FLAME: A Fast Large-scale Almost Matching Exactly Approach to Causal Inference

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Abstract

A classical problem in causal inference is that of matching, where treatment units need to be matched to control units. Some of the main challenges in developing matching methods arise from the tension among (i) inclusion of as many covariates as possible in defining the matched groups, (ii) having matched groups with enough treated and control units for a valid estimate of Average Treatment Effect (ATE) in each group, and (iii) computing the matched pairs efficiently for large datasets. In this paper we propose a fast method for approximate and exact matching in causal analysis called FLAME (Fast Large-scale Almost Matching Exactly). We define an optimization objective for match quality, which gives preferences to matching on covariates that can be useful for predicting the outcome while encouraging as many matches as possible. FLAME aims to optimize our match quality measure, leveraging techniques that are natural for query processing in the area of database management. We provide two implementations of FLAME using SQL queries and bit-vector techniques.

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1 Introduction

Questions of robust causal inference, beyond simple correlations or model-based predictions, are practically unavoidable in health, medicine, or social studies. Causal inference goes beyond simpler correlation, association, or model-based predictive analysis as it attempts to estimate the causal effects of a certain intervention. In the context of the clinical intervention, we are interested in how the binary treatment intervention strategy causes the outcome to change.

While randomized trials are considered the gold standard for causal inference (Rubin, 2008), much of the available data in the clinical and social sciences is observational. In such situations, the benefits of randomization are not available as individuals select into treatment: people who benefit more from pain relievers tend to take them more often, individuals who are likely to succeed in higher education are more likely to enroll in it, and so forth. Estimating causal effects in an observational setting becomes a problem of representing the available data as if it were collected from a randomized experiment. A major benefit of randomization is the covariate balance that it creates between treated and control units. A natural approach to observational studies is the matching of treated and control units such that underlying background covariates are balanced (Chapin, 1947; Greenwood, 1945). In general, the covariate balancing property of matching methods provides a path to proper estimates of causal effects.

Matching increases the interpretability of causal analyses in several ways. In particular, matching highlights issues with overlap between treatment and control populations, allowing for a careful analysis of why some individuals are treated and others are not. This helps us to find the source of uncertainty in the causal estimates, and helps determine what type of additional data must be collected. Exact matching approaches where individuals are matched on raw covariate values further allows the practitioner to interpret causal estimates within matched populations as conditional average treatment effects. This provides a more granular causal analysis that can
provide crucial information on who benefits from treatment most and where resources should be spent for future treatments. Matching can also provide explanations for treatment effect estimates in a way that pure modeling methods (that do not use matching) cannot. A detailed review of the matching literature (e.g. propensity score, coarsened exact, network flow and mixed integer programming) is reserved for Section 4.

We propose a data-adaptive approach to almost-exact matching under the potential outcomes framework with a binary treatment. Our method (FLAME - Fast, Large-scale, Almost Matching Exactly) creates matches that include as many covariates as possible, and iteratively drops covariates that are successively less useful for predicting outcomes. It takes into account an aspect of large samples that past work does not: how to retain as much information as possible when matching, by constructing matches on partial information. This allows the matches to be almost exact, which helps with interpretability, and retains as much important information as possible within each match. It improves over coarsened exact matching and regression methods in that it does not introduce a distance metric on covariate space a priori, since our distance metric is adaptive. It improves over regression and propensity methods in that it does not force a model form, instead it tries to match on covariates almost exactly. It improves over network flow formulations in that it considers covariate balance in the formulation. It improves over mixed integer programming methods in that it considers only variables it deems to be important, and scales nicely with the sample size and number of covariates.

A major benefit of FLAME is that it lends naturally to fast implementations for extremely large datasets. FLAME has two implementations. The first one uses bit vectors, and is extremely fast for data that has been preprocessed and fits in memory. The second implementation leverages database management systems (e.g., PostgreSQL [2016]), and in particular, highly optimized built-in SQL group-by operators that can operate directly on the database, and do not require the data to fit in memory. The use of database systems makes the matching algorithm suitable for
parallel executions. The database implementation is novel in that it is specialized to be efficient; only a few lines of carefully constructed SQL code are needed to perform matching.

By dropping covariates, FLAME increases bias in order to make predictions of conditional average treatment effect. We can calculate FLAME’s bias directly in some cases, and its bias depends directly on how important the dropped covariates are to predicting the output. If only the irrelevant covariates are dropped, the estimates are unbiased. In that case, FLAME’s estimates and the gold standard estimates of exact matches are identical.

In what follows, we first introduce FLAME’s framework of iteratively dropping covariates (Section 2). We then discuss FLAME’s algorithms and implementations (Section 3) and related work (Section 4), provide experiments (Section 5), and a precise theoretical calculation of FLAME’s statistical bias (Section 6).

2 The FLAME Framework

Suppose $D = [X, Y, T]$ is the population table, where $X$ is $n \times p$, $Y$ and $T$ are $n \times 1$, where each row corresponds to a unit (called a tuple in database management). The columns of $X$ correspond to variables (also known as covariates, features, attributes). Data must be categorical in order for exact matches to occur with non-zero probability, but this framework can generalize to binned real-valued data (though we caution on lessons learned from CEM). Treatment assignment variable $T$ takes binary values 1 (for treatment) and 0 (for control). $Y(1), Y(0)$ respectively denote the outcome if the treatment and control were applied to a unit. We make Stable Unit Treatment Value (Rubin, 2005) and strong ignorability (Rosenbaum and Rubin, 1983) assumptions.

Challenges in Observational Studies: The fundamental challenge of an observational study in contrast to a randomized experiment is the lack of control by the scientist of the treatment assignment. In particular, a randomization scheme leads to the strong ignorability of treatment
(Rosenbaum and Rubin [1983]: each individual has a positive probability of being assigned to treatment, and there is conditional independence of potential outcomes \((Y(0), Y(1))\) from \(T\) given relevant covariates \(X\). In an observational setting, it is not known which covariates are relevant for treatment assignment and so common practice is to collect as much pre-treatment information as possible. This in turn leads to a potentially very high dimensional collection of covariates not all of which are relevant for treatment assignment.

While exact matching schemes do not necessarily suffer from the use of superfluous covariates (for example when the estimand of interest is a population quantity) the following represents a desiderata for matched groups in pursuit of any conditional (potentially heterogeneous) causal estimand: (R1) Each matched group contains at least one treatment \((T = 1)\), and one control unit \((T = 0)\). In addition, for a good matching quality, the following properties are desired: (R2) As many covariates in \(X\) as possible are used to define each group. (R3) The chosen covariates are sufficient to create a good predictor of potential outcomes \(Y(1), Y(0)\). (R4) As many units as possible from \(D\) should participate in the final matched groups. (R5) (optional) The size of each group, and possibly the number of treated and control units, should be above a threshold.

(R1) requires that there is in fact information within a group to estimate a group-level estimand. (R2) represents the desire for estimating the most granular causal estimates possible while (R3) addresses the need for matching covariates to be associated with the potential outcomes (Rubin and Thomas [1996], Brookhart et al, 2006). This quality, coupled with (R1) and (R2) makes the conditional independence of potential outcomes from the treatment assignment more plausible. (R4) aims to use as much information as possible from the given dataset. (R5) is a universality condition — if the fraction of data used in the analysis is too small it is unlikely that proper causal inference can proceed. For exact matching, it may not be possible to achieve all the above goals at the same time. If we choose all the covariates in \(X\) to define the matched groups satisfying (R2), the groups may violate (R1) (that is, it would be inappropriate to assume
that every individual, defined by their covariates, had a non-zero probability of being assigned to either treatment or control), the size of the groups may be small (violating (R1) or (R5)), as a result not utilizing many of the original units in the matching (violating (R4)). Thus to achieve (R1), and (R3), we choose a subset of the covariates in defining the matched units.

**Basic Idea of Framework and FLAME:** To achieve a good balance of the properties listed above, we compute matched groups with subsets of variables. First, we match using all variables. The groups that have at least one treatment and one control unit are considered to be complete, since we can directly estimate treatment effects for those groups, and the units are removed for the rest of the analysis. The remaining groups will have either zero treatment or zero control units. If we do not continue trying to match we would violate (R4), but we must reduce the dimensionality of the space in order to match further. The idea of the framework is that when each unit is matched, it is matched on as many relevant dimensions as possible (R2), where relevant dimensions are those useful for prediction (R3). Matching with at least one treatment and one control (R1) is done for as many units as possible (R4).

The FLAME algorithm is a special case of the framework, where after the first level of exact matching when all identical units are removed, a second level of matching is done by omitting one variable from $X$, where the omitted variable is chosen based on optimization criteria for prediction quality (R3). This process is repeated until either all units are matched or until we cannot remove variables without damaging prediction quality, so that (R3) would not be satisfied. Thus, the core of the algorithm is a scheme by which to sequentially reduce the number of variables that are being used to form exact matches without harming prediction quality.

**Matched Quality and Optimization Criteria:** The input to the generic framework is the population table $D$, a holdout training dataset $D^H$, and a match quality measure $MQ(D, D^H)$. The framework determines a selector function, denoted by $\Theta$, which chooses a subset of rows (units) and columns (covariates) of $D$ and $D^H$ that are available when $u$ is matched, i.e., $D_{\Theta,u} =$
$D(\text{rows}_{\Theta,u}, \text{columns}_{\Theta,u})$ denotes the dataset available when $u$ is matched. Here $\text{rows}_{\Theta,u}$ denotes the set of units that can be matched with $u$, and $\text{columns}_{\Theta,u}$ denotes the set of available columns that have been used to match $u$. For the holdout training set (discussed further in what follows), we use the same set of available covariates when $u$ is matched but use the full set of rows, i.e., $D^H_{\Theta,u} = D^H(\cdot, \text{columns}_{\Theta,u})$; we will later describe how we use the holdout training set.

The generic framework aims to optimize the Total Match Quality over selector functions $\Theta$, whereas the FLAME algorithm focuses on $\Theta$-s that are of a certain form (discussed below).

$$\max_{\Theta} \text{TotalMQ}(D, D^H, \Theta),$$

where

$$\text{TotalMQ}(D, D^H, \Theta) = \sum_{u=1}^{n} \text{MQ}(D_{\Theta,u}, D^H_{\Theta,u}) = \sum_{u=1}^{n} \left[ -\text{PE}(D^H_{\Theta,u}) + C \times \text{BF}(D_{\Theta,u}) \right] \quad (1)$$

The function $\text{BF}(D_{\Theta,u})$ is a balancing factor that is maximized when the largest possible fractions of treatment and control populations are matched. This helps with goal (R4), which is to keep the number of unmatched units small. This also helps with goal (R2), which is that throughout the procedure, as many covariates as possible should be used for defining matched groups. This is due to the fact that the framework drops a variable from consideration only when a unit cannot be matched in a valid group satisfying (R1) considering the set of all available covariates. Function $\text{PE}(D^H_{\Theta,u})$ is a prediction error that ensures (R3), which is that the set of covariates available when units are matched is sufficient to maintain prediction quality. A lower prediction error is better, so $\text{PE}$ is negated in (1) since we are maximizing the total matched quality. We define these below, using our class of selector functions $\Theta$. In (1), $C$ is a trade-off parameter between the balancing factor and the prediction error. Note that (R1) is always guaranteed because we will not match any treated unit unless there is a corresponding control unit in the matched group.

**Execution of FLAME:** For FLAME, $\Theta$ sequentially reduces the number of rows and columns used for matching. It eliminates covariates according to a partial permutation $\pi$ over the indices of the covariates $J = \{1, \cdots, p\}$. For a unit $u$ and a subset of indexes $J' \subseteq J$ of covariates, let
\(X(u, J')\) denote the value of the covariates matching the indexes in \(J'\).

At iteration \(l - 1\), \(\Theta\) has dropped covariates \(\pi(1), \pi(2), ..., \pi(l - 1)\). Thus, the set of remaining covariates at time \(l\) is \(J \setminus \{\pi(j)\}_{j=1}^{l-1}\). At iteration \(l\), if \(u\) has not already been matched, and if there is an exact match for unit \(u\) on the covariates that remain, then \(u\) is matched at iteration \(l\), and its MQ comes from iteration \(l\). Said another way, consider conditions:

- (a) \(u\) has not been matched before \(l\), i.e., there is no \(k\) satisfying condition (R1) such that
  \[X(u, J \setminus \{\pi(j)\}_{j=1}^{l-1}) = X(k, J \setminus \{\pi(j)\}_{j=1}^{l-1}).\]

- (b) \(u\) is matched at \(l\): \(\exists k\) satisfying (R1) (i.e., \(T_u = 1 - T_k\)) such that
  \[X(u, J \setminus \{\pi(j)\}_{j=1}^{l-1}) = X(k, J \setminus \{\pi(j)\}_{j=1}^{l-1}).\]

If (a) and (b) hold for unit \(u\), then \(u\) is matched at iteration \(l\). Define \(M_u\) to be the iteration at which \(u\) is matched: \(M_u = l\) such that (a) and (b) both hold at \(l\). If \(u\) is never matched ((b) never holds for any \(l\) before the stopping iteration \(T\)), then set \(M_u = \infty\). Thus, when \(M_u = l\), the columns of data used to match \(u\) are: columns \(\Theta, u = J \setminus \{\pi(j)\}_{j=1}^{l-1}\).

The balancing factor and predictive error of a unit \(u\) depend only on the data available in the iteration when it is matched, and are the same for all \(u\) matched at that iteration. Normalizing by the number of units matched in level \(l\), denoted by \(n_l\), the balancing factor and predictive error of a unit \(u\) are: \(BF(D_{\Theta, u}) = \frac{BF(D_{\Theta, (l)})}{n_l}\) and \(PE(D_{\Theta, u}^H) = \frac{PE(D_{\Theta, (l)}^H)}{n_l}\), where \(BF(D_{\Theta, (l)}), PE(D_{\Theta, (l)}^H)\) are the balancing factor and predictive error at level \(l\). This simplifies expression (1) to:

\[
\text{Total MQ}(D, D^H, \Theta) = \sum_{l \geq 1} \left[ -PE(D_{\Theta, l}^H) + C \times BF(D_{\Theta, l}) \right].
\] (2)

For \(BF\), it is desirable that each dropped set of covariates maximizes the fraction of matched individuals from the available pools of units. If \(BF\) is high in earlier iterations, more of the
matched units will exactly match on almost all covariates (in agreement with (R2)). We write this as follows (# denotes ‘the number of’):

\[
BF(D_{\Theta,(l)}) = \frac{\# \text{ matched control}}{\# \text{ available control}} + \frac{\# \text{ matched treated}}{\# \text{ available treated}} \leq \sum_{u} 1_{T_u=0,M_u=l} + \sum_{u} 1_{T_u=1,M_u=l}. \tag{3}
\]

If we choose covariate to drop using only BF, we may omit covariates that are important for maintaining prediction quality, which could ruin the results of our matching procedure. To counteract this, we associate the matching assignment with the outcome as well as with the treatment assignment (see also Rubin and Thomas, 1996; Brookhart et al., 2006). A natural approach for this considers a holdout training set \( D_H = [X^H, Y^H, T^H] \) that includes both treatment and control units for which predictive quality (predictive error \( PE \)) can be measured. Here we can, for example, use only the covariates available at iteration \( l \), and \( \beta_0 \) and \( \beta_1 \) are vectors of that same size, representing the coefficients obtained by linear regressions on control and treatment units:

\[
PE(D^H_{\Theta,(l)}) = \min_{\beta_0, \beta_1} \left[ \frac{1}{\sum (1 - T_u)} \sum_{u:T_u^H=0} (Y_u^H - X^H(u,J - \{\pi(j)\}_{j=1}^l) \beta_0)^2 + \frac{1}{\sum T_u^H} \sum_{u:T_u^H=1} (Y_u^H - X^H(u,J - \{\pi(j)\}_{j=1}^l) \beta_1)^2 \right]. \tag{4}
\]

The weighted combination of (3) and (4) is our match quality measure \( MQ \). The prediction error \( PE \) is essentially a measure of predictive power of a given subset of covariates. This measure does not need to depend on any specific machine learning model, which makes FLAME less model-dependent. For instance, one can replace \( PE \) with a classification metric if desired.

With the definitions above, selector function \( \Theta \) is uniquely defined by the partial permutation \( \pi \), which is an ordered sequence of a subset of indices \( 1,\ldots,J \). For instance, \( \pi \) might have FLAME drop coefficients \( 6, 13, 2, 8 \) in that order and then keep the remaining coefficients, leaving some units unmatched. Overloading notation, our goal is thus to maximize:

\[
\max_{\pi} \text{TotalMQ}(D,D^H,\pi). \tag{9}
\]
(This notation is overloaded since $\pi$ tells us only the order in which covariates are removed. FLAME’s matching procedure, defined above, is now implicit from this notation.)

Global optimization of total match quality $\text{TotalMQ}$ with respect to partial permutations $\pi$ requires a search over a space that is exponential in the number of covariates, since it requires the choice of a subset of covariates and order of covariates to remove. We instead use a backwards elimination procedure, where we choose the optimal covariate to eliminate at each iteration and optimize parameters in between eliminating covariates. This will allow the method to scale to a huge number of covariates and observations. We have reason to believe that in many cases, the solution FLAME finds is not too far from optimal; it tends to protect features from elimination that are important for prediction or match quality, and the exact order in which the less relevant features are removed does not tend to be important.

For FLAME, $\pi(l)$ is computed at iteration $l$ of the algorithm by performing linear regression on the holdout training set to determine the next feature to drop for backwards elimination. Each remaining feature is checked, and the one that least damages prediction quality is chosen for removal, and that is $\pi(l)$.

3 The FLAME Algorithm and Efficient Implementations

In this section, first we provide a generic FLAME algorithm called $\text{FlameGeneric}$ incorporating the ideas described in the previous section (Section 3.1). We outline two efficient implementations of the matching procedure used in this generic algorithm: (a) using a database management system and database queries (Section 3.2), and (b) using bit vectors (Section 3.3). We also discuss a faster but less adaptable variant of the generic FLAME algorithm (Section 3.4).
### 3.1 The Generic FLAME Algorithm

Algorithm 1 presents the generic matching algorithm FlameGeneric for FLAME. Initially, the input with \( n \) units is given as \( D = (X, Y, T) \), where \( X \) (and \( n \times p \) matrix) denotes the covariates, \( Y \) (an \( n \times 1 \) vector) is the outcome, and \( T \) (an \( n \times 1 \) vector) is the treatment. The covariates are indexed with \( J = 1, \cdots, p \).

At iteration \( l \) of the algorithm, it computes a subset of the matched groups \( MG_l \) such that for each matched group \( mg \in \bigcup_l MG \), there is at least one treated and one control unit. Note that it is possible for \( MG_l = \emptyset \), in which case no matched groups are returned in that iteration. Recall from the previous section that \( M_u \) denotes the iteration when a unit \( u \) is matched. Overloading notation, let \( M_{mg} \) denote the iteration when a matched group \( mg \) is formed. Hence if a unit \( u \) belongs to a matched group \( mg \), \( M_u = M_{mg} \) (although not every \( u \) with \( M_u = M_{mg} \) is in \( mg \)).

We use \( D_l \subseteq D \) to denote the unmatched units and \( J_l \subseteq J \) to denote the remaining variables when iteration \( l + 1 \) of the while loop starts (i.e., after iteration \( l \) ends). Initially \( J_0 = J \). As discussed in Section 2, the algorithm drops one covariate \( \pi(l) \) in each iteration (whether or not there are any valid non-empty matched groups), and therefore, \( J_l = J \setminus \{\pi(j)\}_{j=1}^l \), \( |J_l| = p - l \). All matched groups \( mg \in MG_l \) in iteration \( l \) use \( J_{l-1} \) as the subset of covariates on which to match.

**The first call to BasicExactMatch:** First we initialize the variables \( D_0, J_0, l, \) and \( run \). The variable \( run \) is true as long as the algorithm is running, while \( l \geq 1 \) denotes an iteration. After the initialization step, the subroutine BasicExactMatch (see Algorithm 2) finds all of the exact matches in the data \( D = D_0 \) using all features \( J = J_0 \), such that each of the matched groups \( mg \in MG_1 \) contains at least one treatment and one control observation (i.e., satisfies constraint (R1)). The rest of the iterations in the algorithm aim to find the best possible matches for the rest of the data by selectively dropping covariates as discussed in the previous section.

**The while loop and subsequent calls to BasicExactMatch:** At each iteration of the while loop, each feature is temporarily removed (in the for loop over \( j \)) and evaluated to deter-
mine if it is the best one to remove by running BasicExactMatch and computing the matched quality $MQ$. Since BasicExactMatch does not consider feature $j$ (one less feature from the immediately previous iteration), there are fewer constraints on the matches, and it is likely that there will be new matches returned from this subroutine.

We then need to determine whether a model that excludes feature $j$ provides sufficiently high quality matches and predictions. We would not want to remove $j$ if doing so would lead to poor predictions or if it led to few new matches. Thus, $MQ$ is evaluated by temporarily removing each $j$, and the $j^*$ that is chosen for removal creates the most new matches and also does not significantly reduce the prediction quality. Steps [13] and [14] of the algorithm choose which feature to remove, and remove it. In Step [15] the new matches and matched groups are stored. The remaining unmatched data are used for the next iteration $l + 1$.

**Stopping conditions:** If we run out of unmatched data, the algorithm stops (Step 3). If we choose to include another stopping condition, then we also stop (Step 10). For instance, if the unmatched units are either all control or all treatment observations, we must stop. If there are no more covariates to drop, we also stop. We could also choose to stop when the match quality is too low. Finally, the matched groups are returned along with the units and the features used for each set of matched groups formed in different iterations.

The key component in the FlameGeneric algorithm (Algorithm 1) is the BasicExactMatch procedure (Algorithm 2). The steps of BasicExactMatch can be easily implemented in Java, Python, or R. In the next two subsections we give efficient implementations of BasicExactMatch, one using SQL queries from databases, and the other using bit vector techniques.

### 3.2 Implementation of BasicExactMatch using Database (SQL) Queries

Exact matching is highly related to the GROUP BY operator used in database (SQL) queries, which computes aggregate functions (sum, count, etc) on groups of rows in a two-dimensional...
table having the same values of a subset of columns specified in the query. SQL queries can be run on any standard commercial or open-source relational database management systems (e.g., Microsoft SQL Server, Oracle, IBM DB2, Postgres, etc.). These database systems are highly optimized and robust for SQL queries, can be easily integrated with other languages (we used python and SQL), and scale to datasets with a large number of rows ($n$) or columns ($p$) that may not fit in the available main memory. In addition, SQL queries declaratively specify complex operations (we only specify ‘what’ we want to achieve, like groups on the same values of variables, and not ‘how’ to achieve them, i.e., no algorithm has to be specified), and are therefore succinct. In a recent work (Salimi et al., 2017), various existing causal inference techniques have been efficiently implemented in a database-based engine. In our work, SQL enables us to execute all three steps of the BasicExactMatch procedure outlined in Algorithm 2 (Steps 1, 2, and 3) in a single query as we discuss below.

In this implementation, we keep track of matched units globally by keeping an extra column in the input database $D$ called $\text{is\_matched}$. For every unit, the value of $\text{is\_matched} = \ell$ if the unit is matched in a valid group with at least one treated and one control unit in iteration $\ell$ of Algorithm 1 and $\text{is\_matched} = 0$ if the unit is still unmatched. Therefore instead of querying the set of unmatched data $D_{um}$ at each iteration (as in the input of Algorithm 2), at each iteration we query the full database $D$, and consider only the unmatched units for matching by checking the predicate $\text{is\_matched} = 0$ in the query. Let $A_1, \cdots, A_p$ be the covariates in $J_s$. The SQL query is described below:

WITH tempgroups AS
  (SELECT $A_1$, $A_2$, \ldots, $A_p$  
   MATCHED groups are identified by their covariate values) 
  FROM $D$
  WHERE $\text{is\_matched} = 0$  
  (use data that are not yet matched)  
  GROUP BY $A_1$, $A_2$, \ldots, $A_p$ 
  (create matched groups with identical covariates)
HAVING SUM(T) >= 1 AND SUM(T) <= COUNT(*)-1
    (groups have $\geq$ 1 treated, but not all treated)
),
UPDATE D
SET is_matched = \ell
WHERE EXISTS
    (SELECT D.A_1, D.A_2, \ldots, D.A_p
     FROM tempgroups S  (set of covariate values for valid groups)
     WHERE S.A_1 = D.A_1 AND S.A_2 = D.A_2 AND \ldots AND S.A_p = D.A_p
    )
AND is_matched = 0

The \textit{WITH} clause computes a temporary relation \textit{tempgroups} that computes the combination of values of the covariates forming ‘valid groups’ (i.e., groups satisfying (R1)) on unmatched units. The \textit{HAVING} clause of the SQL query discards groups that do not satisfy (R1) – since treatment $T$ takes binary values 0, 1, for any valid group the sum of $T$ values will be strictly $> 0$ and $< \text{total number of units in the group}$. Then we update the population table $D$, where the values of the covariates of the existing units match with those of a valid group in \textit{tempgroups}. Several optimizations of this basic query are possible and are used in our implementation. Setting the \textit{is\_matched} value to level $\ell$ (instead of a constant value like 1) helps us compute the CATE for each matched group efficiently.

3.3 Implementation of BasicExactMatch using Bit Vectors

In this section we discuss an alternative bit-vector implementation to the SQL query discussed above. We will assign unit $u$’s covariates to a single integer $b_u$. Unit $u$’s covariates, appended with the treatment indicator, will be assigned an integer $b_u^+$. Let us discuss how to compute $b_u$ and
Suppose $|J_s| = q$, and the covariates in $J_s$ are indexed (by renumbering from $J$) as 0 to $q - 1$. If the $j$-th covariate is $k_{(j)}$-ary ($k_{(j)} \geq 2$), we first rearrange the $q$ covariates such that $k_{(j)} \geq k_{(j+1)}$ for all $0 \leq j \leq q - 2$. Thus the (reordered) covariate values of unit $u$, $(a_{q-1}, a_{q-2}, \ldots, a_0)$, is represented by the number $b_u = \sum_{j=0}^{q-1} a_j k_{(j)}^j$. Together with the treatment indicator value $T = t$, the set $(a_{q-1}, a_{q-2}, \ldots, a_0, t)$ for unit $u$ is represented by the number $b_u^+ = t + \sum_{j=0}^{p-1} a_j k_{(j)}^{j+1}$. Since the covariates are rearranged so that $k_{(j)} \leq k_{(j+1)}$ for all $0 \leq j \leq q - 2$, two units $u$ and $u'$ have the same covariate values if and only if $b_u = b_{u'}$. For each unit $u$, we count how many times $b_u$ and $b_u^+$ appear, and denote them as $c_u$ and $c_u^+$ respectively. (The counting is done by NumPy’s `unique()` function.) To perform matching, we compute the $b_u$, $b_u^+$, $c_u$, $c_u^+$ values for all units and mark a unit as matched if its $c_u$ value and $c_u^+$ value differ. Proposition 1 guarantees the correctness of the bit-vector implementation.

**Proposition 1** A unit $u$ is matched if and only if $c_u \neq c_u^+$, since the two counts $b_u$ and $b_u^+$ differ iff the same combination of covariate values appear both as a treated unit and a control unit.

An example of this procedure is illustrated in Table 1. We assume in this population the 0-th variable is binary and the next variable is ternary. In this example, the number $b_1$ for the first unit is $0 \times 2^0 + 2 \times 3^1 = 6$; the number $b_1^+$ including its treatment indicator is $0 + 0 \times 2^1 + 2 \times 3^2 = 18$. Similarly we can compute all the numbers $b_u$, $b_u^+$, $c_u$, $c_u^+$, and the matching results are listed in the last column in Table 1.

**Comparison of two implementations and estimation of treatment effect:** As we will show in our experiments, the bit vector implementation typically outperforms the SQL implementation when the data fits in memory, but for large data and more covariates, SQL performs better. Another limitation of the bit vector implementation is that the magnitude of the numeric representation grows exponentially and can cause overflow problems. This is another reason we recommend FLAME-db when the number of covariates is large. Our final goal is to estimate the
treatment effect for each unit, as well as the average treatment effect (ATE). An estimate of the ATE is straightforward once the treatment effects in each group (conditional average treatment effects – CATEs) are computed.

3.4 Faster Feature Selection

One could precompute the order \( \pi \) in which features are removed in FLAME. This would allow FLAME to run faster at the expense of making it less adaptable. To precompute \( \pi \), we could use Lasso’s regularization path or another backwards selection method to determine the order in which to remove the features before we do any matching or removing of data. This would remove lines 5-9 of the Generic FLAME algorithm, and change lines 13-14 to remove the predetermined next feature. The problem with precomputing \( \pi \) is that it may choose the wrong feature to remove, since it takes into account the full dataset, but does not take into account the data that remain at the iteration when that feature is scheduled to be removed.

If we consider a dataset that has a large number of irrelevant features, it might be beneficial to use Lasso or another technique to choose a pre-determined order to omit the clearly irrelevant features, which provides a computational gain. After that, we can switch back to the Generic FLAME implementation (including the backwards selection loop) to continue removing features.

4 Relationship to Prior Work

Early approaches to matching considered exact matching on covariates but quickly ran into issues of insufficient sample size when the number of covariates was even moderately large; each matched group must include one treatment and one control observation, and in high dimensions, the matches simply do not exist. In the 1970’s and 1980’s, a large literature on different dimension reduction approaches to matching was developed (e.g., [Rubin, 1973a,b, 1976, Cochran and...)]
Rubin (1973) with the extreme being work on propensity score matching, which was later extended to work on penalized regression approaches that leverage propensity (Schneeweiss et al., 2009; Rassen and Schneeweiss, 2012; Belloni et al., 2014; Farrell, 2015). The problem with propensity score methods is that they require a proper specification of either the propensity score model or the outcome model, neither of which is true in practice. The doubly robust literature allows for only one of the two models to be specified correctly, but there is no reason that either of these models would be specified correctly in practice.

An alternative technique, coarsened exact matching, creates matches that attempt to preserve more covariate information. It bypasses the need to fit complicated propensity score models by coarsening or discretizing covariates in such a way that the newly constructed covariates allow for exact matching (Iacus et al., 2011a,b). This approach is appealing when there are many continuous covariates that are naturally amenable to binning. However, when most or all of the covariates are categorical, coarsening becomes impossible without introducing a calculus on all of the covariates. This can be problematic in high dimensions, and tends to have the same problem as nearest neighbor techniques, which are well-known to perform poorly in high dimensions. Further, when categorical variables have two levels, coarsening is equivalent to variable selection. In this setting, coarsened exact matching would lead to the same matches as high dimensional propensity score techniques with variable selection.

A similar problem exists with what is called “optimal” matching in the literature (Rosenbaum, 2016). A distance metric over variables is defined manually, which introduces a calculus on the covariates. That distance metric is used as input to a network flow problem which optimizes match quality. Despite the optimality of the solution network flow problem, the quality of the matches is questionable since it relies on a manually defined distance measure. Network flow problems also cannot directly handle constraints, the user needs to manually manipulate the algorithm in order to obtain desired balance constraints (Zubizarreta, 2012).
The problems with network flow optimization highlight an important concern about non-exact matching methods generally, which is that they implicitly approximate the solution of a hard combinatorial optimization problem. It is possible that high quality match assignments exist, but the standard approximate methods of constructing matches, such as network flow optimization did not find them. To handle the problem of finding suboptimal match assignments, some newer matching schemes use mixed integer programming, which is a flexible framework that can accommodate linear balance constraints (Zubizarreta [2012] Zubizarreta et al., 2014) Keele and Zubizarreta [2014], Resa and Zubizarreta, 2016; Noor-E-Alam and Rudin 2015b,a). However, these methods have two major disadvantages: first they cannot scale to large problems; second, they may be trying to match units on covariates that are not important in any way. In this work, we avoid the introduction of traditional regularization or a measurement scale on the covariates.

In the simulations that follow, we show how the issues with past work heavily affect practical performance of these methods, whereas FLAME, which does not introduce a measurement scale on the covariates, does not seem to have these problems. As we will see in the next section, FLAME balances between producing high quality almost-exact matches and computational efficiency, stemming from the use of bit-vectors and database tools.

5 Experiments

We study the quality and scalability of FLAME on synthetic and real data. The real data we use is the US Census 1990 dataset from the UCI Machine Learning Repository (Lichman 2013). The bit-vector and SQL implementations are referred to as FLAME-bit and FLAME-db respectively. FLAME-bit was implemented using Python 2.7.13 and FLAME-db using Python, SQL, and Microsoft SQL Server 2016. We compared FLAME with several other methods including:
(1) one-to-one Propensity Score Nearest Neighbor Matching (1-PSNNM) (Ross et al. 2015),
(2) Genetic Matching (GenMatch) \cite{DiamondSekhon2013}, (3) Causal Forest (Wager and Athey 2017), (4) Mahalanobis Matching and (5) double linear regression. In double linear regression, we fit two linear regressors, one for the treatment group and one for the control group; the estimate of treatment effect is given by the difference of the predictions of the two regressors. (Unlike the matching methods, the double regression method assumes a model for the outcome making it sensitive to misspecification. Here we correctly specified the linear terms of the generative model in the synthetic data experiments.) We also ran tests with Coarsened Exact Matching (CEM) \cite{Iacus2012} and Cardinality Match \cite{Zubizarreta2012,Zubizarreta2014}. CEM is best suited for numerical data and the R package does not automatically handle more than 15 covariates. Cardinality match does not scale well to the setting of our problem, since it tries to solve a computationally demanding mixed integer programming problem. The computation time results are in Table 2. The experiments were conducted on a Windows machine with Intel(R) Core(TM) i7-6700 CPU processor (4 cores, 3.40GHz, 8M) and 32GB RAM.

5.1 Experiments with Synthetic Data

Since the true treatment effect cannot be obtained from real data, we created simulated data with specific characteristics and known treatment effects. Note that both FLAME-db and FLAME-bit always return the same treatment effects. Four of the simulated experiments use data generated from special cases of the following (treatment $T \in \{0, 1\}$):

$$y = \sum_{i=1}^{10} \alpha_i x_i + T \sum_{i=1}^{10} \beta_i x_i + T \sum_{i=1, \ldots, 5, \gamma=1, \ldots, 5, \gamma \neq i} x_i x_{\gamma},$$

(5)

Here, $\alpha_i \sim N(10s, 1)$ with $s \sim \text{Uniform}\{-1, 1\}$, $\beta_i \sim N(1.5, 0.15)$. 19
Figure 1: Scatter plots of true treatment effect versus estimated treatment effect on every unit in the synthetic data generated. The regression model is misspecified, and performs poorly.

5.1.1 Regression cannot handle model misspecification

We generate 20,000 observations from (5), with 10,000 treatment units and 10,000 control units, where \( U = 5 \) and \( x^T_i, x^C_i \sim \text{Bernoulli}(0.5) \). The nonlinear terms will cause problems for the (mis-specified) linear regression models, but matching methods generally should not have trouble with nonlinearity. We ran FLAME, and all points were matched exactly on the first iteration yielding perfect CATEs. Scatter plots from FLAME and regression are in Figure 1. The axes of the plots are predicted versus true treatment effects, and it is clear that the nonlinear terms ruin the estimates of treatment effects from the regression models, whereas FLAME does not have problems estimating treatment effects.

5.1.2 Most matching methods cannot handle irrelevant variables

Because most matching methods do not consider prediction quality of variables, they might reasonably try to match on all variables equally, including irrelevant ones. This causes matching
methods to perform poorly when there are many irrelevant variables.

We consider 20K units (10K control and 10K treated) generated with (5), with an additional 20 irrelevant covariates (where $\alpha_i = \beta_i = 0$, but the covariates are in the database), with $U = 1$ for the nonlinear terms. We generate $x_i \sim \text{Bernoulli}(0.5)$ for $1 \leq i \leq 10$. For $10 < i \leq 30$, $x_i \sim \text{Bernoulli}(0.1)$ in the control group and $x_i \sim \text{Bernoulli}(0.9)$ in the treatment group.

During the execution of FLAME, irrelevant variables are successively dropped before the important variables. We should stop FLAME before eliminating important variables and the MQ drops to an unacceptable value. In this experiment, however, we also allowed FLAME to continue to drop variables until 28 variables were dropped and there were no remaining possible matches. Figure 2 shows scatter plots of estimated versus true treatment effects for FLAME (Early Stopping), FLAME (Run Until No More Matches) and other methods. In this experiment, Figure 2a is generated by stopping when the MQ suddenly drops from above -1 to below -50. Here 10 covariates are used and more than 15,000 out of 20,000 units are used within the matched groups. FLAME achieves the best performance as shown in Figure 2.

We also compare the execution time of both FLAME-bit and FLAME-db with all the methods listed in Figure 2. The timing results are reported in Table 2. As Table 2a shows, FLAME-bit is faster than most of the other approaches (including FLAME-db) for the synthetic data considered in this experiment. On the other hand, for the larger data analysis (Section 5.2), FLAME-db is much faster than all the other methods as shown in Table 2b illustrating its scalability. We give a more detailed comparison of FLAME-bit and FLAME-db in Section 5.1.5.

Based on the experimental results as well as the algorithm descriptions [Ross et al., 2015; Diamond and Sekhon, 2013; Iacus et al., 2012; Zubizarreta, 2012; Zubizarreta et al., 2014], we summarize the pros and cons of these algorithms in Table 3.

This experiment, and the previous one, illustrate the main general issues with classes of methods for causal inference: propensity score matching (of any kind) projects the data to one dimension.
sion, and thus cannot be used for CATE estimation. GenMatch has similar problems, and cannot be used for reliable CATE estimation. Regression and other modeling methods are subject to misspecification. There are many variations of matching and modeling, leading to similar problems: they generally suffer from one of the two types of issues illustrated in this simulated experiment: model misspecification or projection and loss of information.

**Variance estimation**

While the main thrust of the methodology is in reducing the bias of estimating a CATE, the methodology naturally lends itself for estimating an upper bound on the variance of the CATE. Here we briefly discuss the conditional variance of the estimation in the setting of Figure 2.

As is common in variance estimation we assume that given a unit $x$, the outcome of the treated and the outcome of the control are non-negatively correlated. This assumption allows to bound the conditional variance of the treatment effect using:

$$\text{Var}(y_t - y_c|x) \leq \text{Var}(y_t|x) + \text{Var}(y_c|x).$$

(6)

We then use the sample variance to estimate $\text{Var}(y_t|x)$ and $\text{Var}(y_c|x)$ for each group of units $g$. The estimates of the standard deviation upper bounds are summarized in Figure 3. Each box plot in the figure summarizes the standard deviations of groups in a single iteration of the while loop. They are arranged according to the order in which the variables are dropped. Since the $Y$’s are observed noiselessly, this method estimates a standard deviation of zero for the first few levels as no relevant covariates have been eliminated. The standard deviation increases abruptly once a relevant covariate is dropped since this introduces variability in the treatment effects observed within each group. A sharp increase in the standard deviations thus likely corresponds to the dropping of important covariates and a decay in the match quality. This suggests another heuristic for the early stopping of FLAME.
5.1.3 Decay of performance as less important variables are eliminated

To better understand the behavior of FLAME as it eliminates variables, we created a setting where the variables are all assigned non-zero importance. Again, 30 covariates were used. As FLAME drops variables, prediction quality smoothly degrades. This is meant to represent problems where the importance of the variables decreases according to an exponential or a power-law, as is arguably true in realistic settings. Accordingly, we create 10,000 control units and 10,000 treated units with the outcomes generated as follows:

\[ y = \sum_{i=1}^{20} \alpha_i x_i + 10T, \]  

where \( T \in \{0, 1\} \) is the binary treatment indicator, \( x_i \sim \text{Bernoulli}(0.5) \), \( \alpha_i = 5 \times \left( \frac{1}{2} \right)^i \) for exponential decay (in Figure 4a), and \( \alpha_i = 5 \times \frac{1}{1+i} \) for power-law decay (in Figure 4b). For both exponential and power law decay, variables with smaller indices \((1, 2, \cdots)\) are more important, and variables with higher indices \((20, 21, \cdots)\) are less important. In (7), all of the covariates contribute to the outcome positively. In the real world, variables can contribute to the outcome either positively or negatively, which leads to a smaller estimation bias since the FLAME tends to drop the positive variables and negative variables in alternating order. The case we are considering, where all \( \alpha_i \)'s are positive, is essentially a worst case. However, it allows us to see more easily how prediction quality degrades.

The results from FLAME are shown in Figure 4, which shows that (i) the variability of estimation degrades smoothly as more variables are dropped, and (ii) the bias still remains relatively small. In this experiment, the value of \( C \) is set to be 0.001. The effect of varying the parameter \( C \) is studied in Section 5.1.4. Since (7) is noise free and \( C \) is set to be small, FLAME dropped the covariates in ascending order of importance.
5.1.4 Effect of the $C$ parameter of on the behavior FLAME

This experiment aims to understand how the parameter $C$ would affect the estimation quality. Since the parameter $C$ trades off the Prediction Error (PE) and Balancing Factor (BF), we create a setting where variables that are more important to outcome prediction are less balanced. More specifically, we created 15,000 control units and 15,000 treated units with the outcomes given by

$$y = \sum_{i=1}^{20} \frac{1}{i} x_i + 10T$$

(8)

where $x_i \sim \text{Bernoulli}(0.1 + \frac{3i}{190})$ for the control group and $x_i \sim \text{Bernoulli}(0.9 - \frac{3i}{190})$ for the treatment group, and $T \in \{0, 1\}$ is the treatment indicator. According to (8), we expect that the larger the parameter $C$, the earlier the algorithm eliminates covariates of higher balancing factor.

As we can see from Figure 5 and 6, larger $C$ values encourage FLAME to sacrifice some prediction quality in return for more matches; and vice versa. Better prediction quality leads to less biased estimates while a larger balancing factor leads to more matched units. This is a form of bias-variance tradeoff. Figure 7 summarizes Figures 5 and 6 by plotting the vertical axis of Figure 5 against the vertical axis of Figure 6. Since the percent of units matched in Figure 5 is cumulative, the horizontal axis in Figure 7 also (nonlinearly) corresponds to the dropping of covariates. Each blue dot on the figures represents a matched group. The bias-variance tradeoff between estimation quality versus more matched groups is apparent; the left figure shows fewer but high quality (low bias) matches, whereas the right figure shows more matches that are lower quality (higher bias).

5.1.5 Scalability Evaluation

To evaluate scalability of both implementations of FLAME (FLAME-db and FLAME-bit), we again generate a synthetic dataset using the method described as in (5), but with different values of $n$ and/or $p$. Same as in the previous settings, $x_i^C \sim \text{Bernoulli}(0.1)$ and $x_i^T \sim \text{Bernoulli}(0.9)$ for
We compare the run time of FLAME-bit and FLAME-db as functions of $p$ in Figure 8a (with $n$ fixed to 100K), and of $n$ in Figure 8b (with $p$ fixed to 15). In Figure 8, each dot represents the average runtime over a set of 4 experiments with the same settings; the vertical error bars represent the standard deviations in the corresponding set of experiments (we omit the very small error bars in Figure 8a). The plots suggest that FLAME-db scales better with the number of covariates, whereas FLAME-bit scales better with the number of units, since pre-processing and matrix operations used in FLAME-bit are expensive when the number of columns is large.

5.2 Experiments with Real Data

5.2.1 The Effect of Marriage on Salary

The UCI US Census 1990 dataset [Lichman, 2013] has over 2.4 million units with variables including race, marital status, gender, and citizenship. Using 59 of the variables ($p = 59$), we investigate the causal effect of marital status ($T$) on wage or salary income ($Y$) in the year 1989. The wage variable (dIncome1) is binarized in the following way: 0 for $(0, 15,000]$ (low income), and 1 for larger than 15,000 (high income). This binarization gives 564,755 low income people and 656,127 high income people. The marital status is binarized with 1 for being married and 0 for unmarried (including divorced, widowed and separated). This preprocessing gives 722,688 control units (unmarried) and 498,194 treated units (married). We randomly sampled 10% of these units (122,089 units) as the holdout training set and used the rest (1,098,793 units) to estimate the treatment effect.

**Running time comparison:** Methods in Table 2b other than FLAME-db either did not finish within 10 hours or crashed, whereas FLAME-db took 1.37 hours. In this case, FLAME-bit encounters a overflow problem.

**Average treatment effect and fraction of data matched:** Since FLAME computes Condi-
tional Average Treatment Effect (CATE), we can use it to calculate an average treatment effect with respect to any distribution of interest. If we assume that the married population and unmarried population are similar and weight the CATEs by the number of units corresponding to each CATE, the estimated ATE of marital status on income is 0.534. FLAME utilizes almost all of the units in the dataset (1,061,003 out of 1,098,793 units).

**Analysis of treatment effect on sub-populations:** We studied the treatment effect of marriage on salary for different sub-populations defined by military service record and by citizenship status. We estimated the average treatment effect for each given sub-population by a weighted average of the estimated treatment effects in each group, with the weight being the number of units matched. In Figure 9a, the estimated treatment effect of being married is computed for the subpopulations defined by military record. For the horizontal axis, category 1 is “on active duty;” category 2 is “on duty in the past;” category 3 is “in reserve;” and category 4 is “no service.” Here, the error bars encode the weighted variance. According to our results, being married does affect one’s income. For those on active duty or in reserve, being married has a more positive treatment effect. Meanwhile, being married has approximately the same effect on income of those in active service and those with no service record. In Figure 9b, the estimated treatment effect of being married is computed for the subpopulations defined by citizenship status. For the horizontal axis, category 1 is “born in the U.S.;” category 2 is “born in Puerto Rico, Guam, and Outlying Islands;” category 3 is “born abroad of American parents;” category 4 is “U.S. Citizen by Naturalization” and category 5 is “not a U.S. citizen.” As shown in Figure 9b, being marriage has more positive effect on income for those who are in category 3 and 4, but the effect is not large.

5.2.2 The Effect of Smoking on Natality

In this section, we study the effect of cigarette use on pregnancy outcomes, using a 2010 dataset on Natality in the U.S. (Unknown 2011).
Each unit is a pregnant mother. Treated units are mothers who smoke cigarettes during pregnancy, and there are 2,190,410 units in the dataset, where 204,886 are treated units, and 1,985,524 are control units. The outcome is whether the infant is diagnosed with an abnormal condition after birth, where abnormal conditions include *assisted aentilation, admission to NICU, surfactant therapy received, antibiotics received for for suspected neonatal sepsis and seizures or serious neurologic dysfunction*. Abnormal conditions are assigned outcome ‘1,’ while normal conditions are assigned outcome ‘0.’ There are 86 covariates about the mother and her health history. We reserved 10% of the data as the holdout set, and a linear ridge regressor was used as the regression model for the Prediction Error computation.

Our experiment indicates an approximately 4.8% increase in the chance of abnormal pregnancy outcomes due to smoking. We also study the estimated treatment effects (CATE) on the sub-populations defined by [Unknown (2011)](a) mother’s marital status, (b) pregnancy hypertension, (c) gestational hypertension, and (d) pregnancy diabetes, while all other variables are marginalized out. The results are displayed in Figure [10].

6 Theory

FLAME is an approximately-exact matching algorithm, which means it trades off statistical bias for computational speed. In this section we provide insight into the bias that an oracle version of FLAME induces when estimating heterogeneous causal effects. To evaluate the theoretical behavior of the algorithm we consider the outcome model

$$ y_i = \alpha_0 + \sum_{j=1}^{p} \alpha_j x_{ij} + \beta_0 T_i + T_i \sum_{j=1}^{p} \beta_j x_{ij} $$

that corresponds to a treatment effect $\beta_j$ being associated with every covariate $x_{ij}$ for individual $i$. Here $y_i$ is the observed outcome and $T_i$ is the observed treatment indicator. We are interested
in the bias of FLAME for this simple non-noisy outcome model. We define the Oracle FLAME
algorithm as a simplified version of Algorithm 1 that in addition to the data takes as input the
correct order of importance for the covariates. Without loss of generality let that order be \( p, p - 1, \ldots, 1 \). Given this ordering, we can directly compute the bias of the FLAME estimates for
various combinations of covariates (“bins”).

To compute the overall bias of Oracle FLAME, in theory we would enumerate all possible
covariate allocations and run Oracle FLAME on each of those. For example, in the two-covariate
setting with possible attribute values 0 and 1, there are \( 2^2 \times 2^2 = 16 \) possible covariate allocations
for treatment and for control units leading to \( 16 \times 16 = 256 \) total possible allocations. Since we
are interested only in the bias induced by the algorithm itself, we consider only treatment-control
allocations where our procedure yields an estimate for each covariate combination. In cases
where we do not have an estimate of treatment effect for each covariate combination, we cannot
calculate the bias of the algorithm for any distribution that has support over the full covariate
space; Oracle FLAME’s bias estimates would not be defined on part of the covariate space in
these cases. For example, in the two covariate setting, the allocation of a total of one treated and
one control unit with both having \( x_1 = x_2 = 0 \) would not be considered in our bias calculation
since the exact matching procedure would obtain an estimate for that covariate combination only
and not for the other three. An allocation consists of a set of covariate values, and treatment indi-
cators. (The number of units in each covariate bin does not matter, what matters is that there is at
least one treatment and one control in the bin, so that we can compute the bin’s treatment effect.)
For instance, one of the valid allocations would have at least one treatment and one control unit
in each bin (a bin is a combination of covariates). Another valid allocation would have treatment
and control units in most (but not all) bins, but when the bins are collapsed according to Oracle
FLAME, each bin still receives an estimate.

We perform these computations for two and three binary covariates and use the results to
provide intuition for when we have arbitrarily many covariates. The main results are as follows.

**Theorem 1 (Two covariates)**  (i) There are 59 valid allocations. (ii) Under a uniform distribution over valid allocations the biases (taking expectation over the allocations) are given by:

\[
\text{bias} = (\text{expected TE under FLAME}) - (\text{actual TE}) =
\begin{cases}
  x_1 = 0 & (20\beta_1 + 41/2\beta_2 - 20\beta_1 - 41/2\beta_2) \\
  x_1 = 1 & (20\beta_1 + 41/2\beta_2 - 20\beta_1 - 41/2\beta_2)
\end{cases}
\]

**Theorem 2 (Three covariates)**  (i) There are 38070 valid allocations. (ii) Under a uniform distribution over valid allocations the biases (taking expectation over the allocations) are given by:

\[
\text{bias} =
\begin{cases}
  x_2 = 0 & (5976 + 34/105)\beta_1 + 7854 + 61/210)\beta_2 + 11658\beta_3 \\
  x_2 = 1 & (12755 + 6/7)\beta_1 - (16513 + 4/21)\beta_2 + 19035\beta_3
\end{cases}
\]

**Proof Sketch.** The proofs of these theorems are computer programs. They calculate the bias analytically (rather than numerically). They enumerate all possible covariate allocations. For each allocation, the program checks if the allocation is valid and then runs Oracle FLAME to compute the conditional average treatment effect in each bin. Subtracting these estimate from the true CATE values and averaging (uniformly) over bins yields the bias for that allocation. The theorems report the average over valid allocations.
The FLAME estimates are biased only by fractions of the treatment effects associated with the covariates ($\beta_j$ for $j > 0$) rather than any baseline information (the $\alpha$’s) or a universal treatment effect ($\beta_0$). This is an appealing quality as it suggests that rare covariates that have large effects on baseline outcomes are unlikely to have undue influence on the bias of the treatment effect estimates. Further, this means that in cases where the causal effect is homogeneous (that is, $\beta_j = 0$ for $j > 0$), this effect can be estimated without any bias. This demonstrates that aggregating FLAME estimates naturally adapts to average treatment effect estimation. This provides an advantage over methods that directly target that effect (such as propensity score matching) since FLAME provides an estimate of potential heterogeneity at no additional cost.

Proof by enumeration becomes slow and impractical for higher dimensional problems, but the patterns of bias are evident from Theorems 1 and 2. In higher dimensional settings, the bias remains a function of the $\beta_j$ for $j > 0$ and more importantly, the sign of the bias is a function of the relative signs of the $\beta$’s. These patterns can be leveraged in future algorithmic development and are explored further in Section 7.

7 Discussion

In this paper we introduced FLAME, a novel algorithm for covariate based matching in observational studies.

- It provides a method for approximating the gold-standard performance of exact matching.
- Its efficiency stems from careful bit-vector operations and specialized database queries.
- We can theoretically evaluate the bias under different distributions of the covariates.

The theoretical bias results of Section 6 provide several anchors for future work. Considering the setting of two uniformly distributed covariates: if $\beta_1$ and $\beta_2$ have the same sign then the CATE
for $x_1 = x_2$ sees the greatest bias, while $x_1 \neq x_2$ sees the bias reduced. If the $\beta$s have different signs, the setting is reversed. Knowing these patterns of bias is suggests a natural future direction for algorithm development. In particular, it is possible to mitigate these adverse effects by one of two approaches: first, one can augment the algorithm to perform back-track steps (this would allow covariates to be returned into the potential pool of covariates to drop in line 5 of Algorithm 1). This would allow for multiple estimates of the effect for a single covariate combination — further combining these will likely produce a more efficient estimate. A second approach allows for using the FLAME technique to construct a hierarchical Bayesian model for the CATEs within each bin. This approach can leverage information about easily estimated CATEs using many covariates in order to smooth estimates of harder-to-estimate CATEs without requiring a model for the outcome.

Further generalizations of FLAME can accommodate continuous and other high dimensional covariates. A natural approach for continuous covariates coarsens them to discrete ones and adds them to the existing framework. However, drawbacks of such an approach are that it throws away information during coarsening and that coarsening cannot be accomplished automatically. An alternative approach can leverage the natural metric associated with many continuous and high dimensional covariates by requiring matches in FLAME to be close in that metric. These continuous covariates can be subjected to a similar dropping scheme as FLAME, while tuning the closeness parameter provides a trade-off between the importance of discrete and continuous information. These are ongoing research areas for the authors.

Given FLAME’s large benefits in scalability for massive data, parallelization is a clear future direction. Its SQL queries already handle datasets that do not fit in memory, but we may be able to create a faster parallel version of FLAME that takes advantage of the geometry of the matching problem. For instance, FLAME’s loop over covariates at each iteration can be split among processors, some of its later computations done, and joined afterwards, all using efficient
SQL queries. FLAME’s design inspiration comes both from statistics (matching as exactly as possible) and computationally efficiency (efficient SQL queries). It is part of a next generation of statistical techniques that are explicitly designed for use on huge datasets that take advantage of modern computational machinery.

Code implementing the FLAME algorithm as well as the examples in this paper is available on the authors’ website.

SUPPLEMENTARY MATERIAL

References

Belloni, A., Chernozhukov, V., and Hansen, C. (2014). Inference on treatment effects after selection among high-dimensional controls. *The Review of Economic Studies*, 81(2):608–650.

Brookhart, M. A., Schneeweiss, S., Rothman, K. J., Glynn, R. J., Avorn, J., and Stürmer, T. (2006). Variable selection for propensity score models. *American Journal of Epidemiology*, 163(12):1149–1156.

Chapin, F. (1947). *Experimental Designs in Sociological Research*. Harper; New York.

Cochran, W. G. and Rubin, D. B. (1973). Controlling bias in observational studies: A review. *Sankhyā: The Indian Journal of Statistics, Series A*, pages 417–446.

Diamond, A. and Sekhon, J. S. (2013). Genetic matching for estimating causal effects: A general multivariate matching method for achieving balance in observational studies. *The Review of Economics and Statistics*, 95(3):932–945.

Farrell, M. H. (2015). Robust inference on average treatment effects with possibly more covariates than observations. *Journal of Econometrics*, 189(1):1–23.

Greenwood, E. (1945). *Experimental sociology: A study in method*. King’s crown Press.

Iacus, S. M., King, G., and Porro, G. (2011a). Causal inference without balance checking: Coarsened exact matching. *Political Analysis*, page mpr013.
Iacus, S. M., King, G., and Porro, G. (2011b). Multivariate matching methods that are monotonic imbalance bounding. *Journal of the American Statistical Association*, 106(493):345–361.

Iacus, S. M., King, G., and Porro, G. (2012). Causal inference without balance checking: Coarsened exact matching. *Political analysis*, 20(1):1–24.

Keele, L. and Zubizarreta, J. R. (2014). Optimal multilevel matching in clustered observational studies: A case study of the school voucher system in Chile. *arXiv preprint arXiv:1409.8597*.

Lichman, M. (2013). UCI machine learning repository.

Noor-E-Alam, M. and Rudin, C. (2015a). Robust nonparametric testing for causal inference in natural experiments. *Working paper*.

Noor-E-Alam, M. and Rudin, C. (2015b). Robust testing for causal inference in natural experiments. *Working paper*.

PostgreSQL (2016). *PostgreSQL*.

Rassen, J. A. and Schneeweiss, S. (2012). Using high-dimensional propensity scores to automate confounding control in a distributed medical product safety surveillance system. *Pharmacoepidemiology and drug safety*, 21(S1):41–49.

Resa, M. and Zubizarreta, J. R. (2016). Evaluation of subset matching methods and forms of covariate balance. *Statistics in Medicine*.

Rosenbaum, P. R. (2016). Imposing minimax and quantile constraints on optimal matching in observational studies. *Journal of Computational and Graphical Statistics*, (just-accepted).

Rosenbaum, P. R. and Rubin, D. B. (1983). The central role of the propensity score in observational studies for causal effects. *Biometrika*, 70(1):41–55.

Ross, M. E., Kreider, A. R., Huang, Y.-S., Matone, M., Rubin, D. M., and Localio, A. R. (2015). Propensity score methods for analyzing observational data like randomized experiments: challenges and solutions for rare outcomes and exposures. *American journal of epi-*
Rubin, D. B. (1973a). Matching to remove bias in observational studies. *Biometrics*, pages 159–183.

Rubin, D. B. (1973b). The use of matched sampling and regression adjustment to remove bias in observational studies. *Biometrics*, pages 185–203.

Rubin, D. B. (1976). Multivariate matching methods that are equal percent bias reducing, i: Some examples. *Biometrics*, pages 109–120.

Rubin, D. B. (2005). Causal inference using potential outcomes: Design, modeling, decisions. *Journal of the American Statistical Association*, 100:322–331.

Rubin, D. B. (2008). For objective causal inference, design trumps analysis. *The Annals of Applied Statistics*, pages 808–840.

Rubin, D. B. and Thomas, N. (1996). Matching using estimated propensity scores: relating theory to practice. *Biometrics*, pages 249–264.

Salimi, B., Cole, C., Ports, D. R. K., and Suciu, D. (2017). Zaliql: Causal inference from observational data at scale. *PVLDB*, 10(12):1957–1960.

Schneeweiss, S., Rassen, J. A., Glynn, R. J., Avorn, J., Mogun, H., and Brookhart, M. A. (2009). High-dimensional propensity score adjustment in studies of treatment effects using health care claims data. *Epidemiology (Cambridge, Mass.)*, 20(4):512.

Unknown (2011). User guide to the 2010 natality public use file.

Wager, S. and Athey, S. (2017). Estimation and inference of heterogeneous treatment effects using random forests. *Journal of the American Statistical Association*, (just-accepted).

Zubizarreta, J. R. (2012). Using mixed integer programming for matching in an observational study of kidney failure after surgery. *Journal of the American Statistical Association*, 107(500):1360–1371.

Zubizarreta, J. R., Paredes, R. D., and Rosenbaum, P. R. (2014). Matching for balance, pairing
for heterogeneity in an observational study of the effectiveness of for-profit and not-for-profit high schools in Chile. *The Annals of Applied Statistics*, 8(1):204–231.
Algorithm 1: Generic FLAME Algorithm: FlameGeneric

Input: (i) Input data $D = (X, Y, T)$. (ii) holdout training set $D^H = (X^H, Y^H, T^H)$.

Output: A set of matched groups $\{MG_l\}_{l \geq 1}$ and ordering of covariates $j_1^*, j_2^*, \ldots$, eliminated.

1. Initialize $D_0 = D = (X, Y, T), J_0 = \{1, \ldots, p\}, l = 1, run = True, MG = \emptyset$. ($l$ is the index for iterations, $j$ is the index for covariates)

2. $(D_0^m, D_0 \setminus D_0^m, MG_1) = \text{BasicExactMatch}(D_0, J_0)$.

3. while $run = True$ and $D_{l-1} \setminus D_{l-1}^m \neq \emptyset$ (we still have data to match) do

   4. $D_l = D_{l-1} \setminus D_{l-1}^m$ (remove matches)

   5. for $j \in J_{l-1}$ (temporarily remove one feature at a time and compute match quality) do

      6. $(D_{l}^{mj}, D_l \setminus D_l^{mj}, MG_{temp}) = \text{BasicExactMatch}(D_l, J_{l-1} \setminus j)$.

      7. $D^{Hj} = [X^H(:, J_{l-1} \setminus j), Y^H, T^H]$

      8. $q_{lj} = \text{MQ}(D_{l}^{mj}, D^{Hj})$

   end

   9. if other stopping conditions are met, then

      10. $run = False$ (break from the while loop)

   end

   11. $j_l^* \in \text{arg min}_{j \in J_{l-1}} q_{lj}$: (choose feature to remove)

   12. $J_l = J_{l-1} \setminus j_l^*$ (remove feature $j_l^*$)

   13. $D_l^m = D_l^{mj^*}$ and $MG_l = MG_{temp}$ (newly matched data and groups)

   14. $l = l + 1$

end

15. return $\{MG_l, D_l^m, J_l\}_{l \geq 1}$ (return all the matched groups and covariates used)
Algorithm 2: BasicExactMatch procedure

**Input**: Unmatched Data $D_{um} = (X, Y, T)$, subset of indexes of covariates $J^s \subseteq \{1, \ldots, p\}$.

**Output**: Newly matched units $D^m$ using covariates indexed by $J^s$ where groups obey (R1), the remaining data as $D_{um} \setminus D^m$ and matched groups for $D^m$.

1. $M_{raw} = \text{group-by}(D_{um}, J^s)$ (form groups by exact matching on $J^s$)
2. $M = \text{prune}(M_{raw})$ (remove groups not satisfying (R1))
3. $D^m = \text{Get subset of } D_{um} \text{ where the covariates match with } M$ (recover newly matched units)
4. return $\{D^m, D_{um} \setminus D^m, M\}$.

| first variable | second variable | T | $b_u$ | $b_u^*$ | $c_u$ | $c_u^*$ | is matched? |
|----------------|-----------------|---|-------|---------|-------|---------|-------------|
| 0              | 2               | 0 | 6     | 18      | 1     | 1       | No          |
| 1              | 1               | 0 | 4     | 11      | 2     | 1       | Yes         |
| 1              | 0               | 1 | 1     | 3       | 1     | 1       | No          |
| 1              | 1               | 1 | 4     | 12      | 2     | 1       | Yes         |

Table 1: Example population table illustrating the bit-vector implementation. Here the second unit and the fourth unit are matched to each other while the first and third units are left unmatched.
Figure 2: Scatter plots of true treatment effect versus estimated treatment effect on matched units. Figure 2a is from a typical FLAME run where it stopped before dropping any variable that significantly worsens prediction error; Figure 2b is the result of FLAME when run beyond its natural limit and important variables are eliminated, until no more matches were possible; Figure 2c is the result of 1-PSNNM; Figure 2d is the result of GenMatch; Figure 2e is the result of Causal Forest; Figure 2f is the result of Mahalanobis matching.
| Method          | Time (seconds)   | Method          | Time (hours)   |
|----------------|------------------|----------------|----------------|
| FLAME-bit      | 27.68 ± 0.80     | FLAME-bit      | Crashed        |
| FLAME-db       | 57.93 ± 0.47     | FLAME-db       | 1.37           |
| Causal Forest  | 52.34 ± 1.82     | Causal Forest  | Crashed        |
| 1-PSNNM        | 14.78 ± 0.70     | 1-PSNNM        | > 10           |
| Mahalanobis    | 76.79 ± 0.49     | Mahalanobis    | > 10           |
| GenMatch       | > 150            | GenMatch       | > 10           |
| Cardinality Match | > 150        | Cardinality Match | > 10         |

(a) Timing results of FLAME compared with other methods on the synthetic data generated by the same procedure as in Figure 2, in the format of “average time” ± “standard deviation”. It summarizes 3 runs.

(b) Timing results of FLAME compared with other methods on the US Census 1990 dataset as discussed in Section 5.2.

### Table 2: Timing comparison results.

| Method            | scalability | uses holdout training | provides matches | sensitive to model choice |
|-------------------|-------------|-----------------------|------------------|--------------------------|
| FLAME             | 3           | Yes                   | Yes              | No                       |
| 1-PSNNM           | 3           | No                    | Yes              | Yes                      |
| GenMatch          | 1           | No                    | Yes              | No                       |
| CausalForest      | 2           | Yes                   | No               | No                       |
| Mahalanobis       | 1           | No                    | Yes              | No                       |
| CEM               | 2           | No                    | Yes              | No                       |
| Cardinality Match | 1           | No                    | Yes              | No                       |

Table 3: For columns “scalable”, we use ratings 1-3 with larger number indicating better scalability. For other columns, Yes or No indicates whether that attribute is presented.
Figure 3: This figure plots the standard deviation upper bound estimates. The box plots summarize the estimated standard deviation upper bounds of the groups as the covariates are eliminated. The lower and upper boundaries of the boxes are the first quantile and the third quantile of the distribution, while the upper lower black bar and the upper black bar bound the [0.05, 0.95] confidence interval.
Figure 4: Degradation of treatment effect estimates as FLAME drops variables. *Left:* variable importance decreases exponentially with base being $\frac{1}{2}$. *Right:* the variable importance decreases according to a power-law with exponent -1. The true treatment effect is 10 for all units in both subfigures. Dot size represents the number of units corresponding to that dot. There are fewer matches in high dimensions, and those matches are of higher quality. This shows that the bias of estimation degrades smoothly as we eliminate variables.
Figure 5: This figure shows the percentage of units matched as FLAME eliminates variables with $C$ being 0.1, 0.5 and 1. More units are matched when the value of $C$ is large. The counts in these subfigures are cumulative. The vertical axis denotes the percentage of units matched.

Figure 6: This figure shows how estimation quality changes as FLAME eliminates variables with $C$ being 0.1, 0.5 and 1. The bias is smaller when the value of $C$ is small. As in Figure 4, the size of the dots represents the number of units corresponding to that dot.
Figure 7: Estimated treatment effect versus percentage of units matched. Summary of Figure 5 and Figure 6; the vertical axis of Figure 5 versus the vertical axis of Figure 6.

Figure 8: This figure shows how the runtime scales with the number of units and number of covariates for FLAME-db and FLAME-bit. In general, FLAME-bit is faster when the number of covariates is relatively small so that the multiplication of the bit vectors is not too expensive. On the other hand, FLAME-db is faster when the number of variables is relatively large.
Figure 9: *Left:* estimated treatment effect of marriage on the sub-populations defined by military service record; the categories are “on active duty,” “on duty in the past,” “in reserve,” or “no service,” respectively. *Right:* estimated treatment effect of marriage on the subpopulation defined by citizenship status; the categories are “born in the U.S.,” “born in Puerto Rico,” Guam, and Outlying Islands,” “born abroad of American parents,” “U.S. Citizen by naturalization,” and “not a U.S. citizen.” The dots are weighted averages, and error bars are weighted standard deviations.
Figure 10: In all subfigures, whole on the x-axis corresponds to a plot for the whole population. (a) 0: the mother is not married; 1: is married. (b) 0: pregnancy hypertension is not reported; 1: is reported. (c) 0: gestational hypertension is not reported; 1: is reported. (d) 0: pregnancy diabetes is not reported; 1: is reported. The presence of pregnancy diabetes, pregnancy hypertension or gestational hypertension leads to a higher variance in the treatment effect, and for diabetes and hypertension, a higher treatment effect. Meanwhile, married mothers have a less pronounced treatment effect with a smaller variance.