`rjaf`: Regularized Joint Assignment Forest with Treatment Arm Clustering

November 27, 2024

Summary

Learning optimal assignment of treatments is an important problem in economics and public health, specifically when there are many treatment strategies to choose from. It arises, for example, in settings where a variety of behavioral science informed interventions are tested in a randomized controlled trial (RCT) to identify ones that are most effective at behavior change (Milkman, Gromet, et al. 2021). This has been studied in domains as diverse as encouraging gym visits to vaccine uptake against the coronavirus disease 2019 (COVID-19) or influenza (Milkman, Gromet, et al. 2021; Milkman, Patel, et al. 2021; Dai et al. 2021; Milkman et al. 2022). Most studies focus on identifying interventions which have (on average) the best performance, but ignoring effect heterogeneity can be a missed opportunity or, worse, perpetuate disparities (Bryan, Tipton, and Yeager 2021). Subject-specific covariates/features containing information regarding sociodemographics, past behavior, clinical characteristics, and comorbidities, if available, can be harnessed to identify which interventions works best for different sub-groups in the data. The `rjaf` package provides a user-friendly implementation of the regularized joint assignment forest (RJAF) (Ladhania et al. 2023), a regularized forest-type assignment algorithm based on greedy recursive partitioning (Athey, Tibshirani, and Wager 2019) that shrinks effect estimates across treatment arms. The algorithm is augmented by outcome residualization (to reduce baseline variation) and a clustering scheme (Hartigan and Wong 1979) that combines treatment arms with consistently similar outcomes. Personalized treatment learning is achieved through optimizing a regularized empirical analogue of the expected outcome. The integration of `R` (R Core Team 2024) and `C++` (Stroustrup 2013) substantially boosts the computational efficiency in tree partitioning and aggregating. This package is especially suitable in RCT settings where a large number of treatment arms are present, with potential overlap among the arms, and constrained sample sizes.

Statement of Need

There is an ever-growing literature at the intersection of machine learning and causal inference attempting to address the problem of optimal treatment assignment through heterogeneous treatment effect estimation (Athey and Imbens 2016; Wager and Athey 2018; Hitsch and Misra 2018; Athey, Tibshirani, and Wager 2019; Sverdrup et al. 2020; Athey and Wager 2021). Other methods focus on maximizing the benefit (empirical welfare) from treatment assignment (e.g., Kitagawa and Tetenov 2018), or the chance of assigning an individual to an optimal treatment arm (e.g., Murphy 2005; Zhou, Wang, and Zeng 2018). Most of these methods perform well with a limited number of treatment and control groups. A large number of arms renders the identification of best arm increasingly difficult, and assignments based on separate arm-wise estimation are inefficient. Commonly used implementations such as the multi-arm causal forest (Tibshirani et al. 2022) and random forest (Wright and Ziegler 2017) might lead to suboptimal assignment, particularly in settings with high noise. By contrast, the RJAF yields elevated empirical outcome estimates closer to the optimal level from the oracle assignment than the multi-arm causal forest approach in high noise settings, and performs at the same level in low-noise ones. Despite the methodological advantage over existing approaches,

the incorporation of machine learning and causal inference techniques such as recursive tree partitioning, bootstrap aggregating, and treatment arm clustering makes it challenging to implement the RJAF from scratch even for well-trained data scientists. The `rjaf` is an open-source software package in `R` and `C++` that efficiently implements the RJAF, offering data scientists a user-friendly analytic toolbox for learning personalized treatment rules in real-world settings.

Workflow

Figure 1 outlines the workflow for using the `rjaf` package to perform personalized treatment assignment and honest outcome estimation. The process begins with partitioning the input data–consisting of outcomes, treatment arms, covariates, individual identifiers, and optional probabilities of treatment assignment–into two parts, one for model training and estimation, and the other is the heldout set on which personalized assignment rules are obtained. The `rjaf` function first checks whether outcome residualization for reducing baseline variation should be performed via the `residualize` function, using the `resid` argument. If `resid` is set to `TRUE` (the default), a new column of residualized outcomes is added to the input data and used for tree growing on the training set. Next, the `rjaf` function evaluates whether treatment clustering should be performed on the training-estimation set during tree growing using the `clus.tree.growing` argument. If `clus.tree.growing` is `TRUE`, the `rjaf_cpp` function is employed to estimate cross-validated counterfactual outcomes for the $K+1$ treatment arms, after which k-means clustering is used to learn $M+1$ treatment arm clusters. The optimal number of treatment clusters is determined using the elbow method. After clustering, the `rjaf_cpp` function is reapplied to the preprocessed data, with assignment forest fitted on $M+1$ treatment clusters and counterfactual outcomes estimated for the original $K+1$ arms. If `clus.tree.growing` is `FALSE`, the `rjaf_cpp` function is employed to estimate counterfactual outcomes for the $K+1$ arms. Lastly, `rjaf_cpp` function is used to obtain optimal treatment arms and predicted counterfactual outcomes under all treatment arms for individuals in the heldout set.

Figure 2 provides a detailed description of the `rjaf_cpp` function, which grows a large number of trees through the `growTree` function. `growTree` begins by taking the training and estimation set as input, splitting it into two separate training and estimation subsets proportionally by treatment arms or clusters. Initially, utility is set at the root node, where optional inverse probability weighting (IPW) can be applied. A tree is then grown via recursive partitioning of the training subset based on covariate splits. Each potential split is generated by the `splitting` function, where regularization tuned by the `lambda1` parameter can be performed along with IPW to calculate average outcomes across treatment arms or clusters. A potential split is retained if it meets three criteria: (1) each child node contains at least the minimum number of units specified by the `nodesize` argument, (2) the utility gain is at least `eps` times the empirical standard deviation of outcomes in the entire input data, and (3) the child nodes have different optimal treatment arm or cluster assignments. Recursive partitioning ends when no potential split meets these criteria. Once terminal nodes are determined on the training subset, the same splitting rules applied to the estimation subset to obtain its terminal nodes. Outcomes from the estimation subset are then used to calculate treatment-specific average outcomes in each terminal node, with optional regularization tuned by `lambda2` and imputation controlled by `impute`. The validation set undergoes the same splitting, with treatment-specific outcomes from the estimation subset assigned to corresponding terminal nodes to achieve honest outcome estimates, thus concluding the `growTree` function. The final step in `rjaf_cpp` is bootstrap aggregation of a large number of trees grown via `growTree`, where the total number of trees is set by the `ntree` parameter of the `rjaf_cpp` function.

As in the implementations of other forest-based methods, built-in hyper-parameter tuning (e.g., `eps`, `lambda1`, and `lambda2`) is not provided in the `rjaf` package. Interested users are referred to the `caret` package (Kuhn 2008) for details.

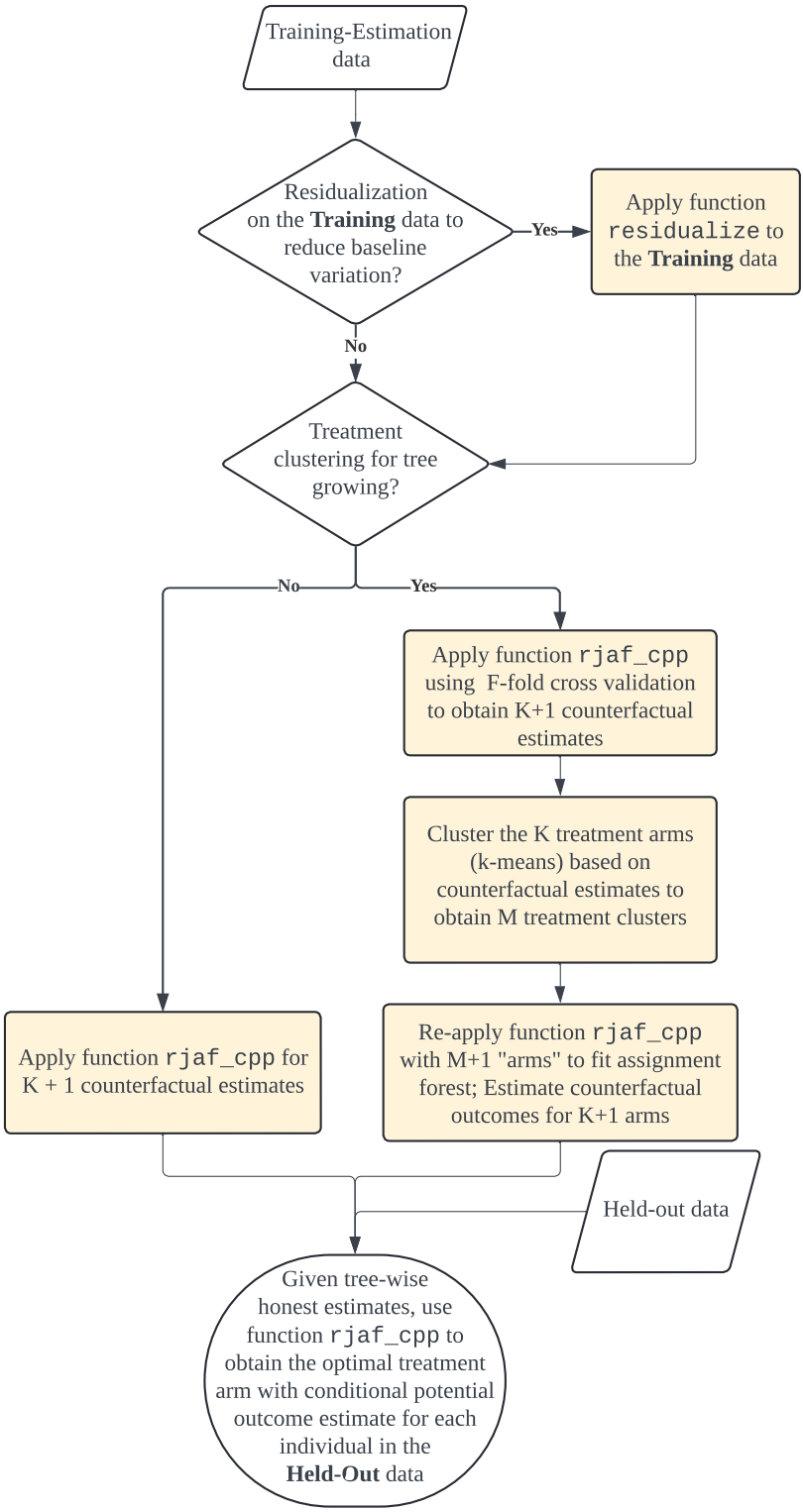

Figure 1: A sketch of the `rjaf` package.

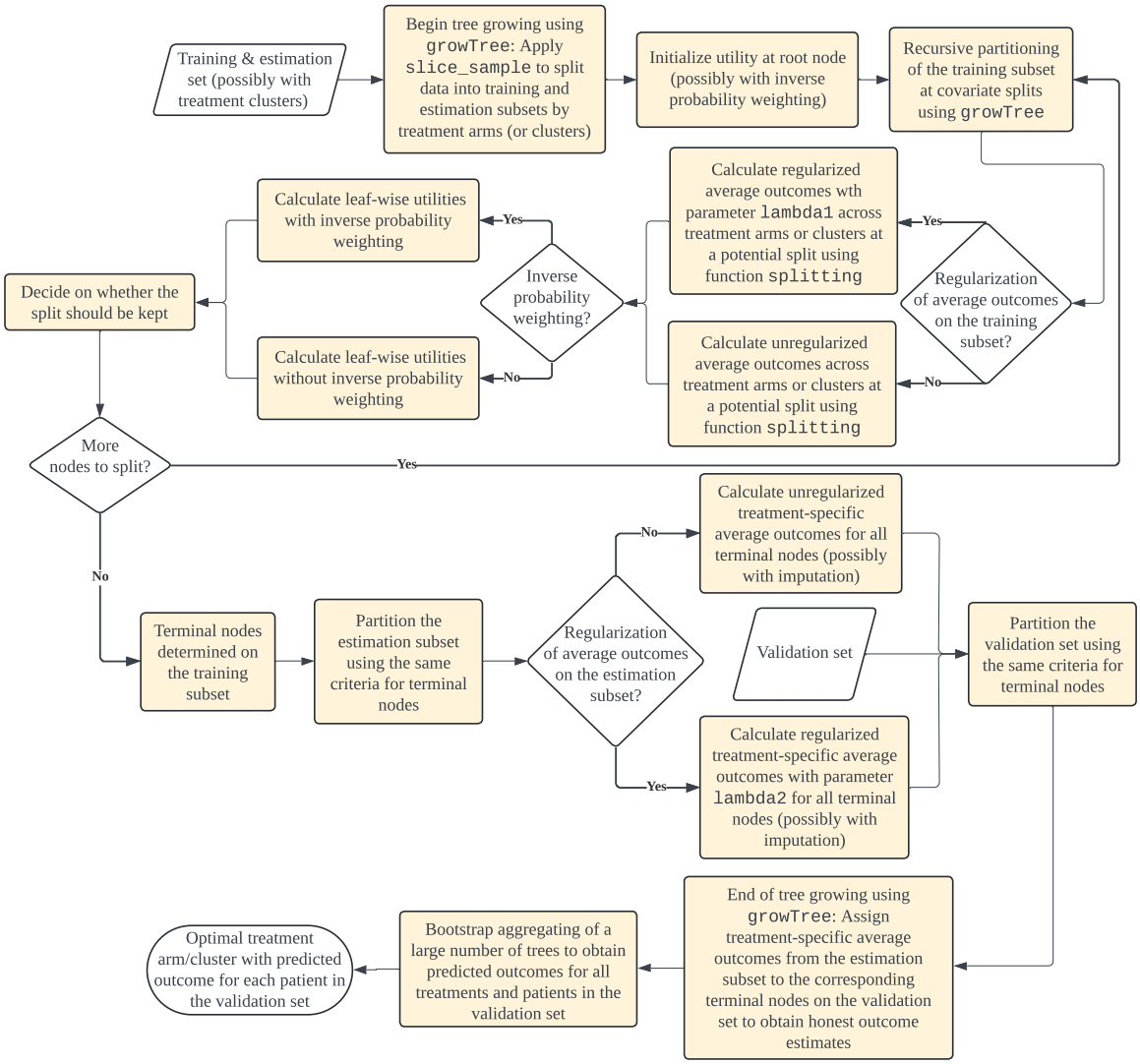

Figure 2: A description of the `rjaf_cpp` function.

Quick Start

The `rjaf` package is publicly available on GitHub, where the use of the `rjaf` package, including installation instructions and an example, has been documented in the `README.md` file. The package is also available on the Comprehensive R Archive Network. This section provides an introduction to the basics of `rjaf`. One can install and load the `rjaf` package by executing the following `R` commands:

```
install.packages('rjaf')
library(rjaf)
```

Example

Next we present an example that illustates the usage of the package. A function `sim.data` used for simulating a synthetic data set with three covariates is provided below, where `n` indicates the sample size, `K`+1 represents the number of treatment arms, `gamma` denotes the strength of treatment effects, `sigma` is the noise level, and `probability` is a vector of sampling probabilities of treatment arms. This function depends on two widely used `R` packages `MASS` and `dplyr`. The output of the `sim.data` function is a data frame, containing a column (named `id`) of individual IDs, a column (named `Y`) of outcomes, three columns of covariates `X1`, `X2`, and `X3`, a column (named `trt`) of treatment arms, and a column (named `prob`) of probabilities of treatment assignment. Readers are referred to Ladhania et al. (2023, sec. 4.1) for more details about the simulation setup.

```
sim.data <- function(n, K, gamma, sigma, probability = rep(1,K+1)/(K+1)) {
  options(stringsAsFactors=FALSE)
  data <- left_join(data.frame(id=1:n,
                               trt=sample(0:K, n, replace=TRUE, probability),
                               mvrnorm(n, rep(0,3), diag(3))),
                    data.frame(trt=0:K, prob=probability), by="trt")
  data <- mutate(data, tmp1=10+20*(X1>0)-20*(X2>0)-40*(X1>0&X2>0),
                 tmp2=gamma*(2*(X3>0)-1)/(K-1),
                 tmp3=-10*X1^2,
                 Y=tmp1+tmp2*(trt>0)*(2*trt-K-1)+tmp3*(trt==0)+rnorm(n,0,sigma))

  Y.cf <- data.frame(sapply(0:K, function(t)
    mutate(data, Y=tmp1+tmp2*(t>0)*(2*t-K-1)+tmp3*(t==0))$Y))
  names(Y.cf) <- paste0("Y",0:K)
  return(mutate(bind_cols(dplyr::select(data, -c(tmp1,tmp2,tmp3)), Y.cf),
                across(c(id, trt), as.character)))
}
```

Using the `sim.data` function, we generate two data sets: one for training and estimation, and the other held out for validation, both of which have a sample size of 5000. The number of treatment arms is set to 30 (`K`=29), with a treatment effect strength of `gamma`=10 and a noise level of `sigma`=20. Treatment arms are uniformly assigned to all individuals across both data sets. Calling the `rjaf` function returns a tidyverse tibble (Müller and Wickham 2023) containing individual IDs, optimal treatment arms, counterfactual outcomes, predicted outcomes, and treatment arm clusters.

```
library(MASS)
library(dplyr)
K <- 29; gamma <- 10; sigma <- 20; probability <- rep(1,K+1)/(K+1)
n.heldout <- n.trainest <- 5000
```

```
data.trainest <- sim.data(n.trainest, K, gamma, sigma, probability)
data.heldout <- sim.data(n.heldout, K, gamma, sigma, probability)
fit <- rjaf(data.trainest, data.heldout, y = "Y", id = "id", trt = "trt",
            vars = paste0("X", 1:3), prob = "prob", ntrt = K+1, nvar = 3,
            lambda1 = 0, lambda2 = 0.5, nodesize = 3, eps = 0.5, reg = TRUE,
            impute = FALSE, clus.tree.growing = TRUE, clus.max = 5)
head(fit)
# A tibble: 6 × 5
  id    trt.rjaf  Y.cf Y.rjaf clus.rjaf
  <chr> <chr>    <dbl>  <dbl>     <int>
1 1     29        20     11.6         1
2 2     29        40     11.5         1
3 3     3         18.6   10.3         3
4 4     3         38.6   10.4         3
5 5     3         18.6   10.4         3
6 6     3        -21.4   10.3         3
```

To demonstrate the advantage of treatment arm clustering, we conducted a series of simulated data experiments following the above setup. In each experiment, 500 simulated Training-Estimation sets were generated, while the same heldout data set was used for validation across all Training-Estimation sets. The number of treatment arms was set to 10, 30, 50, and 100, respectively. Figure 3 displays boxplots of 500 simulations comparing the average outcome of the heldout set from unclustered and clustered RJAF. "Oracle Optimal Assignment" denotes the assignment strategy derived from the ground truth in simulations, ensuring the best possible outcomes. "Random Assignment" involves randomly distributing units across treatment arms in each simulation. "Global Best Assignment" refers to assigning all units to the treatment in a simulation that demonstrates the highest average performance. Across all settings, the clustered RJAF is associated with a higher average outcome than the unclustered RJAF; the RJAF (both clustered and unclustered) consistently outperforms "Random Assignment" and "Global Best Assignment," while closely approximating the performance of the "Oracle Optimal Assignment."

Acknowledgments

Wenbo Wu and Xinyi Zhang contributed equally to the project. Wenbo Wu and Rahul Ladhania were partially supported by a research grant from the Robert Wood Johnson Foundation titled *Informing Strategies to Increase Use of COVID-19 and Flu Vaccines by Different Racial and Ethnic Groups to Improve Health Equity during Health Crises* (award number 78416).

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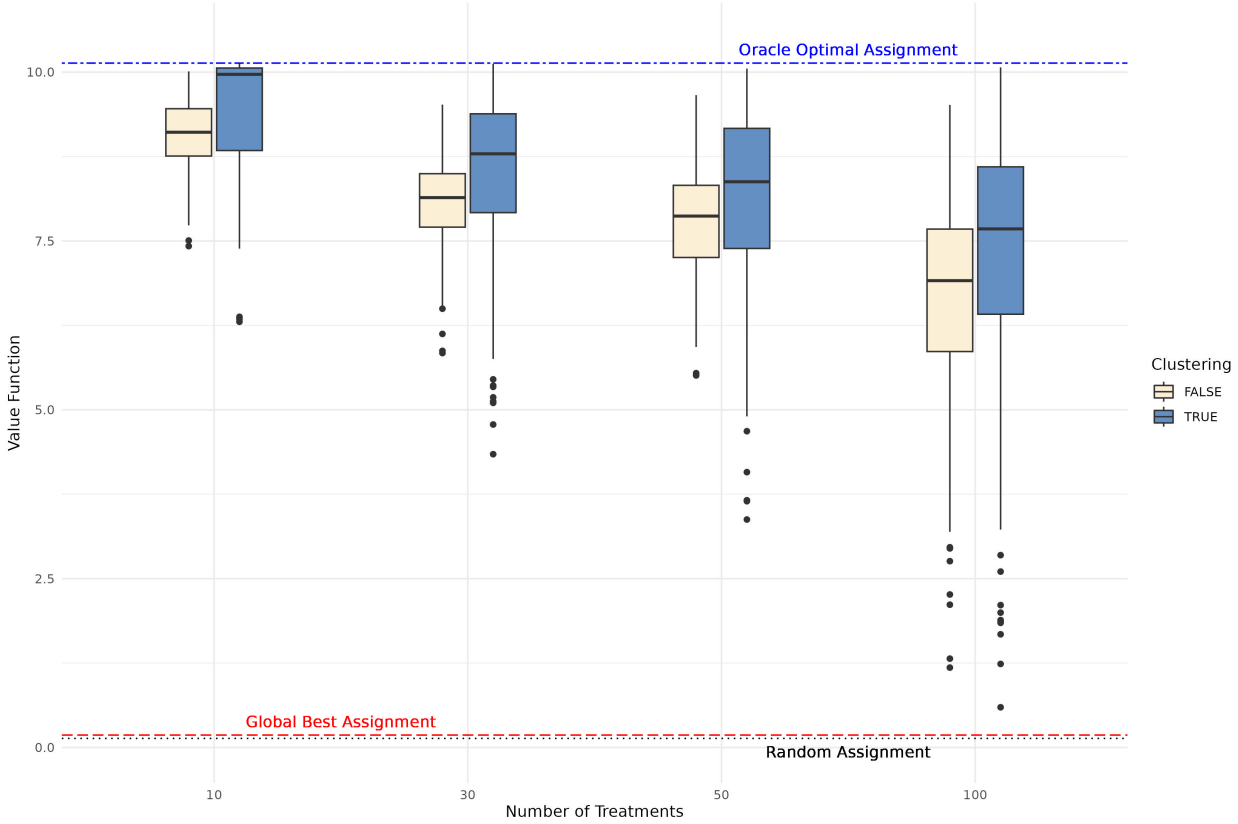

Figure 3: Boxplots of 500 simulations comparing the average outcome of the heldout set from unclustered and clustered RJAF. "Oracle Optimal Assignment" denotes the assignment strategy derived from the ground truth in simulations, ensuring the best possible outcomes. "Random Assignment" involves randomly distributing units across treatment arms in each simulation. "Global Best Assignment" refers to assigning all units to the treatment in a simulation that demonstrates the highest average performance.

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