Machine Learning for Experimental Design: Methods for Improved Blocking

Brian Quistorff∗ and Gentry Johnson†

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Abstract

Restricting randomization in the design of experiments (e.g., using blocking/stratification, pair-wise matching, or rerandomization) can improve the treatment-control balance on important covariates and therefore improve the estimation of the treatment effect, particularly for small- and medium-sized experiments. Existing guidance on how to identify these variables and implement the restrictions is incomplete and conflicting. We identify that differences are mainly due to the fact that what is important in the pre-treatment data may not translate to the post-treatment data. We highlight settings where there is sufficient data to provide clear guidance and outline improved methods to mostly automate the process using modern machine learning (ML) techniques. We show in simulations using real-world data, that these methods reduce both the mean squared error of the estimate (14%-34%) and the size of the standard error (6%-16%).

Keywords: Machine Learning, Big Data, Experimentation, Causality, Blocking, Stratification, Pair-wise matching, Rerandomization

1 Introduction

In the design of experiments, the method of treatment randomization can be used to reduce the variance of the estimated treatment effect so as to improve efficiency, protect against type I errors, and increase power (Bruhn and McKenzie, 2009)—particularly for small- and medium-sized experiments. This is achieved by improving variable balance (similarity of a variable’s distribution between the treated and control groups) for variables that are important predictors of the post-treatment outcome.

For illustrative purposes we first look at the most common randomization method, blocking (sometimes called stratifying†), originally proposed by Fisher (1935). Blocking creates a partition of the sample, separating pre-treatment data into blocks with a minimum size \( c_B \) (typically four, Kernan 1999) and assigning an equal number of treated and control units within each block. By dividing an important variable’s extent with these blocks, one can increase balance along this variable. For example, if we ensure that units with different values of an important categorical variable are partitioned into separate blocks, then we can ensure that, even in finite-sample (not just in expectation), treatment will be uncorrelated with this variable.

Existing guidance on how to use pre-treatment data is not fully data-driven and so involves many decisions by the experimenter, wasting time and potentially resulting in sub-optimal treatment effect estimation. There are two main existing strategies for picking blocks. We show

∗Microsoft Technology + Research. Contact: Brian.Quistorff@microsoft.com.
†Amazon, AWS Central Economics. Contact: gentryaj@amazon.com.
‡In some settings “stratification” refers to the drawing the experimental sample from the population and “blocking” refers to assigning treatment.
how both can be improved by using modern off-the-shelf machine learning (ML) solutions that make our proposed procedures mostly data-driven. We also show how to choose among the available strategies.

The most common approach for determining blocks is what we will refer to as variable selection. This strategy attempts to select variables that will be strongly related to the post-treatment outcome. Blocks are then defined by a (potentially uneven) grid from splitting each variable separately and taking the Cartesian product. The number of selected variables is kept small as there is a cost to stratifying on unimportant variables. Imbens et al. (2009) show that while stratification on a variable can not increase the true expected squared error of the estimate, it does increase the estimate of its variance when accounting for stratification due to a degrees-of-freedom adjustment as discussed below (one could use the variance estimator which ignores the stratification, but this is overly conservative). In their survey of this approach, Bruhn and McKenzie (2009) recommend selecting at least the pre-treatment outcome variable—as most outcomes have some unit-level persistence—and a geographic variable, as outcome shocks are likely to be correlated within geographic regions (i.e., the data generating process (DGP) is time-varying). With multiple pre-treatment periods of data, they suggest that one could determine which additional variables to include based on how each early variable is correlated with later pre-treatment outcomes. Even if there are many related variables, they caution against including too many since each new variables decreases the balance on existing ones (given that blocks have a minimum size so that the granularity along existing dimensions must decrease). In their simulation studies, they include four blocking variables. They recommend splitting variables by a roughly even number of quantiles. Overall, the guidance leaves some areas unspecified (how exactly to determine which variables to include, how many quantiles to split variables by) and some areas sub-optimal (partitioning by a grid is sub-optimal when units are unevenly distributed across multiple selected variables as increasing the granularity of the grid quickly causes some grid cells to reach the minimum cell size).

An alternative strategy for blocking has been to use an estimated prediction model to determine which units to group together. Barrios (2014) and Aufenanger (2017) both suggest, in different settings, using pre-treatment data to build a model of the pre-period outcome using pre-period covariates and then generating predicted values—so-called pre-period prognostic scores (Hansen, 2008). Blocks are formed by ordering units by their prognostic score and then sequentially allocating blocks of a common size. The guidance here is well specified, though we note that there may be more optimal ways to partition based on the prognostic score, given that the default method may create more blocks than is helpful for minimizing treatment effect error and therefore result in larger than necessary standard errors.

The approaches differ due to their assumptions about the DGP, particularly about its temporal properties. If the DGP is constant over time and well estimated by the predictive model in terms of available predictors and functional form, then the prognostic score approach is optimal. It efficiently uses pre-treatment information both by utilizing weakly related covariates discarded by the variable selection strategy and also by collapsing all covariates to a single dimension and thus making it easier to find an optimal partition. Reducing to a single dimension, however, often results in units with similar prognostic scores that have very different covariates. If the DGP changes over time, units with similar pre-treatment prognostic scores may not have similar future prognostic scores. In this case, it is beneficial to block instead on a handful of fixed characteristics (e.g., geographic and demographic variables). Similarly, if the predictive model cannot closely approximate the functional form of the DGP, it may be more beneficial to block on separate variables rather than a composite index. If the predictive model is missing variables, then there may be persistence in the outcome variable over time not captured by the model, making it beneficial to block on the actual value of the pre-treatment outcome as this is informative in addition to $\hat{y}_{pre}$.

\footnote{For example suppose you estimate a model with a squared covariate term. Then a unit will be put close to one with the opposite value, which may differ significantly from the true model.}
We show that, when there are multiple pre-treatment periods of data, there are ways to choose between the variable selection and prognostic score strategies. We also apply standard ML tools to automate both. This includes a strategy for determining the number of blocks, again an area with little guidance, where we balance the goals of improving estimate accuracy and reducing standard errors. Most of the improvements can be made using off-the-shelf ML tools, though we detail some areas where custom solutions would be helpful.

We note that there are additional situations in which one would want to block an experiment. It is commonly done if subgroup analysis is expected to be performed, as (a) the pre-specification guards against claims of searching indiscriminately for statistically significant subgroups and (b) it improves the precision of these estimates. We show how to include these extra block-constraints in the strategies we present. Finally, it is noteworthy that in the context of two-stage randomized trials, which we do not study here, one can form blocks in the second stage (using data from the first stage) to vary the treatment percentage across blocks in ways that can increase estimation precision—the so-called Neyman Allocation (Tabord-Meehan, 2018).

We discuss the basic ML tools involved and our proposed strategies in Section 2. In Section 3 we discuss the application of these tools to the other most common methods of randomization. In Section 4 we use real-world data to compare our proposed strategies to hand-built blocking. We conclude in Section 5.

2 Algorithms

We first describe our notation and review basic goals. Then we discuss a few standard general ML tasks and highlight the most common method used currently for each. We then outline our proposed automated strategies that use these methods and then how to select the optimal one. Finally, we propose modified strategies when different types of data are available.

2.1 Econometric setup

Suppose the following data generating process (DGP)

\[ y_{it} = \beta d_{it} + h_t(X_i) + u_{it} \]

where \( i \in [1, ..., n] \) indexes experimental units (e.g. customers), \( t \) indexes time, and, as above, \( d \) is the binary treatment (zero for all units in the pre-periods and treatment only changes in one time period), \( h \) is potentially time-varying, \( X_i \) are the observed covariates, and the \( u_{it} \) are independent across units but may be correlated across time for an individual as we do not measure all characteristics. We assume we have one post period and at least one pre-period (i.e. a baseline) of data. We also assume that we will analyze the experiment using data from post and include dummy variables for each block. 3

In this paper, as is widely accepted in the literature on experimentation and causal inference more broadly, we follow the potential outcomes framework (Cochran and Rubin, 1973; Holland, 1986). More formally, if we just consider the post period, then we have outcome \( y_i \) of unit \( i \). When unit \( i \) receives treatment \( d_i = 1 \), her outcome is \( y_{i1} \), and when she receives treatment \( d_i = 0 \), her outcome is \( y_{i0} \). The identification problem is that we cannot observe unit \( i \) in both states, meaning that we must use different units altogether to serve as the counterfactual for \( i \). The average treatment effect (ATE) is defined as \( \beta = E[y_{i1} - y_{i0}] = E[y_{i1}] - [y_{i0}] \). Without any source of randomization we would estimate

3Though Bruhn and McKenzie (2009) note that in practice blocking dummies are often not included, they show empirically that this leads to overly conservative standard errors. CPMP (2004) similarly states that “analysis should reflect the restriction on randomisation implied by the stratification.”
The first term on the right-hand side is the average treatment effect on the treated. The second is often referred to as selection bias. To eliminate selection bias the Conditional Independence Assumption, \( \{y_{0i}, y_{1i}\} \perp \perp d_i|X_i, \) must be met (Rosenbaum and Rubin, 1983). In non-experimental causal inference settings, the intuition underlying this assumption is that, after controlling for observable characteristics, treatment is as good as random. It also implies that \( E[y_{1i}|X_i, d_i = 1] = E[y_{0i}|X_i, d_i = 0] = E[y_{1i} - y_{0i}|X_i], \) and therefore \( \beta = \beta. \)

In experimental settings, it can be easily seen that random assignment to treatment implies the Conditional Independence Assumption. In fact, conditioning on \( X_i \) is not even necessary for the assumption to hold, and thus inference in experimental settings is generally far more convincing than in observational settings. While pure randomization provides identification of \( \beta, \) more sophisticated treatment assignment mechanisms such as blocking bring other advantages, as mentioned briefly above and described in more detail below.

The standard benefits mentioned to motivate blocking include reducing Type I error, reducing Type II error (increasing power), and increasing efficiency. Type I error refers to the chance of a false-positive result given no effect exists. This can happen if there is a finite sample correlation between the assigned treatment and a prognostic factor. Blocking will reduce the chance of such a correlation, and while some experimenters may address this with an ex-post adjustment, ex-ante restrictions are more efficient (Bruhn and McKenzie, 2009). We, therefore, can reduce Type I errors by reducing the mean-squared error (MSE) of the estimated treatment effect. Type II error refers to the chance of failing to detect an effect when one exists. This is directly related to the variance of the outcomes between the two treatment arms. Blocking on prognostic factors reduces the sample variances. We, therefore, can increase power by reducing the standard error of the estimated treatment effect. Efficiency refers to the number of observations required to detect an effect for a given experimental setup. While dependent on many factors, it is typically thought of along the dimension of power. The more power required, the larger the experiment must be. We will therefore think about statistical efficiency in terms of reducing standard errors.

Blocking would, therefore, ideally reduce the estimate’s MSE and the estimate’s standard error. These two goals are typically, but not always, aligned. Blocking on the most important expected prognostic factors typically improves both, but as mentioned above there is a degree-of-freedom cost in the estimate’s standard error. For example, using the OLS regression formula, \( \hat{\beta} = \sqrt{s^2(\hat{X}'\hat{X})^{-1}}, \) where \( s^2 = \hat{u}'\hat{u}/(n-b-1), \) \( \hat{u} \) are the fitted residuals, there are \( b \) blocks, and \( \hat{X} \) includes \( d \) and along with all the blocking variables. Suppose two blocking partitions, with \( b \) and \( b+1 \) blocks respectively. As treatment is assigned orthogonal to the blocking factors, we can ignore differences in the \( (\hat{X}'\hat{X})^{-1} \) term.\(^4\) The extra blocking may reduce the residuals \( \hat{u}'\hat{u}, \) but might increase the standard error through the \( \sqrt{1/(n-b-1)} \) term. If the extra blocking does not improve the residuals then the cost in terms of the relative increase in standard error is

\[
\frac{s.e.(\hat{\beta}_{b+1})}{s.e.(\hat{\beta}_{b})} = \sqrt{\frac{n-b-1}{n-b-2}}.
\]

This cost decreases with sample size, and conditional on sample size, each additional block is increasingly costly (though bounded as the maximum number of blocks is roughly \( n/c_B. \)) For

\[\hat{\beta} = E[y_{1i}|d_i = 1] - E[y_{0i}|d_i = 0]
= (E[y_{1i} - y_{0i}|d_i = 1]) + (E[y_{0i}|d_i = 1] - E[y_{0i}|d_i = 0]).\]
a sense of scale, with \( n = 200 \) and \( c_B = 4 \), the first partition block increases the standard error by roughly 0.25\% and the \( n/c_B \) block increases the standard error by 0.34\%. For a sample of \( n = 400 \) the numbers are 0.13\% and 0.14\%. The partition, therefore, that minimizes the estimate’s standard error can have fewer blocks than the one that minimizes the estimate’s MSE. If any block in the partition that minimizes the effect standard error has a size of at least \( 2c_B \) then splitting it would improve the estimate’s MSE.

An additional motivation for blocking can emerge if the experimenter expects to perform subgroup analysis across a particular variable to look for heterogeneity. In this case, the experimenter would have selected \( \tilde{X} \) variables with an existing partition (likely a grid) \( \Pi \) for this analysis. For example, in the simplest case, all \( \tilde{X} \) variables could be split at their median values creating \( 2|\tilde{X}| \) initial blocks. In Section 2.3 and Section 2.4, we suggest minor adaptations to the procedures in this paper when an ex-ante subgroup analysis plan motivates blocking.

Given the two goals (of reducing the estimate’s MSE and standard error) might diverge, one must decide on an overall strategy. Ex-post one could optimally select among candidate partitions given a weighting between the two goals, but ex-ante this is much harder. While we note later how to do this when data is available (see Section 2.6.2), typically the data will not be available or can be put to better use. We, therefore, put forward a simple and reasonable approach that tries to balance them without explicitly optimizing the two goals. We create a sequence of partitions (discussed below) and find the partition where its fitted outcome model (fitting \( y \) to the block variables) has the best expected out-of-sample accuracy. This naturally limits the partition complexity to some degree, as when building a predictive model, a partition that is too fine-grained will over-fit to its training data and perform badly out-of-sample (e.g., a partition with a block for every observation has clearly gone beyond finding generalizable patterns and instead memorizes the idiosyncrasies of the current sample). This strategy, of estimating the out-of-sample performance of a model, can be done efficiently using the same data via a procedure called cross-validation (discussed below).

The value of blocking decreases with sample size. As the sample size increases, the chance of a finite-sample correlation between treatment and a prognostic factor decreases. Therefore the concern about the estimate’s MSE becomes less important. For statistical efficiency, it is commonly believed that blocking in larger samples is less important (Kernan, 1999), but this will depend more on the nature of the data. Overall, many clinical trialists suggest blocking is less important with samples over 400 (Kernan, 1999). Our view, however, is that if the process can be made easy, then the benefits may outweigh the costs at many sample sizes.

We focus first on the situation of having at least two pre-periods worth of data \( t \in \{\text{pre1}, \text{pre2}\} \) as this is the cleanest setup for the models. Both strategies will model the relation between \( y_{\text{pre2}} \) and \( [X, y_{\text{pre1}}] \) to form partitions, and we show how to use an out-of-sample method to pick between them. After deciding which strategy to use, given there is likely some temporal dependence, we proceed with estimation by using the selected model to generate partitions when using \( [X, y_{\text{pre2}}] \), rather than \( [X, y_{\text{pre1}}] \).

### 2.2 Standard ML methods

Before we detail the ML methods, we first discuss a general difference with more common methods used in economics. ML models typically have hyper-parameters, which often control the model’s overall complexity. One benefit of many ML methods is that they can be quite complex, but increasing their complexity too much can mean that they overfit to the sample data, essentially memorizing the idiosyncrasies of the current sample and behaving badly out of sample. Experimenters and practitioners have therefore developed procedures to modulate model complexity and limit overfitting. The main procedure is cross-validation (CV), which simulates the out-of-sample error. CV randomly split the data into \( K \) “folds” (usually 5 or 10). Out-of-sample predictions are made for each observation using a model that was trained on all data but the fold for that observation (so there are \( K \) separately trained sub-models). One can
then fit the model with different values of the hyper-parameter and pick the hyper-parameter value based on the one with the lowest mean squared prediction error (MSPE).\footnote{An alternative is the “1se” rule (Friedman et al., 2010), which is the simplest model that has a MSE no more than one standard error above the minimum. This is typically used if there is a strong reason to believe that the model will be used with new data drawn from a different distribution.}

We list three common ML tasks and identify for each a method that is common, simple, and can be used off-the-shelf:

- **Partitioning**: This task is to create a partition, $\Pi$, with cells $\ell$, from a feature-space $X$ to a variable level of complexity. The goal when constructing the partition is that the set of dummy variables covering each block maximizes their predictive power for $y$ (i.e., the predicted value for each block is the block’s mean outcome). Finding the globally optimal partition is too computationally intensive, so the most common method (Hastie et al., 2009) for this task is Classification and Regression Tree (Cart, Breiman 1993). Cart starts with the whole feature space as a single block and recursively splits each block into two using rectilinear cuts. To split a block, it searches over each dimension and possible values in that block and finds the split that reduces the overall MSE of the outcome of the two sub-blocks. Intuitively, it finds a split such that the two sides have very different mean outcomes. The main hyperparameters are the tree depth (which we choose through CV) and the minimum leaf size (which we set as $c_B$).

- **Feature selection**: In this task, we have a generic outcome $y$ and features $X$ and we would like to find the subset $X^*$ that is most important for determining $y$. The most common method (Taddy, 2019) is the Least Absolute Shrinkage and Selection Operator (Lasso, Tibshirani 1996). Lasso is a linear model that adds to the OLS objective function a penalty for the $L_1$-norm of the coefficients, solving $\min_\beta \|y - X\beta\|^2_2 + \lambda \|\beta\|_1$. The Lasso solution will typically set many coefficients to exactly zero due to the geometry of the $L_1$ penalization. If the true DGP is sparse in terms of the non-zero coefficients, then under certain conditions the Lasso can achieve the oracle property and be consistent in terms of selecting the true subset (Zou, 2006). We highlight three usage notes. First, as the absolute sizes of the coefficients are all penalized, we typically normalize all features to have a standard mean and variance. Second, as it’s a linear model, variables that interact or affect the outcome non-linearly may not be selected.\footnote{The partitioning methods introduced above may also be used as a non-linear variable-selection procedure by generating a partition and then selecting the variables that were used to split on at least once. With many variables, however, the performance of decision trees suffers (Hastie et al., 2009) and so in these cases especially, Lasso is preferred.} To help address this, a common practice is to augment $X$ with common transformations. Third, we will follow common practice and set the $\lambda$ hyperparameter using CV.\footnote{We note that for Lasso, some plug-in estimates for setting $\lambda$ have attractive theoretical properties (Belloni et al., 2012).}

- **Prediction**: In this task we wish to form a robust prediction in the face of potential non-linearities, learning $y \approx \hat{g}(X)$. There are many options for this task, but in most statistical data (i.e., not visual or text data) applications, the Random Forest (Breiman, 2001) is common, simple, and performs well (Taddy, 2019). A Random Forest is the average of a large number of separate tree models (typically Cart). Each tree is trained
on a slight modification of the original data (the data is bootstrapped and then at each splitting decision a random number of features are selected as candidates for splitting), to yield different trees adding smoothness and robustness.

We note that, while we have picked a popular, widely available, and simple method for each purpose, there are alternatives (e.g., Best Subset instead of Lasso and Boosted Trees instead of Random Forests). If there are data or computational reasons to pick an alternative, that should be explored by the experimenter. The above can be thought of as default choices to operationalize the below algorithms. In the description of the algorithms, we will use the generic task name—partitioning, feature selection, or prediction—rather than any particular method. Finally, as with most ML methods, the ones noted here can function even when there are more features than observations. They are therefore quite useful in settings where, despite a small sample size, we nonetheless have rich data on individuals.

2.3 Strategy: Variable selection (VS)

As mentioned above, we can use a dedicated feature selection method initially or directly use the partitioning algorithm. The choice will depend on the number of covariates, $K$, and the experimenter’s prior on the sparsity of the covariates in the DGP. If $K$ is relatively small, then the partitioning algorithm can be used directly on the variables to create blocks. If $K$ is relatively large, then the performance of partitioning algorithms tends to suffer. In that case, and especially if the experimenter’s prior is that only a sparse subset of the variables matter for predicting the outcome, we can use a preliminary feature selection method.

Note that in addition to the standard variables, we could pre-generate $\hat{y}_{\text{pre1}}$ (from a prediction model of $y_{\text{pre1}} \approx g_{PS}^{\text{pre1}}(X)$) and include it as well. Its inclusion might improve performance and focuses this strategy on alleviating issues rising from model misspecification and dynamic DGPs. Performance improvements will result if there is a long tail of covariates in $X$ that are weakly related to $y_{\text{pre1}}$ and can therefore be compactly represented in $\hat{y}_{\text{pre1}}$. An orientation towards the issue of dynamic DGPs will result insofar as $\hat{y}_{\text{pre1}}$ captures information from $X$ that explains the static components of the DGP, meaning the covariates selected from $X$ when $\hat{y}_{\text{pre1}}$ is included in the model will be those whose influence may vary over time. Concisely, if $y_{\text{pre1}}$ is selected, this is evidence of persistence (unspecified variables), and if some of $X$ is selected, then this is evidence of a dynamic DGP.

In some circumstances, blocking on real variables (even if chosen by a model) may be preferred for interpretability and trustworthiness reasons to using a synthetic feature such as $\hat{y}_{\text{pre1}}$. Using a synthetic measure such as these can result in unintuitive groups (units that, while having similar prognostic scores, have very different covariates). This concern is raised similarly in the matching literature (King and Nielsen, 2016) in the context of propensity-score matching. If interpretable blocks are required, then the experimenter may prefer to leave $\hat{y}_{\text{pre1}}$ out of the Variable Selection strategy.

Full details are in Algorithm 1. This algorithm has multiple advantages over the existing manual process:

1. This algorithm has a common method for selecting among $y_{\text{pre1}}$, geographic variables, and other features. It also focuses on predictive power in a joint setting rather than using bivariate correlations. While the feature selection method does not jointly pick blocking variables and partition, it does have an automatic stopping rule (the cross-validated $\lambda$) for limiting the selected set of blocking variables.

2. In general, a tree-based partition is preferred to a grid-partition as it can have increased granularity while adapting to densely and sparsely populated regions of the covariate space.\footnote{Technically the minimum blocks size is only used on the pre2 data, but blocks could be made smaller for...}
Algorithm 1 Variable Selection Blocking Strategy

Inputs: $y_{pre1}, y_{pre2},$ and $X$.

1. Estimate a prediction model $y_{pre1} \approx \hat{y}_{PS}^{pre1}(X)$ and generate $\hat{y}_{pre1}$. Define $M = \{y_{pre1}, \hat{y}_{pre1}, X\}$.
2. Estimate a prediction model $y_{pre2} \approx \hat{y}_{PS}^{pre2}(X)$ and generate $\hat{y}_{pre2}$.
3. If $K$ is large (or assuming sparsity): Use a feature selection method predicting $y_{pre2}$ using $M$. Redefine $M$ as the selected set of features. (If needed for a downstream task, return the importance weights).
4. Perform partition (with CV tree depth) predicting $y_{pre2}$ using $M$, yielding partition $\Pi$.
5. Assign blocks based on updated data: $b = \Pi(y_{pre2}, \hat{y}_{pre2}, X)$. Ensure that the partition did not create blocks smaller than $c_B$ with updated data (if so, prune back the tree complexity until this constraint is satisfied).

Return: $b$

3. As the partition algorithm ensures that there is expected benefit to a finer partition, we naturally balance the trade-off between increased granularity and the downstream degrees-of-freedom adjustment.

If the experimenter is unsure whether to use an initial variable selection method in Algorithm 1, one can create both versions of the variable selection strategy and use the procedure in Section 2.5 to decide between them. If the experimenter is motivated to block in order to carry out a pre-specified subgroup analysis, then we suggest the following modification to Algorithm 1: in the partitioning step, we start with the existing partition $\tilde{\Pi}$ as described in Section 2.1 and recursively partition cells from that point. If the experimenter is using an initial feature selection, then the procedure should be constrained to only allow new splits on selected dimensions.

Remark 1. (Adaptive Grid Alternative) The partition created by Cart will subdivide the space into hyperrectangles, but the partition can still be quite irregular and hard to understand. If the partition needs to be understandable on its own, then an alternative is to use an adaptive grid partition. This grid can be built by dividing (when possible) covariates on quantiles. There should be more blocks across variables that are more important. Therefore, attempt to make the number of blocks across variables roughly proportional to their importance weights. The overall granularity is a hyperparameter that can be set by CV (and assuming a minimum block size of $c_B$).

Remark 2. (Misfits) Blocks for experiments often contain an odd number of units, preventing a perfect even distribution of treatment in the block. One of the units (typically at random) is held-out and labeled the “misfit” and the rest are randomized event across treatments. One may want to ensure that the treatment assignment of the misfits is also even across the distribution. If blocks span only a single dimension then we can iterate across the blocks in order and assign misfits to alternating treatments. If blocks span multiple dimensions, however, there are no simple solutions. (If the misfits themselves form a rectangular lattice then this is possible, but this is highly unlikely). Practice varies in this situation and non-random solutions are typically slow and approximate.

One approach, with any progressive partition method, is to view just the misfit units from a higher, coarser-level of partitioning and re-do blocking at this higher level. With Cart, this can be done easily by simply iterating across the tree leaves in order and assigning misfits to the pre1 data as well. In practice, typical decision trees have minimum node leaf sizes of around 6 so as to not estimate means from very small samples. As a result, this variant is unlikely to be helpful.
alternating treatments. Subsequent misfits will come from the same part of the original partition and would therefore be in the same cell at a higher level.

**Remark 3. (Feature learning)** In ML, a related task to feature selection is **feature learning**. This focuses on generating (often a small set of) synthetic features that are transformations or combinations of the original features that can perform better than the original features for some downstream estimation. This is a task that many experimenters already do manually (e.g., constructing composite indexes, averages, and log/polynomial transformations of existing features), but feature learning performs this in an automated way. Learned features are often constructed using neural networks (Hinton and Salakhutdinov, 2006). A full treatment of the theory and application of feature learning is beyond the scope of this paper, so we note here merely situations where feature learning might be helpful. It would be a case where FPS will not perform the best (the true DGP is difficult to approximate or the DGP is dynamic), but where VS does not perform as well as should be expected (e.g., because there are too many variables to select, so some combination is helpful). We note that given the procedure must learn an additional set of transformations, the task usually requires a larger sample size, potentially limiting its usefulness. To our knowledge, feature learning has not yet been applied to experimental blocking.

### 2.4 Strategy: Future Prognostic Score (FPS)

We construct a **Future Prognostic Score (FPS)** by using a prediction model to approximate

\[
y_{\text{pre2}} \approx g_{FPS}(X, y_{\text{pre1}}).
\]  

Note that this is different from the simple prognostic score models of Barrios (2014) and Aufenanger (2017), as it is looking one step ahead and incorporates a past outcome value. This ensures that this strategy uses the same data as the variable selection strategy. With the past outcome value, FPS can now deal with outcome persistence, though since it collapses the match-space to a single index it cannot deal with a dynamic DGP. We must still also consider the fact that our model may be misspecified.

As with the above, blocking is carried out on the predicted value using updated features \(g_{FPS}(X, y_{\text{pre2}})\). The existing standard method, which we call **Sequential Allocation**, is to arrange units according to their FPS and generate groups of size \(c_B\). Groups can be made larger to incorporate segments of units with identical predicted values. This ensures that extra blocks are only created when there is a benefit to (in-sample) predictive performance. This might create more odd-sized cells, but misfits are less of a problem in this approach as we can ensure an even distribution of the treatment arms across the span of the prognostic scores by iterating across the misfits in order and alternately assigning treatment. In the case of blocking motivated by a pre-planned subgroup analysis, the experimenter should start with the existing partition \(\tilde{\Pi}\) as described in Section 2.1, arrange units within each block by their FPS, and proceed partitioning from that point (ensuring no cell with size below \(c_B\)).

**Remark 4. (Alternate score-based partitioning)** The existing approach of taking prognostic scores and performing Sequential Allocation may create too many blocks since it focuses on in-sample predictive performance. The first-stage predictive method for learning \(g_{FPS}\) does use tools to control for overfitting (so that \(\hat{y}\) is not too influenced by \(y\)), but will likely still create too many unique levels of \(\hat{y}\) and that is all the Sequential Allocator focuses on. We need to treat the joint process of learning \(\hat{y}_{FPS}\) and constructing the allocation as a combined partition method using CV to control for the final complexity (the number of blocks). Given we want a second-stage partitioning method that can create a partition with a less-than-maximal number of blocks, we may want more complexity than the Sequential Allocator. Options include:

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10A pre-generated \(\hat{y}_{\text{pre1}}\) could be used here as well, but it would not improve performance unless it were estimated using a different algorithm.
• Simple: A Scaled Sequential Allocator that creates fewer blocks than $N/c_B$, but still roughly evenly sized. This is simple, but far from optimal.\footnote{We note that another simple alternative would be to use Cart targeting $y_{pre2}$ and blocking on $\hat{y}_{pre2} = \hat{g}_{FPS}(X, y_{pre1})$ to create the partition. This solution likely does not offer any benefit in single-dimensional partitioning as the greedy solution will results in a very uneven distribution of sizes (some blocks roughly twice the size of others).}

• Complex: Since we are only dealing with a single dimension, there will be many fewer possible partitions, and we can jointly optimize the splitting rules rather than use a greedy solution such as Cart. A straightforward approach would start with quantile splits and then use coordinate-descent to sequentially optimize each split until no changes are made.

Regardless of the actual partitioning method used, the complexity should still be tuned for CV performance. As this is a two-stage process, for each iteration $f$ we learn a separate $\hat{g}_{FPS}$ and partition using all data but fold $f$ creating an outcome prediction of the average prognostic score in each block and then see the out-of-sample performance on fold $f$.

### 2.5 Deciding between FPS and VS

There are different ways to determine which strategy to use depending on the available data:

- If there is another pre-treatment period, $pre3$, we can empirically see which resulting partition has the best predictive performance on $y_{pre3}$.

- If not, then we can compare performance using cross-validation, where here we choose between different model types rather than between different hyper-parameters for a single model type.\footnote{Note that comparing directly the performance of the partitions from the above models on $y_{pre2}$ will be biased as the ML models were trained on that data.}. Given we need to have sufficient units per block, a 2-fold CV version is best to maximize the size of the held-out fold. One can average the results over multiple random splits to reduce noise. Note that this works best with larger datasets.

After deciding which strategy to use, given there is likely temporal dependence, we use the model to generate partitions when using $y_{pre2}$ rather than $y_{pre1}$.

### 2.6 Different pre-period data

#### 2.6.1 Time-varying covariates

If there are time-varying covariates $Z_{it}$, then they should be used in the same way as $y_{pre}$. $Z_{pre1}$ would be used when modeling $y_{pre2}$, and then updated values $Z_{pre2}$ would be used to construct the final partition.

#### 2.6.2 3+ pre-periods

With more time-periods, we can improve several parts of the process. One option is to use the above strategies with additional look-ahead predictions.

- Variable selection: Use variables $M = \{y_{pre2}, y_{pre1}, X, \hat{y}_{pre1}, \hat{y}_{pre2}\}$ and either construct the partition directly or via an initial feature selection method targeting $y_{pre3}$.

- FPS: Generate prediction values from $y_{pre3} \approx g_{FPS}(y_{pre2}, y_{pre1}, X)$

A second option is to use $y_{pre3}$ to find an optimal trade-off between the goal of reducing the estimate’s MSE and its standard error. For every candidate partition created using data from $\{y_{pre2}, y_{pre1}, X\}$, one could simulate $S$ different randomizations and then calculate the average
standard error and MSE (given there was no actual treatment in pre3). Given an optimal weight between the two goals, the best partition could be selected.

When data is scarce, using the extra information to inform the ML models is likely more beneficial. If there are strong reasons to believe that the default partition complexity is non-optimal (e.g., idiosyncratic research preferences) then the latter option may be preferred.

3 Other randomization methods

We review here the other main randomization methods, pair-wise matching and rerandomization, and how the above strategies can be modified when either are preferred to blocking.

3.1 Pair-wise matching

Pair-wise matching divides the sample into similar pair with each pair randomly assigned to have a treated and control unit. If the experimenter wants to improve balance along a certain variable, this can be explicitly achieved through including that variable in the match criteria.

Application of Strategies:

- Variable selection: It is straightforward to use the feature selection method above to select a match space and then construct pairs. Each unit has values for its selected features, $M$, and so our task becomes to divide the units into pairs with a method that attempts to minimize the overall within-pair differences (where we define distance as geometric distance in $M$, but where we weight each dimension by its importance $w_k$). This is similar to the problem of matching treated to control units in 1-1 matching estimators. Similar to that domain, the optimal solution (Greevy, 2004) is quite difficult, so most implementations take the approach of finding the “nearest available match” (King et al., 2007). We, therefore, suggest the same: select available units randomly and pair them to their nearest available unit.

- Future prognostic score: Use a prediction model to generate prognostic scores, order units by their score, and then sequentially put them into pairs.

Selection between strategies: As we can produce pair-level dummies similar to the block-level dummies, the selection procedure is the same as with blocking.

3.2 Rerandomization/Minimization

Rerandomization techniques (Taves, 1974; Pocock and Simon, 1975) repeatedly randomize units to treatment and control arms until the imbalance across important variables meets some criterion. There are two methods commonly used: “big stick” which rerandomizes until no important variable has a significant difference at a pre-specified level (commonly 5%) and “min-max” which computes for a pre-specified $R$ number of draws (commonly 1000) the maximum $t$-statistic difference for the important variables and then chooses the randomization with the minimum maximum. Notice that, in contrast to the other methods, this ensures a parametric rather than non-parametric form of balance as we explicitly specify the moments (typically means) that should be matched. We will focus on the min-max strategy, but it is straightforward to adapt the methods for the “big stick” approach. Let $\theta_{rk}$ be the $t$-statistic for the difference in means of the $k$th variable between the two treatment arms in the $r$th randomization, so that the standard min-max strategy selects $r^* = \arg\min_r [\max_k \theta_{rk}]$.

Application of strategies:

- Variable Selection: Proceeding as we have above in the variable selection setting, we use the feature selection method as to get selected variables $M$. This will constitute the set of
variables for which we will compare the t-statistics of mean differences across treated and control units. We suggest taking into account the relative importance of the variables by finding the ideal randomization via \( r^* = \arg \min_r \max_k \omega_k \theta_{rk} \).

- **Future Prognostic Score**: Use a prediction model to generate future prognostic scores. Let \( \theta_r \) be the t-statistic for the difference in means of the future prognostic scores for the \( r \)th randomization. As we have collapsed the dimensions we now simply choose \( r^* = \arg \min_r \theta_r \).

Selection between strategies: If we have access to an additional pre-period of data, then we can choose between the above methods in a similar way by taking both approaches and seeing how well they do at minimizing average differences in \( y_{pre3} \) between treatment and control groups. If we do not, we can use the method for blocking using CV and see the average difference between the arms in the hold-out samples.

### 4 Simulations

To analyze empirically how well our strategies perform, we use the data and framework of Bruhn and McKenzie (2009), comparing their manually constructed blocks against our blocking strategies. We use the two datasets from their framework containing more than two pre-treatment outcomes periods: a panel survey of microenterprises in Sri Lanka (de Mel et al., 2008) and a sub-sample of the Mexican employment survey (ENE). In both of these, the subgroup studied received no treatments. We treat the first two periods as pre1 and pre2 and the third as post. For both, we estimate results using the \( n=100 \) and \( n=300 \) samples. The Sri Lanka dataset has 29 covariates and the Mexican sample has 30 covariates. The benefit of the ML strategies we propose typically increases with the number of covariates. We perform 10,000 simulations of placebo assignments to units and assess the performance of the strategies above as compared to the strategy of Bruhn and McKenzie (2009) that constructs 48 blocks by hand-picking four variables and then manually determining a grid.

We analyze our results in terms of MSE of the treatment effect (given we know the true effect is zero) and the size of the standard error. Table 1 reports the MSE of the estimated coefficient. We see that all of our strategies perform better than the manual method across all samples. The reduction in the MSE from using the best ML method ranges from 16%-34%. The Future Prognostic Score strategy performed best on the Mexican ENE sample with \( n=100 \) sample whereas the Variable Selection strategy with initial Feature Selection performed best on the Mexican ENE sample with \( N = 300 \) and both Sri Lankan samples.

Table 2 reports the length of the standard error for the estimate, a measure of increased precision. All ML algorithms again perform better than the manual strategy across all samples. The reduction in the MSE from using the best ML method ranges from 6%-16%. All three automated strategies performed best in at least one context.
### Table 2: Size of Coefficient Standard Error

| Method          | Mexico, n=100 | Mexico, n=300 | Sri Lanka, n=100 | Sri Lanka, n=300 |
|-----------------|---------------|---------------|------------------|------------------|
| FPS: Random Forest | 509.4455      | 268.1693      | 917.4573         | 515.8929         |
| Manual: 48 blocks | 611.7684      | 300.0989      | 964.0424         | 537.3345         |
| VS: CART        | 525.2979      | 274.4434      | 925.6401         | 499.0057         |
| VS: Lasso + CART | 514.9183      | 264.9388      | 905.8749         | 500.7876         |

### 5 Conclusion

Restricting randomization in experiments to reduce treatment-control imbalances on variables that are important for predicting the post-treatment outcome improves efficiency, protects against type I errors, and increases power for the estimated treatment effect (Bruhn and McKenzie, 2009), particularly for small- and medium-sized samples. Existing guidance for this process has been conflicting and demands many ad hoc decisions. We show that this incompleteness in guidance is due to differing views on the dynamics of the data generating process (DGP). In the case of having at least two pre-periods worth of baseline data, we outline methods that resolve these differences and automate the process using modern, and off-the-shelf machine learning (ML) techniques. For the main type of randomization restriction, blocking, we determine what are the important dimensions to create blocks along, how to create blocks, and how many should be made. Crucially, for determining how many blocks to create, we provide a way to balance the goal of improving the estimators true accuracy, which improves with more blocks, and the goal of reducing the estimated standard error, which can increase due to a degree-of-freedom correction if the extra blocks are only marginally helpful. Applications are also show to the other main types of randomization restrictions: pair-wise matching and rerandomization. With real-world data, we see reductions in the mean squared error of the estimated coefficient of 14%-34% and reductions in the standard error of the estimate of 6%-16%. We also detail custom tools that may improve performance even more.

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A Alternative tree splitting rule for partitions

While partitioning algorithms are fit on one set of data, they are designed to not overfit to the sample and are instead tuned to do well on the general population of data that the sample was drawn from. The standard way to do this is to fit a full sequence of partitions of increasing granularity, each focusing on in-sample fit, and then to pick the one that does best on CV OOS predictions. An alternative way, pioneered by Athey and Imbens (2016), is to incorporate this out-of-sample focus directly into each splitting decision in cases where we know the size of the auxiliary sample on which the partition will be used. Taking the example of Cart, one can write the typical objective function as finding the partition $\Pi$ that minimizes the “modified” MSE

$$\text{MSE}(\Pi; S^{pre}) = -\frac{1}{N} \sum_{\ell \in \Pi} N_{\ell} \hat{\mu}^2(\ell; S^{pre}, \Pi).$$

Athey and Imbens (2016) show that if we take the auxiliary sample into account during the split we should minimize the Expected MSE, which can be estimated as

$$\hat{\text{EMSE}}(\Pi; S^{pre}) = -\frac{1}{N} \sum_{\ell \in \Pi} N_{\ell} \hat{\mu}^2(\ell; S^{pre}, \Pi) + \frac{2}{N} \sum_{\ell \in \Pi} N_{\ell} \hat{\gamma}(\hat{\mu}(\ell; S^{pre}, \Pi))$$

where we now penalize blocks that have high variance in their estimates. Using this for partitioning requires custom tools (Athey and Imbens (2016) provide tools for partitioning on estimated treatment effect, not estimated outcome), so we leave this for future work.

B Alternative available data

B.1 1 pre-period

This is the typical case studied in the previous literature. We can automate a few portions of the standard strategies, but we can not deal with the general temporal dynamics of the DGP:
- Variable selection: Since we only have a single outcome, we do not have a separate target to jointly pick the best variables from $[X, y_{\text{pre1}}]$. We, therefore, take the guidance of Bruhn and McKenzie (2009) and force the inclusion of $y_{\text{pre1}}$ and separately select the features $X^*$ from a feature selection model targeting $y_{\text{pre1}}$ with $X$. Similarly, we no longer can construct a partition based on a joint predictive model. We could construct an *adaptive grid* (as above). The experimenter would have to give a relative weight for $y_{\text{pre1}}$ compared to the variables in $X^*$. Obvious candidates would be $\sum_{k \in X^*} w_k$ (so that $y_{\text{pre1}}$ has equal weight to all of $X^*$) or $\frac{1}{|X^*|} \sum_{k \in X^*} w_k$ (the average weight from $X^*$).

- Prognostic score: Construct the simple prognostic scores from a model of $y_{\text{pre1}} \approx g_{PS}(X)$. Then order units by their prognostic score and partition them into groups of $c_B$.

Selection between strategies: Here the experimenter would have to take a stand on the amount of temporal dependence in the DGP (which could potentially be assessed in another data source).

Remark 5. (Auxiliary sample) If there is an auxiliary sample with improved data (e.g., $[X, y_1, y_2]$ and no treatment was applied) then we can construct the partition tree using the auxiliary sample and bring the partition over to the main sample. If the main sample is smaller, then it can be pruned back until the minimum cell has at least $c_B$ units. As there is not sufficient data to tune this new partition to out-of-sample performance, it might result in slightly more blocks than are optimal.

**B.2 Zero pre-period outcomes**

If no pre-treatment outcomes exist, but there are covariates $X$, then one alternative would be to use an unsupervised dimension reduction technique such as principal component analysis or neural-network autoencoders to select the blocking variables (choosing the number of dimensions by identifying when the marginal explained variance begins to diminish). The partition could be constructed as an evenly-distributed quantile-based grid granular enough that the smallest cell has size $c_B$. This might result in slightly more blocks than optimal.