset of $D_{um}$ where the covariates match with $M$ (recover newly matched units)

return $\{D_m, D_{um} \setminus D_m, M\}$. (matched units, unmatched units, and matched groups)

D-AEMR keeps track of two sets of covariate-sets: (1) The set of **processed sets** $\Delta$ contains the covariate-sets whose main matched groups (if any exist) have already been formed. That is, $\Delta$ contains $s$ if matches have been constructed on $J \setminus s$ by calling the GroupedMR procedure. (2) The set of **active sets** $\Lambda$ contains the covariate-sets $s$ that are eligible to be dropped according to Proposition 3.1. For any iteration $i$, $\Lambda(i) \cap \Delta(i) = \emptyset$, i.e., the sets are disjoint, where $\Lambda(i), \Delta(i)$ denote the states of $\Lambda, \Delta$ at the end of iteration $i$. Due to the monotonicity property Proposition 3.1 if $s \in \Lambda(i)$, then each proper subset $r \subset s$ belonged to $\Lambda(j)$ in an earlier iteration $j < i$. Once an active set $s \in \Lambda(i-1)$ is chosen as the optimal subset to drop $s^*_i$ in iteration $i$, $s$ is excluded from $\Lambda(i)$ (it is no longer active) and is included in $\Delta(i)$ as a processed set. In that sense, the active sets are generated and included in $\Lambda(i)$ in a hierarchical manner similar to the apriori algorithm. A set $s$ is included in $\Lambda(i)$ only if all of its proper subsets of one less size $r \subset s$, $|r| = |s| - 1$, have been processed.

Figure 1 shows an example of the earlier steps of the D-AEMR algorithm.
Figure 1: Example of the first few steps of D-AEMR. The red number in an oval is a count of how many times the covariate in the left of the same oval has been within a dropped set of the size indicated on the left of the oval's row. **Step1**: Find the optimal set to drop from the set of active sets and form the matched groups. **Step2**: Add the dropped set to the corresponding set of processed sets. **Step3**: If new sets become active, add them to the set of active sets. Otherwise, return to Step1. Repeat until no more active sets or units to match.

**Algorithm 2**: The D-AEMR algorithm

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Theorem 4.1. (Correctness) The algorithm D-AEMR solves the AEMR problem.
5 Simulations

We present results under a variety of data generating processes. We show that D−AEMR produces higher quality matches than popular matching methods such as 1-PNNSM and Nearest Neighbor matching with Mahalanobis distance, and can produce better treatment effect estimates than black box machine learning methods such as Causal Forest (which is not a matching method, and is not interpretable). The ‘MatchIt’ R-package ([8]) was used to perform 1-Propensity Score Nearest Neighbor matching (1-PSNNM) and Nearest Neighbor with Mahalanobis distance (Mahalanobis). For Causal Forest, we used the ‘grf’ R-package ([2]). D−AEMR also improves over the original FLAME [3] with regards to the quality of matches in high dimensions. Other matching methods (optmatch, cardinality match) do not scale to large problems and thus needed to be omitted. We use "FLAME" to represent original FLAME algorithm. Throughout this section, the outcome is generated with

$$y = \sum_i \alpha_i x_i + T \sum_i \beta_i x_i + T \cdot U \sum_{i, i'>i} x_i x_{i'}$$

where $T \in \{0, 1\}$ is the binary treatment indicator. We vary the distribution of the covariates, coefficients ($\alpha$'s, $\beta$'s, and $U$), as well as the fraction of treated units.

5.1 Presence of irrelevant covariates

A basic sanity check for matching algorithms is how sensitive to irrelevant covariates they are. To that end, we run experiments with a majority of the covariates being irrelevant to the outcome. This simulation generates 15000 control units, 15000 treatment units, 5 important covariates and 10 irrelevant covariates. For important covariates $1 \leq i \leq 5$ let $\alpha_i \sim N(10s, 1)$ with $s \sim \text{Uniform}\{-1, 1\}$, $\beta_i \sim N(1.5, 0.15)$, $x_i \sim \text{Bernoulli}(0.5)$. For unimportant covariates $5 < i \leq 15$, $x_i \sim \text{Bernoulli}(0.1)$ in the control group and $x_i \sim \text{Bernoulli}(0.9)$ in the treatment group.

Figure 2: D−AEMR perfectly estimates the CATTs when stopped early i.e. before dropping important covariates. D−AEMR and FLAME find all the good matches early on and should not be run all the way to the end. If run to the end, poor matches are introduced. All the other methods are sensitive to irrelevant covariates and give poor estimates.
Results: As Figure 2 shows, D-AEMR and FLAME achieve the optimal result before dropping any important covariates. They respectively match 79% and 95% of units on all important covariates. When imposing that the FLAME algorithms find all the possible matches even if important covariates are dropped (not recommended), poor matches are introduced. However, their worst case scenario is still substantially better than the comparative methods, all of which perform poorly in presence of irrelevant covariates. Causal Forest is especially ill suited for this case.

5.2 Exponentially decaying covariate importance

A notable advantage of D-AEMR over FLAME is that it should produce more high quality matches before resorting to lower quality matches. To test that theory, in this experiment we consider covariates of decaying importance (letting the $\alpha$ parameters decrease exponentially, $\alpha_i = 64 \times \left(\frac{1}{2}\right)^i$). We evaluate the performance of the algorithms when $\approx 30\%$, $50\%$ and $60\%$ of the units are matched.

Results: As Figure 3 shows, in all instances (each threshold in each column) D-AEMR matches on more covariates, yielding better estimates than FLAME.

![Figure 3](image)

Figure 3: D-AEMR makes higher quality matches early on. Furthermore, on all thresholds (each column), D-AEMR consistently matches on more covariates than FLAME and minimizes the Hamming distance between matched units.

5.3 Imbalanced Data

Imbalance is a common situation in observational studies: there are often substantially more control than treatment units. The data considered in this experiment has covariates with decreasing
importance and does not include unimportant covariates. A fixed batch of 2000 treatment units was generated as well as a batch of 40000 control units. We sample from the batch of controls to construct different imbalance ratios: 40000 in the most imbalanced case (ratio1), then 20000 (ratio2) and, finally, 10000 (ratio3). This experiment was run reusing control units to amplify the high dimensional matching of D−AEMR and to find the best possible match for each treatment unit. 

Results: A check reveals that FLAME and D−AEMR outperform the neareast neighbor matching methods, which produce poor estimates regardless of the degree of imbalance. A second check highlights that D−AEMR is distinctively better than FLAME when the data are imbalanced. D−AEMR yields better results when the data is extremely imbalanced. Additionally, D−AEMR has an average of 4 covariates not matched on, with ≈ 84% of units matched on all but 2 covariates. On the other hand, FLAME averages 7 covariates not matched on and only ≈ 25% units matched on all but 2 covariates.

Figure 4: (1) Estimated CATT vs True CATT from less imbalance (bottom) to more imbalance (top). In all cases, D−AEMR outperforms 1-PSNNM and Mahalanobis, which produce poor quality estimates. (2) D−AEMR estimation quality increases with the imbalance. The best results are produced when the data is extremely imbalanced. Within each ratio of the imbalance, D−AEMR outperforms FLAME.
Figure 5: For all the different imbalance ratios, D-AEMR consistently matches on more covariates than FLAME.

5.4 Running Time Evaluation

In this section, we compare the running time of our dynamic approach to solving the AEMR problem with a brute force solution (AEMR solution 1 described in Section 3). We also compare with FLAME which does not solve the AEMR problem. All experiments were run on a MacBook Pro with Intel Core i5 Processor (Cores: 2, Speed: 2.4 GHz), 8 GB RAM. 

Results: As shown in Figure 6, FLAME provides the best running time performance because it utilizes a bit vector implementation and incrementally reduces the number of covariates. D-AEMR resets the pool of covariate sets to consider at each round of the algorithm, which takes more time. However, as shown in the previous simulations, D-AEMR produces high quality matches that the other methods do not. Our proposed method substantially reduces the running time to solve the AEMR as compared to brute force. The running time for D-AEMR can be further optimized through simple parallelization of the checking of active sets. Additional results are available in Section E in the supplement.

Figure 6: Runtime comparison
5.5 Effect of Noise

In Section D of the supplement, we study how D-AEMR performs in the presence of noise. We show that D-AEMR outperforms Causal Forest on all noise levels constructed. While Causal Forest with small amount of noise (low noise coefficient and low noise variance) performs better than Causal Forest without noise, it still produces worse estimates than D-AEMR. The relative ordering of the methods remains unchanged.

5.6 Missing Data

We consider the case when data are missing at random. We compared performance of FLAME and D-AEMR both with and without multiple imputation.

To generate covariates $X$ we first sample $Z \sim N_p(\mu, \Sigma)$, where $\Sigma$ is not the identity matrix (provided in the supplement) and then let $X_j = f_j(Z_j)$ where $f_j(z) = 1_{z>0}$. This creates correlated binary variables so methods that impute the missing values are expected to perform well. We generate 15000 control and 5000 treated units; 20% of the data are missing at random.

To allow for missing values in D-AEMR and FLAME we construct an $n \times p$ matrix $O$ where $o_{ij} = 1$ if covariate $j$ is unobserved for unit $i$. Treating “missing” as just another category for each variable we proceed with the algorithm by adding a condition for a matched group to be valid: if covariates $J' = \{j_1, \ldots, j_{p'}\}$ are being matched on then $\sum_{j \in J'} o_{ij} = 0$ for a unit $i$ in the group. If the sum is greater than 0 then the group matched on the level “missing” for at least one covariate, making it invalid. We compare this approach to multiply imputing 10 datasets using the Multiple Imputation Chained Equations algorithm in the `mice` R package and averaging the estimates over the datasets. The correlation matrix $\Sigma$ that defines the relationship among the covariates $X$ is given in Figure 7.

![Correlation Matrix of 20% Missing Data](image)

Figure 7: Correlation matrix that defines the relationship among the covariates $X$.

We generate a dataset with 20% missing values, and Figures 9 and 8 contain the results with and without imputation. D-AEMR outperforms FLAME in terms of CATE estimation. D-AEMR with imputation yields a MSE of 1.11 vs. MSE without imputation of 5.08 compared to FLAME which has 2.77 (MSE with imputation) vs. 195.63 (MSE without imputation). This suggests that for datasets that are too large to undergo multiple imputation, D-AEMR still produces reasonable causal estimates. The result is more interpretable when there is no imputation, because it matches only on covariates that the observation actually possesses rather than imputed covariates.
6 Breaking the cycle of drugs and crime in the United States

Breaking The Cycle (BTC) \cite{7} is a social program conducted in several U.S. states designed to reduce criminal involvement and substance abuse, and improve health and employment among current offenders. A survey \cite{7} was conducted in Alabama, Florida, and Washington regarding the program’s effectiveness, with high quality data for over 380 individuals. These data (and this type of data generally) can be a powerful tool in the war against opioids, and our ability to draw interpretable, trustworthy conclusions from it depends on our ability to construct high-quality matches. For the survey, participants were chosen to receive screening shortly after arrest and participate in a drug intervention under supervision. Similar defendants before the start of the BTC program were selected as the control group. Covariates used for matching are detailed in Table \ref{table:covariates}.

6.1 Covariate Importance

The features used for the BTC data are listed in Table \ref{table:covariates}. Each feature has a variable importance score associated with it, the ratio of the loss of a ridge regression model trained with and without randomly permuting that feature. To obtain the values within the table, we randomly shuffled the values of that feature 100 times, retraining ridge regression, and each time compared with the unshuffled loss of ridge regression:

\[
\text{average}\left(\frac{\hat{\text{loss}}_{\text{removing } i}}{\text{loss}}\right).
\]
In Table 1, the mean variable importance values are reported. These calculations were performed on a holdout training set, not on the test data. As Table 1 shows, all covariates have similar values of the importance score, which suggests that all covariates are almost equally important.

| Covariate                                      | Importance Score |
|------------------------------------------------|------------------|
| Live with anyone with an alcohol problem       | 0.958458         |
| Have trouble understanding in life             | 0.983272         |
| Live with anyone using nonprescribed drugs     | 0.984558         |
| Have problem getting along with father in life | 0.989829         |
| Have a automobile                              | 0.990346         |
| Have driver license                            | 0.990732         |
| Have serious depression or anxiety in past 30 days | 0.992095       |
| Have serious anxiety in life                   | 0.994400         |
| SSI benefit Last 6 Months                      | 1.001295         |
| Have serious depression in life                | 1.003302         |

Table 1: Features for BTC data, and importance score of each feature, learned from a holdout training set.

6.2 Order of Dropping Covariates
The order in which D−AEMR and FLAME process covariates is different. Table 2 shows the order in which the covariates were processed for both algorithms. We used the formulations of FLAME and D−AEMR where variable importance is recomputed for only the variables we are considering at that iteration, since variable importance values change in the absence of various covariates. Covariates in FLAME are not eliminated on variable importance alone, there is a balancing factor that prefers not to eliminate too many units from either treated or control at once. Because D−AEMR eliminates one variable at a time, it tends to process the least relevant covariate in the earlier rounds. For example, at the first round, both algorithms drop the covariate “Live with anyone with an alcohol problem” which has the lowest importance score in Table 1. At the second round, D−AEMR process the covariate “Have trouble understanding in life” because this covariate has the lowest importance score aside from “Live with anyone with an alcohol problem.” On the other hand, at that same second round, FLAME processes “Have serious anxiety in life” which now is dropped along with “Live with anyone with an alcohol problem.” Once “Live with anyone with an alcohol problem” was removed, “Have serious anxiety in life” has a lower importance score than “Have trouble understanding in life,” which is why it was dropped.

6.3 Analysis of the matches
We compare the quality of matches between FLAME and D−AEMR in terms of the number of covariates used to match within the groups. Many of the units matched exactly on all covariates and thus were matched by both algorithms at the first round. For the remaining units, D−AEMR matches
| Order | FLAME                                      | D−AEMR                                      |
|-------|-------------------------------------------|---------------------------------------------|
| 1st   | Live with anyone with an alcohol problem  | Live with anyone with an alcohol problem    |
| 2nd   | Have serious anxiety in life              | Have trouble understanding in life          |
| 3rd   | Live with anyone using nonprescribed drugs| Have serious depression or anxiety in past 30 days |
| 4th   | Have trouble understanding in life        | Live with anyone using nonprescribed drugs  |
| 5th   | Have problem getting along with father in life | Have serious anxiety in life                |
| 6th   | Have serious depression in life           | Have driver license                         |
| 7th   | Have driver license                       | Have problem getting along with father in life |
| 8th   | Have a automobile                         | Have serious anxiety in life                |
| 9th   | Have serious depression or anxiety in past 30 days | Have a automobile                          |

Table 2: Order in which features were processed for FLAME and D−AEMR.

on more covariates than FLAME. Figure 10 shows the results. In particular, D−AEMR matched many more units on 9 variables, whereas FLAME matched more units on only one variable.

![Figure 10: Number Matched: Number of units matched per covariates for the BTC data](image-url)
6.4 Comparison of D-AEMR with SVM based method Minimax Surrogate Loss

We wanted to use D-AEMR as a tool to double check performance of a black box machine learning approach. There is no ground truth, so there will not be formal accuracy evaluation (see simulations for accuracy comparison). We chose a recent method that predicts whether treatment effects are positive, negative, or neutral, using a support vector machine formulation [20]. We ran D-AEMR on the BTC dataset and saved the CATE for each treatment and control unit that were matched. Units with a positive CATE have a negative treatment effect and vice versa. We also implemented the SVM approach and recorded a prediction of positive, negative, or neutral treatment effect for each unit. Figure 11 in the main manuscript shows that D-AEMR and the SVM approach agree on most of the matched units.

Figure 11: Matched Units Analysis: CATE estimates for the BTC dataset. The colors represents the labels from the SVM method.

To see this, the units for which D-AEMR predicted approximately zero treatment effect all have a “neutral” treatment effect label from the SVM approach. Most positive CATE’s corresponded to negative treatment effects from the SVM. Only one matched group seems to have a different prediction than the SVM: a negative CATE with a negative treatment effect prediction. The easiest way to explain the discrepancy between the two methods is that D-AEMR is a matching method, not a statistical model. Usually if one wanted to estimate CATEs, one would smooth the treatment effect estimates with a regression model after matching, however, we did not do this. Thus, if the negative SVM group happened to be closer in proximity to the matched groups with positive CATEs, it would completely resolve the discrepancy between the two models: the SVM simply smoothed out the treatment effect estimates so that there was a negative predicted treatment effect, even though the CATE may have been negative for that matched group.

In order to determine whether this was true, we computed the Hamming distance between the units in that unusual group to units in other groups to investigate. As it turned out, the units within that matched group were much closer to the units with negative treatment effect than other units, and as such, the difference between the results of the two methods is because there was no smoothing in the matching method. We similarly investigated the blue group at x=0.5 CATE estimate in Figure 11 and again, the covariates of its units were closer in Hamming distance to other blue groups than to
other points.

Smoothing the matched groups is beyond the scope of this paper, but can be done with any regression method once the groups are formed if desired. The combination of matched groups with regression techniques for treatment effect can easily handle data with highly nonlinear baseline effects and smooth treatment effects; matching methods allow us to create such models without having to model the nonlinear baseline at all since the matching accounts for it.

Further, in the BTC dataset, we observed a decline in the match quality after about 30 out of the 43 covariates were dropped. We suggest stopping when the match quality MQ (which considers both prediction error and balancing factors in groups) becomes low, since in that case, either prediction error is bad (∼drop of > 5%) or the treatment and control samples have become too imbalanced (∼> 10% ratio difference). This all changes with highly imbalanced data, in which case, running D-AEMR to the end will generally find the best match for each treatment unit and there is no need to stop early (see Section F).

7 Conclusion

The algorithm presented here produces better matches than any other published algorithm for matching. Not only are the matches high quality, the predictions of treatment effect from the matches are as good as, if not better than, the (black box) machine learning methods we have tried on the problems we have encountered. This algorithm stands to have an impact in the social sciences, as it produces much higher quality results than the methods used for studies within the realms of law, economics, sociology, psychology, and criminology, management, as well as in many areas of healthcare where observational studies are conducted. Unlike matches from other methods, which match individuals whose covariates can be nothing like each other, the matches from D-AEMR are meaningful, as they are almost exact. Code is publicly available at https://github.com/almostexactmatch/daemr.
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A Group-by Implementation using Bit-Vectors

We implement the "Group-by" operation by bit-vector manipulation\[3\]. Assume there are p covariates in the dataset. If the $i$-th covariate is $k_i$-ary ($k_i \geq 2$), we at first rearrange the $p$ covariates such that $k_i \leq k_{i+1}$ for all $0 \leq i \leq p - 2$ and get reordered covariates values of unit $u_i$ to be $(a_{p-1}, a_{p-2}, \ldots, a_0)$. Then for each unit $u$, we compute two values.

$$b_u = \sum_{j=0}^{q-1} a_j k_j^j$$  \hspace{1cm} (3)

Together with the treatment indicator value $T = t$:

$$b_u^+ = t + \sum_{j=0}^{p-1} a_j k_j^{j+1}$$  \hspace{1cm} (4)

Since the covariates are rearranged so that $k_i \leq k_{i+1}$ for all $0 \leq i \leq p - 2$, two units $u$ and $u'$ have the same covariate values if and only if $b_u = b_{u'}$. For each unit $u$ with values $b_u$ and $b_u^+$, we compute how many times these two values occurs for all the units in the dataset(using unique() function of Numpy package in Python) and denote them as $c_u$ and $c_u^+$ respectively. To guarantee each matched group has at least one treatment and one control, we mark a unit $u$ as matched if its $c_u$ and $c_u^+$ differs. More rigorous proof can be found in \[3\].

B Adjustment of weights

One noticable feature of D–AEMR resides in its ability to dynamically adjust the weight of the covariates throughout the run of the algorithm. This property is important as covariates become more or less relevant in presence of other covariates. To recompute the weight ie the importance score of each covariate, D–AEMR utilizes a hold-out training set $D_H$ whose covariate space is restricted to the subset of the covariates being considered ($J \setminus s$). Using the hold-out set $D_H = [X^H, Y^H, T^H]$ that includes both treatment and control units, we obtain the vectors representing the weights $\beta_t$ and $\beta_c$ by linear regressions on control and treatment units. The readjusted weights are used to compute a prediction error $\mathcal{PE}$ measure to determine which subset of covariates leads to the best estimation quality. Specifically, $\mathcal{PE}$ is computed for each active set considered by

$$ \mathcal{PE}(D_{\Theta,s}^H) = \min_{\beta_t, \beta_c} \left[ \frac{1}{\sum_{u:T_u^H=0} (1 - T_u^H)} \sum_{u:T_u^H=0} (Y_u^H - X^H(u, J \setminus s)\beta_c)^2 ight. $$

$$+ \left. \frac{1}{\sum_{u:T_u^H=1} T_u^H} \sum_{u:T_u^H=1} (Y_u^H - X^H(u, J \setminus s)\beta_t)^2 \right] $$  \hspace{1cm} (5)

Notation: $D_H$ is the holdout dataset, $\Theta$ represents a selector function on the rows and columns of the input dataset for any given matched unit $u$. In other words, $D_{\Theta,u}$ consists of a subset of rows and
covariates that match with \( u \) (maximizing \( \Theta \) gives the main matched group for any unit \( u \)), \( T^H_u \) and \( T^H_u \) are respectively the treatment indicator and the outcome for unit \( u \) in the hold-out dataset.

Other criteria for optimization in addition to optimizing over \( v^T w \) is giving preference to subsets of attributes that allow better balancing of treatment and control units in the matched group. That balancing factor \( BF \) depends only on the number of units matched at each iteration by dropping \( s \) and the remaining unmatched units.

\[
BF_{\Theta,s} = \frac{\text{# of matched controls by dropping } s}{\text{# of remaining controls}} + \frac{\text{# of matched treatments by dropping } s}{\text{# of remaining treatments}}
\]

A matched quality quantity consisting of a trade off between these two measures ensures that \( D\text{-AEMR} \) only processes sets that maintain good prediction quality while the matched groups contain enough units to yield good estimate of treatment effects.

C Omitted Proofs

C.1 Proof of Proposition 4.1

**Proposition 4.1** If for a superset \( r \) of a newly processed set \( s \) where \( |s| = k \) and \( |r| = k + 1 \), all subsets \( s' \) of \( r \) of size \( k \) have been processed (i.e. \( r \) is eligible to be active after \( s \) is processed), then \( r \) is included in the set \( Z \) returned by GenerateNewActiveSets.

**Proof.** Suppose all subsets of \( r \) of size \( k \) are already processed and belong to \( \Delta^k \). Let \( f \) be the covariate in \( r \setminus s \). Clearly, \( f \) would appear in \( \Delta^k \), since at least one subset \( s' \neq s \) of \( r \) of size \( k \) would contain \( f \), and \( s' \in \Delta^k \). Further all covariates in \( r \), including \( f \) and those in \( s \) will have support at least \( k \) in \( \Delta^k \). To see this, note that there are \( k + 1 \) subsets of \( r \) of size \( k \), and each covariate in \( r \) appears in exactly \( k \) of them. Hence \( f \in \Omega \), the ‘if’ condition to check minimum support for all covariates in \( s \) is satisfied, and the final ‘if’ condition to eliminate false positives is satisfied too. Therefore \( r \) will be included in \( Z \) returned by the procedure. \( \square \)

C.2 Proof of Theorem 4.1

**Theorem 4.1 (Correctness)** The algorithm \( D\text{-AEMR} \) solves the AEMR problem.

**Proof.** Consider any treatment unit \( t \). Let \( s \) be the set of covariates in its main matched group returned in \( D\text{-AEMR} \) (the while loop in \( D\text{-AEMR} \) runs as long as there is a treated unit, and the GroupedMR* returns main matched group for every unit when it is matched for the first time). Let \( v_s \) be the indicator vector of \( s \) (see (2)). Since the GroupedMR* procedure returns a main matched group only if it is a valid matched group containing at least one treated and one control unit (see Algorithm 1), and since all units in the matched group on \( s \) have the same value of covariates in \( J \setminus s \), there exists a unit \( \ell \) with \( T(\ell) = 0 \) and \( x_\ell \circ v_s = x_t \circ v_s \).

Hence it remains to show that the covariate set \( s \) in the main matched group for \( t \) corresponds to the maximum weight \( v^T w \). Assume the contradiction that there exists another covariate-set \( r \) such that \( v^T r w > v^T s w \), there exists a unit \( \ell' \) with \( T(\ell') = 0 \) and \( x_{\ell'} \circ v_r = x_t \circ v_r \), and gives the maximum weight \( v^T r w \) over all such \( r \).
(i) $r$ cannot be a (strict) subset of $s$, since $D$-AEMR ensures that all subsets are processed before a superset is processed to satisfy the downward closure property in Proposition 3.1.

(ii) $r$ cannot be a (strict) superset of $s$, since it would violate the assumption that $v_r^T w > v_s^T w$ for non-negative weights.

(iii) Hence assume that $r$ and $s$ are incomparable (there exist covariates in both $r \setminus s$ and $s \setminus r$). Suppose the active set $s$ was chosen in iteration $i$. If $r$ was processed in an earlier iteration $j < i$, since $r$ forms a valid matched group for $t$, it would give the main matched group for $t$ violating the assumption. We argue that in this case $r$ must be active at the start of iteration $i$, and will be chosen as the best covariate set in iteration $i$, leading to a contradiction.

Note that we start with all singleton sets as active sets in $\Delta(0) = \{\{1\}, \ldots, \{p\}\}$ in the $D$-AEMR algorithm. Consider any singleton subset $r_0 \subseteq r$ (comprising a single covariate in $r$). Due to the downward closure property in Proposition 3.1, $v_{r_0}^T w \geq v_r^T w$, hence $v_{r_0}^T w \geq v_r^T w > v_s^T w$. Hence all of these singleton subsets of $r$ will be processed in earlier iterations $j < i$, and will belong to the set of processed covariate sets $\Lambda_{(i-1)}$.

Repeating the above argument, consider any subset $r' \subseteq r$. It holds that $v_{r'}^T w \geq v_r^T w > v_s^T w$. Hence all subsets $r'$ of $r$ will be processed in earlier iterations $j < i$ starting with the singleton subsets of $r$. In particular, all subsets of size $|r| - 1$ will belong to $\Lambda_{(i-1)}$. As soon as the last of those subsets is processed, the procedure GenerateNewActiveSets will include $r$ in the set of active sets in a previous iteration $j < i$. Hence if $r$ is not processed in an earlier iteration, it must be active at the start of iteration $i$, leading to a contradiction.

Hence for all treatment units $t$, the covariate-set $r$ giving the maximum value of $v_r^T w$ will be used to form the main matched group of $t$, showing the correctness of the $D$-AEMR algorithm.

\section{D Effect of Noise}

We use 15000 treated units, 15000 control units, 5 important covariates and 8 unimportant covariates. We change our generative process in the following way to add noise:

$$y = \sum_i \alpha_i x_i + T \sum_{i=1} \beta_i x_i + T \cdot U \sum_{i,\gamma > i} x_i x_\gamma + \tau \epsilon, \quad (6)$$

where the noise coefficient $\tau \in \{0.25, 0.5, 1, 2\}$ and $\epsilon$ denotes noise chosen as either $\epsilon_1$, $\epsilon_2$, $\epsilon_3$ below:

- Noise1: $\epsilon_1 \sim N(mean = 0, sd = 1)$
- Noise2: $\epsilon_2 \sim N(mean = 0, sd = 2.5)$
- Noise3: $\epsilon_3 \sim N(mean = 0, sd = 5)$

First, we run $D$-AEMR and Causal Forest on all noise models to study how noise affect each method in terms of CATE estimations. Then, we compare the CATE estimates of $D$-AEMR and Causal Forest on the noise model in which Causal Forest achieves its best results.
Results: As Figure 12 shows, D-AEMR outperforms Causal Forest on all noise levels constructed. While Causal Forest with small amount of noise (low noise coefficient and low noise variance) performs better than Causal Forest without noise (see Figure 15), it still produces worse estimates than D-AEMR. The relative ordering of the methods remains unchanged. Additionally, Figure 13 show that D-AEMR is robust to small amount of noise but a high noise coefficient (> 2) and/or high variance (sd > 5) can lead to poorer results. To add smoothing of the estimates for D-AEMR, one can either: (i) smooth after matching by doing regression afterwards, or (ii) increase the minimum number of units in each match (which is a parameter in our code) to induce smoothing.

Figure 12: comparison of D-AEMR and Causal Forest for different noise levels. Noise coefficient $\tau = 0.25$. Each row represents a different standard deviation (from top to bottom: sd = 1, sd = 2.5, sd = 5)
Figure 13: effect of noise on CATE estimation for D-AEMR when stopped early (before dropping important covariates. Each column represents a different noise coefficient (from left to right: \(\tau_0 = 0\) (nonoise), \(\tau_1 = 0.25\), \(\tau_2 = 0.5\), \(\tau_3 = 1\), \(\tau_4 = 2\)). Each row represents a different standard deviation (from top to bottom: \(sd = 1\), \(sd = 2.5\), \(sd = 5\)).
Figure 14: effect of noise on CATE estimation for $D$–AEMR when run until no more matches. Each column represents a different noise coefficient (from left to right: $\tau_0 = 0$ (no noise), $\tau_1 = 0.25$, $\tau_2 = 0.5$, $\tau_3 = 1$, $\tau_4 = 2$). Each row represents a different standard deviation (from top to bottom: $sd = 1$, $sd = 2.5$, $sd = 5$)
Figure 15: effect of noise on CATE estimation for Causal Forest. Each column represents a different noise coefficient (from left to right: $\tau_0 = 0$ (no noise), $\tau_1 = 0.25$, $\tau_2 = 0.5$, $\tau_3 = 1$, $\tau_4 = 2$). Each row represents a different standard deviation (from top to bottom: $sd = 1$, $sd = 2.5$, $sd = 5$)
E  More runtime evaluation of $\text{D-AEMR}$

The running time of $\text{D-AEMR}$ varying the number of units is given in Figure 16.

![Figure 16: Run time of $\text{D-AEMR}$ with variations on the number of units.](image)

F  Evolution of the match quality (MQ) in the BTC dataset

Figure 17 shows how the prediction error (PE) and balancing factor (BF) change over iterations for the BTC dataset with 43 covariates when we run $\text{D-AEMR}$. The prediction error suddenly drops after 30 iterations. This leads to a drop in the matching quality and can serve as a stopping criteria in practice.

![Figure 17: Evolution of Match Quality (MQ = PE + C*BF) where C is a trade off parameter](image)

(a) Evolution of the Prediction Error  
(b) Evolution of the Balancing Factor