Trees-Based Models for Correlated Data

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Abstract

This paper presents a new approach for regression trees-based models, such as simple regression tree, random forest and gradient boosting, in settings involving correlated data. We show the problems that arise when implementing standard regression trees-based models, which ignore the correlation structure. Our new approach explicitly takes the correlation structure into account in the splitting criterion, stopping rules and fitted values in the leaves, which induces some major modifications of standard methodology. The superiority of our new approach over trees-based models that do not account for the correlation is supported by simulation experiments and real data analyses.

Keywords: random forest, linear mixed models, Gaussian process regression, prediction error for correlated data, model selection

1. Introduction

Trees-based models are widely used for tabular data due to their high prediction accuracy and their inherent model selection functionality (Hastie et al., 2009). Commonly, trees-based models are fitted without assuming any distributional setting on the dependent variable. While the distribution of the dependent variable is mostly unknown and therefore it is tempting to avoid distributional assumptions, the correlation structure, which relates to the sampling mechanism (e.g., clustered data, time-series data, longitudinal data, spatial data), is frequently known and therefore it is not reasonable to ignore it. Unlike in trees-based models, the correlation structure is an essential component in many machine learning models, for example kernel covariance functions are used in Gaussian processes regression (Rasmussen, 2003), which is frequently implemented for modeling data sets with spatial correlation structure, such as neuroscience data sets (Caywood et al., 2017) and climatography data sets (Goovaerts, 1999). Another example is linear mixed model, which is used for data involving longitudinal correlation structure, as is common in health (Coull et al., 2001) and trading (Westveld et al., 2011) applications.

In this paper we develop a method which combines the concepts of random effects and random fields, which are convenient platforms for analyzing correlated data, and trees-based models such as: regression tree, random forest and gradient boosting. The desired result is that the trees-based part results a high prediction accuracy and model selection capabilities and the random effects part enables to boost the model performance by using
the correlation structure and even to exact statistical inference. The idea of integrating between random effects/random field and trees-based methods has previously been explored (see Sela and Simonoff 2012, Stephan et al. 2015, discussed in more detail in Section 4). However, we propose a novel approach which takes advantage of recent developments in model evaluation and selection methodologies for correlated settings, and yields improved results as demonstrated below.

Section 2 gives relevant background for the proposed method. The background contains a brief description of trees-based methods, linear mixed model (which is based on random effects) and prediction error estimation for correlated data, which has a key role in our approach. Our new algorithm, REgression Tree for COorrelated data (RETCO), is presented and discussed in Section 3. Section 4 compares RETCO with other algorithms that were introduced in recent years. Section 5 presents simulation and real data analyses that support our proposed algorithm.

2. Theoretical Background

This section presents briefly regression trees-based models, linear mixed models and prediction error estimation for correlated data. Additional information can be found in Appendix A and in resources which are cited below.

2.1 Trees-Based Models

Given a vector of covariates $\mathbf{x}^* \in \mathbb{R}^p$ a regression tree estimates the corresponding response, $y^* \in \mathbb{R}$, as follows:

$$f(\mathbf{x}^*) = \sum_{s=1}^{S} I(\mathbf{x}^* \in g_s) \mu_s,$$

where $g_s \subseteq \mathbb{R}^p$ and $\mu_s \in \mathbb{R}$, for all $s \in \{1, ..., S\}$. $\{g_s\}_{s=1}^{S}$ define a partition of the covariate space, that is $g_s \cap g_t = \emptyset$ for $s \neq t$ and $\cup_{s=1}^{S} g_s$ is the entire covariates space. $\mu_s$ is the predictor for covariate vectors that are in $g_s$. The nodes, $\mathcal{S} = \{\mu_s, g_s\}_{s=1}^{S}$ are selected using a recursive optimization process that can be diagrammed as a tree, where $\mathcal{S}$ are the terminal nodes (the leaves). The recursive optimization for selecting $\mathcal{S}$ is based on the training set, $\{y_i, x_i\}_{i=1}^{n} = \{\mathbf{y}, \mathbf{X}\}$, where $\mathbf{y} \in \mathbb{R}^n$ and $\mathbf{X} \in \mathbb{R}^{n \times p}$ is the design matrix, and it is implicitly assumed that the prediction points, $y^*$ and $\mathbf{x}^*$, are drawn from the same distribution as $y_i$ and $\mathbf{x}_i$. Each step in the tree’s recursive optimization process is a model selection of linear models, where a threshold of one of the available covariates is selected in order to minimize a loss function, $Loss(\cdot, \cdot) : \mathbb{R}^2 \rightarrow \mathbb{R}$. Also, stopping rules that follow predefined hyper-parameters, e.g., maximal depth of the tree and minimal number of training set observations in a node, are enforced on the recursive optimization and limit the tree’s depth and affect other properties of the tree’s structure in order to avoid overfitting.

Random forest (RF) and gradient boosting (GB) predictor are based on averaging an ensemble of trees. More information about regression tree, RF and GB, as well a formalized regression tree algorithm, is available in Appendix A and can also be found in Freund et al. (1999); Friedman (2001); Breiman (2001); Hastie et al. (2009).
2.2 Linear Mixed Model

In linear mixed models (LMM) there are two covariate vectors: fixed effects covariates, \( x^* \in \mathbb{R}^p \), and random effects covariates, \( z^* \in \mathbb{R}^q \). Commonly, \( y^* \) is assumed to be normally distributed and decomposed as follows:

\[
y^* = \beta^t x^* + b^t z^* + \epsilon^*,
\]

where \( \beta \) is the fixed effects vector of coefficients, \( b \sim N_q(0, G) \) is the random effects vector and \( \epsilon^* \sim N(0, \sigma^2) \) is the residual. \( \beta^t x^* \) is the marginal mean of \( y^* \), \( \mathbb{E}(y^*|x^*) \), and \( \beta^t x^* + b^t z^* \) is the conditional mean of \( y^* \) given \( b \), which is commonly denoted as \( \mathbb{E}(y^*|x^*, z^*, b) \).

\( \beta \) and \( b \) are estimated using the training sample, \( \{y_i, x_i, z_i\}_{i=1}^n = \{y, X, Z\} \), which follows the same model:

\[
y = X\beta + Zb + \epsilon,
\]

where \( \epsilon \sim N_n(0, \sigma^2 I_n) \), and \( X, Z \) are the fixed effects and random effects covariate matrices, respectively. Since \( y^* \) and \( y \) share the same random effects, \( b \), they are correlated, and estimating \( b \) by the training sample can later be used for improving the prediction accuracy of \( y^* \). Given \( G \) and \( V := \text{Var}(y) = ZGZ^t + \sigma^2 I_n \), \( \beta \) and \( b \) can be estimated as follows:

\[
\hat{\beta} = (X^t V^{-1} X)^{-1} X^t V^{-1} y
\]

\[
\hat{b} = GZV^{-1}(y - X\hat{\beta}).
\]

Harville et al. (1976) showed that given the true covariance matrices, \( G \) and \( V \), the estimated conditional mean, \( \hat{\mathbb{E}}(y^*|x^*, z^*, \hat{b}) = \hat{\beta}^t x^* + \hat{b}^t z^* \), is the best linear unbiased predictor (BLUP) of \( y^* \). In practice, the covariance matrices are mostly unknown and therefore are estimated using maximum likelihood or restricted maximum likelihood (Verbeke, 1997). Note that given the covariance matrices, LMM is linear in \( y \), i.e., the LMM predictor satisfies:

\[
\hat{y}^* = h^* y,
\]

where \( h^* \), the hat vector, does not contain the training response vector \( y \), and the element \( h^*[i] \) is the weight of \( y_i \) in predicting \( y^* \), \( \forall i \in [1, \ldots, n] \).

2.2.1 \( b^* \neq b \) Scenario

In many cases the random effects of \( y^* \) are not the same as the random effects of \( y \), i.e.,

\[
y^* = \beta^t x^* + b^* t z^* + \epsilon^*, \quad b^* \neq b.
\]

That means that the correlation between the observations in \( y \) is not the same as the correlation between \( y^* \) and the observations in \( y \). In case \( b^* \perp b \), which implies \( \text{Cov}(y^*, y) = 0 \), estimating \( b \) does not improve the prediction accuracy of \( y^* \). Therefore, in this case \( y^* \) is predicted by the marginal mean, \( \hat{\mathbb{E}}(y^*|x^*) = \hat{\beta}^t x^* \). This model, which is a special case of LMM, is also called generalized least squares model (GLS). A simple example for this scenario, is when the prediction set contains different clusters than in the training set. Several prediction tasks that follow this scenario setting are analyzed in Section 5.2. For example, using FIFA data set from Kaggle website, a predictive model for footballs players’
market-value was trained using GLS, where the prediction goal is to predict the market-value of players that belong to clubs that do not appear in the training set. This data set has a clustered correlation structure, where cluster is the players’ club, i.e., market-values of players that belong to the same club are correlated, while market-values of players that belong to different clubs are uncorrelated. Given the prediction goal of predicting the market-value of players from new clubs, this setting follows exactly the \( b^* \perp b \) setting.

Another scenario is when \( b^* \not\perp b \) (although \( b^* \neq b \)) and therefore \( \text{Cov}(y^*, y) \neq 0 \). This can happen for example when some of the random effects of \( y \) and \( y^* \) are the same and some are not. In this case, the elements in \( b \) that are in \( b^* \) should be estimated and used for predicting \( y^* \). Examples where \( b^* \not\perp b \) although \( b^* \neq b \), and more information about this scenario can be found in Rabinowicz and Rosset (2020). This scenario, of \( b^* \neq b \), is common and should be taken into account when developing trees-based methods for correlated data, as will be developed in Section 3.

2.3 Prediction Error Estimation and Model Selection for Correlated Data

Once a predictive model is fitted, it is often evaluated by its prediction error estimator. Moreover, when there is a set of alternative models (e.g., for LMM: models with different covariates, for trees-based models: models with different hyper-parameters) the ‘best’ model can be selected based on minimizing the prediction error estimator. It is important to note that common prediction error estimators, e.g., AIC (Akaike, 1974), Cp (Mallows, 1973), and even cross-validation (Stone, 1974, CV) are biased in some settings involving correlated data. Naturally, their corresponding model selection criteria are also biased in those scenarios. This bias was studied in the recent years, mostly for linear models. Here we present Cp, AIC and CV versions for correlated data. For description of the original Cp and AIC versions, that do not address correlation structure, see Appendix A.

2.3.1 Cp

In Cp, the goal is to estimate the squared prediction error:

\[
\mathbb{E}_{y,y^*} \frac{1}{n} \| y^* - Hy \|_2^2,
\]

where \( H \) is the hat matrix, and \( y^* \in \mathbb{R}^n \) is a vector of new observations measured at the same covariate values as \( y \), \( \{X,Z\} \), but with new independent noise and potentially different random effects realizations. This type of prediction error, when both \( y \) and \( y^* \) relate to the same covariate points, \( \{X,Z\} \), is called in-sample prediction error. In this setting, it is natural to consider \( \{X,Z\} \) as fixed matrices rather than random variables. Hodges and Sargent (2001) extended Cp to LMM with \( b^* = b \), here we employ a more general formulation which reduces to Hodges and Sargent (2001) when \( b^* = b \) but also covers the case that they are different:

\[
C_p = \frac{1}{n} \| y - \hat{y} \|_2^2 + \frac{2}{n} \text{tr} \left( H \left( \text{Var}(y) - \text{Cov}(y^*, y) \right) \right).
\]

2.3.2 AIC

Similarly to Cp, AIC is also an in-sample error, however its loss function is based on likelihood. Vaida and Blanchard (2005) presented the conditional AIC (cAIC) and marginal
AIC (mAIC) which are suitable for the scenarios where \( b^* = b \) and \( b^* \perp b \), respectively. Here we will use the name AIC for our formulation which subsumes cAIC and mAIC, but also covers the \( b^* \neq b \cap b^* \not\perp b \) scenario:

\[
AIC = -\frac{2\ell(y; \hat{E}(y|X, Z, \hat{b}), V_c)}{n} + \frac{2\text{tr}\left(H(\text{Var}(y) - \text{Cov}(y, y^*))V_c^{-1}\right)}{n},
\]

where \( \ell(y; \hat{E}(y|X, Z, \hat{b}), V_c) \) is the conditional likelihood of \( y \) given \( \hat{b} \), and \( V_c = \text{Var}(y^*|b) \).

### 2.3.3 Cross-Validation (CV)

Unlike Cp and AIC, CV estimates the generalization error:

\[
\mathbb{E}_{X, X^*, Z, Z^*}\mathbb{E}_{y^*, y}\sum_{i=1}^{n} \frac{1}{n} \text{Loss}(y^*_i, \hat{y}^*_i(x^*_i, z^*_i; y, X, Z)),
\]

where \( y^* \) is drawn from the same marginal distribution as \( y \), but relates to new covariate values, \( \{x^*_i, z^*_i\}_{i=1}^{n} = \{X^*, Z^*\} \), which were drawn from the same distribution as \( \{X, Z\} \).

For simplicity, a special case of CV algorithm, leave-one-out (LOO), is presented:

1. For simplicity, a special case of CV algorithm, leave-one-out (LOO), is presented:
   - For all \( i \in [1, ... , n] \), fit a model using the whole sample besides the \( i^{th} \) observation. Denote the sample without the \( i^{th} \) observation as \( \{y_{-i}, X_{-i}, Z_{-i}\} \).
   - Predict \( y_i \) by the fitted model and denote the predictor as \( \hat{y}_{i} = \hat{y}_i(x_i, z_i; y_{-i}, X_{-i}, Z_{-i}) \).

   For a squared errors loss function and linear predictor of \( y \), the CV error is

\[
CV = \frac{1}{n} \|y - H_{cv}y\|^2_2,
\]

where \( H_{cv} \), the CV hat matrix, is

\[
H_{cv} = \begin{bmatrix}
0 & h_{1,2} & \cdots & h_{1,n} \\
h_{2,1} & 0 & \cdots & h_{2,n}
\vdots & \vdots & \ddots & \vdots \\
h_{n,1} & h_{n,2} & \cdots & 0
\end{bmatrix},
\]

\( h_{k,k'} \in \mathbb{R} \forall k, k' \in \{1, ..., n\} \). In this presentation, the vector \( [h_{1,2}, ..., h_{1,n}] \) is the hat matrix of \( \hat{y}_i^{-1} \). K-fold CV generalizes LOO, by partitioning \( \{y, X, Z\} \) into K equal size subsets, \( \{y_k, X_k, Z_k\}_{k=1}^{K} \), where \( K \leq n \) (rather than \( K = n \) as in LOO).

Rabinowicz and Rosset (2020) presented a generalization of CV, \( CV_c \), which is suitable for scenarios involving correlated data:

\[
CV_c = CV + \frac{2}{n} \text{tr}\left(H_{cv}(\text{Var}(y) - \text{Cov}(y^*, y))\right).
\]

In the LMM settings, when \( b^* = b \), \( CV_c = CV \). For more information see Rabinowicz and Rosset (2020).

Cp and \( CV_c \) do not assume a specific distributional setting and can be applied for any linear model, while AIC is suitable for LMM, however it can also be adjusted for other linear models that assume normality, such as Gaussian process regression (GPR). Table 1 summarizes the prediction error estimators that are described in this section.
3. Trees-Based Models for Correlated Data

This section presents the main algorithm of this paper, REgression Tree for COrrrelated data (RETCO), and discusses the main differences between RETCO and the standard regression tree algorithm.

3.1 RETCO Algorithm

A simple approach for integrating between trees-based methods and random effects is replacing the marginal mean in LMM, $\beta' x^*$, by a trees-based model, $f(x^*)$:

$$ f(x^*) + b' z^*, $$

where $f(x^*)$ is created in a way that does account for the correlation structure (unlike in the standard regression tree algorithm). The power of the model in expression (1) can be perceived from different points of views. From the LMM point of view, the additive representation of marginal and conditional means is preserved, however the marginal mean is non-linear and therefore more expressive than in standard LMM. From the regression tree point of view, this approach differentiates between the two types of covariates—fixed effects, which are used for splitting the tree’s nodes, and random effects that are added linearly to the fitted tree—enabling expressing and using the correlation structure. This also enables using inference tools that do not exist for standard regression trees but exists in LMM, for example, comparing between the variance components, $\sigma^2$ and $G$. Note that expression (1) assumes that the effect of the random effects on $y$ is linear, however it can be generalized.

The template in expression (1) was already suggested (for literature review see Section 4), however here we present a new algorithm, RETCO, for fitting $f(x^*)$ that follows the theoretical aspects that were presented in the previous section. The algorithm formulation is general, and is not based on a specific prediction error type or distributional setting. Also, the algorithm refers to a case when $f(\cdot)$ is a single regression tree, the extension to RF and GB will be discussed in Section 3.1.1.

Algorithm 1, which presents RETCO use the following notations:

- $f(x_i|S)$, the intermediate predictor of $y_i$ during the tree fitting.

$$ f(x_i|S) = \sum_{s \in S} I(x_i \in g_s) \eta(\mu_s), $$

where

- $\mu_s$ is the GLS predictor of $\{y_i | x_i \in g_s\}$, $\forall s \in S$
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- $\eta(\cdot)$ is the identify function for the setting of $b^* \perp b$, and the BLUP for $b^* \neq b$.

Of course, after fitting the tree $f(x_i) = f(x_i | S)$.

- $f(x_i | j, c, S/s)$, the predictor of $y_i$ when splitting node $s$ using covariate $j$ at the threshold $c$:

$$f(x_i | j, c, S/s) = I(\{x_i \in g_s \cap x_{i,j} \leq c\}) \eta(\mu^l_s(c)) + I(\{x_i \in g_s \cap x_{i,j} > c\}) \eta(\mu^r_s(c)) + \sum_{l \in S/s} I(\{x_i \in g_l\}) \eta(\mu_l),$$

where $\mu^l_s(c)$ and $\mu^r_s(c)$ are the GLS predictors of $\{y_i | x_i \in g_s \cap x_{i,j} \leq c\}$ and $\{y_i | x_i \in g_s \cap x_{i,j} > c\}$, respectively.

Algorithm 1 REgression Tree for COrelated Data (RETCO)

**Input:** $y$, $X$, $Z$.

**Output:** $f(\cdot)$.

**High level setting:**

- select a prediction error estimator loss function—$C_p$, AIC or $CV$—from Table 1
- define the relation between $b^*$ and $b$ ($b^* = b$ versus $b^* \neq b$)
- define the stopping rules

**Initialization:** $S = \{g_1, \mu_1\}$, where $g_1 = \mathbb{R}^p$ and $\mu_1$ is the GLS estimator.

repeat

Given the predefined stopping rules, find the best node for splitting ($\tilde{s}$), the best covariate ($j_{\tilde{s}}$) and the best threshold ($c_{\tilde{s}}$) as follows:

$$\tilde{s}, j_{\tilde{s}}, c_{\tilde{s}} = \arg\min_{s \in S, j \in J_s, c \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^{n} Loss(y_i, f(x_i | j, c, S/s))$$

subject to:

$$\frac{1}{n} \sum_{i=1}^{n} Loss(y_i, f(x_i | j, c, S/s)) < \frac{1}{n} \sum_{i=1}^{n} Loss(y_i, f(x_i | S)), \quad (2)$$

where $J_s$ is the set of available covariates for splitting node $s$.

if $\{\tilde{s}, j_{\tilde{s}}, c_{\tilde{s}}\}$ exist then

Update $S$: replace $(g_{\tilde{s}}, \mu_{\tilde{s}})$ by the new two nodes, $(g_{\tilde{s}} \cap x_{j_{\tilde{s}}} \leq c_{\tilde{s}}, \mu^l_{\tilde{s}}(c_{\tilde{s}}))$, $(g_{\tilde{s}} \cap x_{j_{\tilde{s}}} > c_{\tilde{s}}, \mu^r_{\tilde{s}}(c_{\tilde{s}}))$, where $x_{j_{\tilde{s}}}$ is the covariate $j_{\tilde{s}}$.

end if

until $\{\tilde{s}, j_{\tilde{s}}, c_{\tilde{s}}\}$ do not exist or stopping rules are satisfied $\forall s \in S$.

As can be seen in Algorithm 1, RETCO covers various settings including different prediction error measures and correlation structures. Before analyzing its properties, here are some technical details for RETCO:
• Predefined stopping rules: stopping rules, such as maximal tree’s depth and minimal number of observations in a node, are commonly applied when fitting regression trees (for more details, see Section 2.1).

• Variance estimation: the variance components, needed for calculating \( f(x_i|j, c, S/s) \), \( f(x_i|S) \) and the loss function, can be estimated in different ways, for example using maximum likelihood or restricted maximum likelihood. For clustered data, simple closed-form equations that estimate the variance components are available and presented in Appendix B.

• Main optimization part:
  – the GLS predictors, \( \mu^l_s(c) \), \( \mu^r_s(c) \) and \( \{ \mu_l \}_{l \in S/s} \) are estimated using dummy variables for the current leaves: \( \{ i | x_i \in g_s \cap x_{i,j} \leq c \} \), \( \{ i | x_i \in g_s \cap x_{i,j} > c \} \) and \( \{ i | x_i \in g_l \}_{l \in S/s} \)
  – for every potential split, the variance components are estimated using the whole sample (rather than only \( \{ y_i | x_i \in g_s \} \))
  – the condition of eq. (2) is required since the loss function is not a training error (as in the standard regression tree algorithm) and therefore splitting a node may increase the loss

• Algorithm’s Output: since the tree estimates the marginal mean, its predictors are \( \{ \mu_l \}_{l \in S} \) rather than \( \{ \eta(\mu_l) \}_{l \in S} \).

There are two main conceptual differences between RETCO and the standard regression tree algorithm. The first is the use of a prediction error estimator: \( \text{Cp}, \text{AIC} \) or \( \text{CV}_c \) as loss functions. Unlike in the standard regression tree, where the loss function is the training error, here the loss function is prediction error estimator for correlated data. As was mentioned in Section 2.1, although the regression tree model is a non-linear function of \( y \), each split is a model selection problem of linear models. Due to the linearity, \( \text{Cp}, \text{AIC} \) and \( \text{CV}_c \) can be implement. More details about the effect of using these prediction error estimators on the selected thresholds and variables are given in Section 3.2. The second conceptual difference is the iterative approach that is used here instead of the recursive approach that is used in the standard regression tree model. The iterative approach is expressed by selecting the optimal node, \( \tilde{s} \), for splitting, rather than splitting each node independently. The reason for using an iterative approach is that observations in different paths are dependent. The dependency is accounted in the GLS predictors as well as in other expressions in the loss function (e.g., bias correction and likelihood, depending on the correlation setting and the selected loss function), therefore splitting one node may affect the splitting of the other. This is in contrast to i.i.d setting with training error loss function, where a recursive approach can be used since observations in different paths are independent and therefore splitting one node does not affect the splitting of the other.

For LMM-like setting, when \( b^* = b \), once \( f(\cdot) \) was fitted, the random effects can be estimated using the BLUP formula:

\[
\hat{b} = \hat{\text{Cov}}(y^*, y)\hat{V}^{-1}(y - f(X)),
\]
where \( f(X) = [f(x_1), ..., f(x_n)] \).

RETCO is formalized in context of LMM: \( \{\mu_s\}_{s=1}^S \), are GLS predictors and the variance is decomposed as in LMM, \( V = ZGZ^t + \sigma^2 \times I_n \). However these properties are not fundamental in the algorithm and can easily be generalized. For example, the covariance matrices, \( \text{Cov}(y^*, \ y) \) and \( \text{Var}(y) \), can be expressed using a kernel covariance function as is common in Gaussian process regression (and will be analyzed numerically in Section 5). Also, other linear models instead of GLS can be used for estimating the marginal means, \( \{\mu_s\}_{s=1}^S \). Moreover, the random effects, \( b \), can be estimated in different ways than using the BLUP formula.

Due to the iterative approach the complexity is higher than the complexity of a standard regression tree. Assuming \( x_{i,j} \neq x_{i',j}, \forall i \neq i' \in [1,...,n], \ j \in [1,...,p] \), the loss function is evaluated less than \( n \times p \times 2^d \) times, where \( d \) is the tree’s depth. Practically, due to hyper-parameters that restrict the number of potential splitting values (e.g., such as minimum observations at each node) and due to the constraint in inequality (2), which frequently shortens the depth of paths, the number of evaluations is smaller. The complexity of each loss function evaluation depends on the loss function, the predictor type and the correlation structure. For example, in Cp loss function, GLS predictor and clustered data, each evaluation complexity is \( O(n_c^3) \), where \( n_c \) is the cluster size, and therefore the overall computational complexity is \( O(n \times p \times 2^d \times n_c^3) \). The amount of memory required is quadratic in \( n \), due to storing of \( \text{Var}(y) \).

### 3.1.1 RETCO for RF and GB

Extending RETCO to RF and GB is done by averaging ensemble of implementations of RETCO, while taking into account the special adjustments that RF and GB require. The random effects are estimated in the same way. Several aspects should be noted when implementing RF and GB:

- **Training set sampling**: sampling with replacement cannot be implemented naively when the loss function involves calculation of \( \text{Var}(y)^{-1} \) (as when GLS predictor or marginal likelihood loss are used) since in that case \( \text{Var}(y) \) might be a singular matrix due to duplication. Therefore, a half-sample method should be used.

- **Number of trees**: since the trees in RF and GB are correlated, then in order to reduce the variance the number of trees should be large, especially when the trees are deep. When correlated data are involved, the trees are even more correlated due to the correlation between the observations. Therefore, the number of trees should be even larger than in the i.i.d sample setting. RF based on RETCO is demonstrated in Section 5.

- **Response in GB**: in common regression GB the trees are fitted consecutively to the residual of the previous tree. Therefore, the input of the algorithm in all the trees except the first one is not \( y \). Correspondingly, the estimated variance matrices relate to the residual of the previous tree, rather than to \( y \).
3.1.2 Using CV Loss in Regression Tree

In typical predictive modeling settings, generalization error is the primary objective of learning, hence CV loss is the natural choice. Surprisingly, there is not much previous work on using CV loss in trees, even without correlation. Notable exceptions are the ALOOF algorithm (Painsky and Rosset, 2016) and approximations used in CatBoost (Prokhorenkova et al., 2017). The main drawback in using CV-based loss function is increasing the computational cost compares to Cp loss function. Moreover, since RETCO is iterative rather than recursive, the number of evaluations of the loss function can remain large for all the splits along the tree.

3.2 The Bias Correction Effect

As explained in the previous sections, we suggest to add a bias correction term to the training error such that the loss function estimates the prediction error. This section illustrates the effect of the bias correction on split selection. Extensive numerical analysis is presented in Section 5.

3.2.1 \( b^* \perp b \) Scenario

Observations with positive correlation are similar in higher probability than uncorrelated observations. Therefore, loss functions that do not take into account the correlation, tend to split a node based on the correlation structure of the training set observations rather than their mean. Splitting based on the correlation of the training data is not useful for predicting uncorrelated observations. Therefore, when \( b^* \perp b \) it is important to fit the regression tree based on the marginal mean only. The corrections in Cp and \( CV_c \), which take into account the correlation structure, balance this tendency. Examples 3.1 and 3.2 demonstrate this mechanism. The code for the examples, as well as for the numerical part in Section 5, is written in Python and is available in https://github.com/AssafRab/RETCO.

Example 3.1 Consider the setting of \( b^* \perp b \) and a training data containing four observations from two clusters with the covariance matrix \( \text{Var}(y) = \begin{pmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 0 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{pmatrix} \), i.e., observations 1 and 2 belong to the first cluster and observations 3 and 4 belong to the second cluster. The \( CV_c \) correction is reduced in this setting to \( 2 \text{tr}(H_{cv} \text{Var}(y))/n \). Two models with the GLS predictor are tested:

- Model A, which splits the training set into the two clusters. Given the covariance matrix:

\[
H_{cv} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \rightarrow \frac{2}{n} \text{tr}(H_{cv} \text{Var}(y)) = 2.
\]
• Model B, that mixes between the clusters and selects observations 1 and 3 for one subset and 2 and 4 for the other subset. Given the covariance matrix:

\[ H_{cv} = \begin{pmatrix} 0 & 0.25 & 1 & -0.25 \\ 0.25 & 0 & -0.25 & 1 \\ 1 & -0.25 & 0 & 0.25 \\ -0.25 & 1 & 0.25 & 0 \end{pmatrix} \]  

\[ \frac{2}{n} \text{tr}(H_{cv} \text{Var}(y)) = 0.5. \]

As we can see in Example 3.1, decomposing the penalty, \( \frac{2}{n} \text{tr}(H_{cv} \text{Var}(y)) \), shows that the weights that relate to observations from the same cluster are multiplied by their positive covariance values and therefore contribute to the penalty, while weights that relate to observations from different clusters are multiplied by zero and therefore do not contribute to the penalty. As a result the penalty of model A, which gives the whole weight for observations from the same cluster, is larger than for model B. Therefore, while \( CV \) selects model A when \( CV(A) < CV(B) \), \( CV_c \) selects model A when \( CV(A) < (CV(B) - 1.5) \). In that way \( CV_c \), as well as \( Cp \), balance the tendency to split based on the correlation structure of the training set. Obviously, as much as the observations in the training set are more correlated, the penalty effect is stronger, and the superiority of RETCO over the standard algorithm is more prominent (see also Section 5).

Example 3.2 Consider the setting of \( b^* \perp b \) and \( y \sim N_{100}(0.1 \times x_1, V) \), where

\[ \text{Var}[i, j] = \begin{cases} 
2, & \text{when } i = j \\
1, & \text{when } i \neq j \text{ and } (i, j \leq 50 \text{ or } i, j > 50), \\
0, & \text{o.w} 
\end{cases} \]

and

\[ x_1[i] = \begin{cases} 
0.5 + \epsilon_x, & \text{when } i \text{ is odd}, \quad \epsilon_x \sim N(0, 0.1) \\
-0.5 + \epsilon_x, & \text{when } i \text{ is even}, 
\end{cases} \]

i.e., \( y \) contains two clusters of 50 observations each, and its mean is not correlated with the clusters.

Two models are tested, model A which uses the threshold \( x_1 = 0 \) and model B which uses \( x_2 = 0 \), where \( x_2 \) is highly correlated with the clusters:

\[ x_2[i] = \begin{cases} 
0.5 + \epsilon_x, & \text{when } i \leq 50, \quad \epsilon_x \sim N(0, 0.1) \\
-0.5 + \epsilon_x, & \text{when } 50 < i.
\end{cases} \]

A simulation of this setting is visualized in Figure 1. In this simulation \( CV(A) = 1.47 \) and \( CV(B) = 1.04 \), while \( CV_c(A) = 2.47 \) and \( CV_c(B) = 3.04 \). Therefore, in case \( b^* \perp b \), while \( CV \) selects model B, \( CV_c \) selects model A. \(^1\)

Unlike \( Cp \) and \( CV_c \), whose penalties depend on \( \text{Var}(y) \), the penalty of AIC in this setting \( (b^* \perp b) \) is fixed regardless of the training covariance structure at \( 2p/n \). Therefore, we can conclude that in AIC the likelihood, \( \ell(y; \hat{E}(y|X), V) \), is responsible for mixing uncorrelated training set observations in the different paths, while the penalty only affects the stopping rule.

\(^1\) For the setting \( b^* = b \), which will be discussed next, \( CV_c = CV \) and both select model B.
3.2.2 \( b^* = b \)

When \( b^* = b \) the correlation between \( y^* \) and \( y \) is the same as the correlation between observations in \( y \). Therefore, unlike in the \( b^* \perp b \) setting, here there is no clear motivation to restrict the tendency to split the nodes based on the correlation structure of the training set (as appears in standard regression trees). Correspondingly, the bias corrections in this setting are also different than in the \( b^* \perp b \) setting. For example, \( CV \) is not biased in this setting, i.e., \( CV_c = CV \) (for more details see Section 2.3). The penalty in \( Cp \), \( 2\sigma^2 \text{tr}(H)/n \), depends on \( \text{Var}(y) \) through \( H \) for some models (e.g., for LMM), however for other models it does not depend implicitly on \( \text{Var}(y) \). In any case, the effect of \( \text{Var}(y) \) is much less prominent than in \( b^* \perp b \) setting, where the bias is \( 2\text{tr}(HV\text{Var}(y))/n \). Similarly with the penalty in \( \text{AIC} \), \( 2\text{tr}(H)/n \). Therefore, in this setting, both \( \text{Cp} \) and \( \text{AIC} \) penalties mainly affect to the stopping rule rather than mix between uncorrelated observations. Given additional stopping rules (e.g., tree depth, minimal number of training set observations in each node), we can conclude that the effect of using prediction error estimator instead of training error is limited. A numerical analysis of this scenario is presented in Section 5.1.2. Still, it is important to emphasize that the proposed model—\( f(x^*) + b^* z^* \)—is recommended also because of the inference and the use of a solid statistical perspective that the random effects framework enables.

3.2.3 \( b^* \not\perp b \) but \( b^* \neq b \) Scenario

From a qualitative perspective, this scenario is the same as the \( b^* \perp b \) scenario. In both scenarios, the correlation structure of \( y \) is not preserved in the prediction problem. As a result, the bias correction has a key role in balancing the tendency of standard regression trees to split based on the correlation structure of \( y \). The main difference between the scenarios is quantitative and is explicitly expressed in the bias corrections formulas, for
example the bias correction in \( \text{Cp} \) is \( 2 \text{tr} \left( H \left( \text{Var}(y) - \text{Cov}(y, y^*) \right) \right) / n \). This setting of \( b^* \not\perp b \) but \( b^* \neq b \) is demonstrated in Section 5.2.

4. Comparison With Other Algorithms

To our knowledge Sela and Simonoff (2012) were the first to propose integration between LMM and regression tree by introducing the RE-EM algorithm. The main idea in RE-EM is generating \( \{g_s\}_{s=1}^S \) using a standard regression tree that is fitted to the residual, \( y - Z\hat{b} \). Given \( \{g_s\}_{s=1}^S \), \( \{\mu_s\}_{s\in S} \) are estimated by GLS. Therefore, the correlation is taken into account in estimating \( \{\mu_s\}_{s\in S} \), but it is ignored in selecting \( \{g_s\}_{s=1}^S \). RE-EM algorithm is presented in Appendix C. Hajjem et al. (2014) proposed a RF algorithm which is based on the same logic as RE-EM algorithm. For numerical comparison between RE-EM and RETCO, see Section 5.1.4.

Stephan et al. (2015) proposed the Mixed Random Forest (MRF), that does not ignore the correlation structure when selecting \( \{g_s\}_{s=1}^S \), however still does not address the correlation correctly. The goal in MRF (which is also presented in Appendix C) is fitting a model that estimates accurately the variance components, rather than optimizing prediction accuracy, as in RETCO. Also, MRF assumes a specific data type and is based on strong distributional assumptions (\( y \) is normally distributed and \( G = \sigma^2_b I_q \)). Besides the difference in goals and the assumed settings, the main difference in the tree fitting approach is that MRF uses likelihood loss function for finding \( \{g_s, \mu_s\}_{s=1}^S \), rather than estimated prediction error for correlated data (i.e., training error plus a bias correction) as in RETCO. Also, MRF is based on a standard recursive approach, while RETCO is based on an iterative approach (for the motivation of using an iterative approach see Section 3). For numerical comparison between MRF and RETCO, see Section 5.1.4.

Extensions of these papers, where the response is binary or count data, as in generalized linear mixed model (Wolfinger and O’connell, 1993), where proposed by Fokkema et al. (2018); Hengl et al. (2018); Ngufor et al. (2019); Speiser et al. (2019).

5. Numerical Results

This section compares the performance of RETCO with the standard regression tree algorithm and relevant modifications of it that will be described. The analysis is performed using both simulated data and real data sets for different correlation settings. The simulation part is based on random effects framework and presents results for \( b^* = b \) as well as for \( b^* \not\perp b \) correlation settings. The \( b^* \neq b \) but \( b^* \not\perp b \) correlation setting is analyzed in the random field context using a real data set with spatial correlation. Also, different prediction error estimator types (Cp, CV_\text{c} and AIC) and different trees-based models (regression tree and RF) are analyzed. The code is available in \url{https://github.com/AssafRab/RETCO}.

5.1 Simulation

The training set was generated from the following model:

\[
y = I(x_1 > 0) + I(x_2 > 0) + I(x_3 > 0) + I(x_1 > 0)I(x_2 > 0)I(x_3 > 0) + Zb + \epsilon,
\]

where
• $I(x_{j,i} > 0), \forall j \in [1, 2, 3]$ is the indicator vector for $x_{j,i} > 0, \forall i \in [1, ..., n]$.

• The sample contains $C$ clusters, each one of size $n_c = n/C$. $Z \in \mathbb{R}^{n \times C}$ indicates the clusters, i.e., for the first column the first $n_c$ elements are 1, and the rest are zero, for the last column the last $n_c$ elements are 1 and the rest are zero.

• $b \in \mathbb{R}^C$ is the random effects vector, distributed $N_C(0, \sigma^2 b I_C)$, and $\epsilon \sim N_n(0, I_n)$.

• $x_1, x_2$ and $x_3$ are $Z \gamma + \eta$, where $\gamma \sim N_C(0, \sigma^2 \gamma I_C)$ and $\eta_i$ are uncorrelated and distributed uniformly, $U(-1, 1)$, $\forall i \in [1, ..., n]$.

5.1.1 New Random Effects ($b^* \perp b$)

As was mentioned in Section 2.2, when $b^* \perp b$, i.e., when $\text{Cov}(y^*, y) = 0$, GLS estimator should be used instead of LMM. Here, $C_p$ prediction error estimator is analyzed and therefore $y^*$ should be related to the same covariate values as in the training set, $\Phi = \{x_1, x_2, x_3, Z\}$. In order to reduce the variance of the prediction error estimate, the test sample contains 300 replicates of $\Phi$. RETCO is compared to a standard regression tree with squared error loss function, which is the same loss as in $C_p$ but without the bias correction term. In both algorithms, the stopping rules are depth of tree smaller than 4, and number of observations in the terminal node greater than 2. The relative difference between the RETCO test error and its alternative:

$$\text{error difference} \% = \frac{\text{error(RETCO)} - \text{error(standard tree)}}{\text{error(standard tree)}},$$

is calculated repeatedly for 100 simulation runs. The average simulation run time is 82.1 seconds, where RETCO takes on the order of 3-8 fold longer to run due to its iterative approach. For more details about RETCO’s computational complexity, see Section 3.1.

Figure 2, left panel, presents boxplots of error difference$\%$ for different $\sigma^2 b$. As expected, when $\sigma^2 b$ is larger (i.e., the correlation is stronger), the improvement in using RETCO over the standard regression tree algorithm is bigger. However, also for relatively small $\sigma^2 b$ values RETCO outperforms the standard regression tree algorithm. Additional comparisons for different sample sizes ($n$) and cluster sizes ($n_c$), and similar analyses for generalization error setting using $CV_c$, are given in Appendix D.

As was mentioned in Section 3.2, RETCO balances the tendency of standard tree to split based on the correlation structure of the training sample. Therefore, we expect that RETCO mixes training set observations from different clusters in the leaves more than the standard regression tree. The following measure quantifies this mixing property:

$$\text{homogeneity} = \sum_{s \in S} \sum_{c=1}^{C} |n(c, s) - n(s)/C|,$$

where $n(c, s)$ is the number of training set observations in leaf $s$ that belong to cluster $c$ and $n(s) = \sum_{c=1}^{C} n(c, s)$. Smaller homogeneity means bigger mixing. Figure 3 plots the training sample homogeneity difference$\%$:

$$\frac{\text{homogeneity(RETCO)} - \text{homogeneity(standard tree)}}{\text{homogeneity(standard tree)}},$$
5.1.2 Same Random Effects ($b^* = b$)

For the $b^* = b$ scenario, the training set is the same as in Section 5.1.1, but the prediction set is different, such that the random effects realizations from the training set are also used for constructing $y^*$. 

For RETCO, AIC loss function with LMM predictor for $y$ is used for splitting. As presented in Section 3, the predictor in the tree’s leaves is GLS and the random effects term is added after fitting the tree. For the standard regression tree, normal likelihood loss
function is used with no distinction between random and fixed effects, i.e., all the covariates, including the cluster, can be selected for splitting. Correspondingly, the minus log likelihood of i.i.d normal distribution (which is effectively the same as squared error loss) is used as a loss function for the standard regression tree algorithm. The middle panel of Figure 2 compares between the algorithms for different $\sigma^2_b$ values (when $n = 300$ and $n_c = 50$). As we can see, RETCO outperforms the standard tree algorithm. For $\sigma^2_b = 0.5$ and $\sigma^2_b = 1$, the average error difference [%] is relatively small. As was mentioned in Section 3.2.2, this phenomenon is expected.

5.1.3 RF - New Random Effects

RF is analyzed for $b^* \perp b$ and Cp loss function setting. The training sample model is:

$$
\mathbf{y} = \mathbf{I}(x_1 > 0) + \mathbf{I}(x_2 > 0) + \mathbf{I}(x_3 > 0) + \mathbf{I}(x_4 > 0) \mathbf{I}(x_5 > 0) \mathbf{I}(x_6 > 0) + Z\mathbf{b} + \mathbf{e},
$$

where $x_i \forall i \in \{1, ..., 6\}$, $Z \mathbf{b}$ and $\mathbf{e}$ have the same distribution as in Section 5.1.1. Additional parameters that are relevant for RF are:

- The maximal tree depth is 10
- The number of regression trees is $T = 100$
- A random half-sample method is used for sampling the training set for each tree (i.e., the training sample size for each tree is 250 without duplicates)
- Three covariates are randomly selected at each split, following the rule of thumb of selecting randomly $\text{round}(\log_2(p))$ potential covariates at each split.

Also, two versions of RETCO are tested: the first uses the stopping rule constraint as presented in RETCO inequality (2), the second does not enforce the constraint, and therefore results in deeper trees. The prediction set contains new random effects realizations, such that $\text{Cov}(\mathbf{y}^*, \mathbf{y}) = 0$. The covariates of the prediction set are 200 replicates of the covariates of the training set. The analysis was repeated 50 times. The right panel in Figure 2 presents boxplots of the error difference [%] for different $\sigma^2_b$. As we can see, both versions of RETCO outperform the standard algorithm. Also, forcing the stopping rule gives better results.

5.1.4 Comparison With Previous Algorithms

The competitors in the left and the right graphs in Figure 2 preserve the main characteristics of the MRF algorithm: taking into account the correlations structure by using GLS estimator and differentiation between random and fixed effects. The exact MRF algorithm, which was designed for a genetic application, is not implemented here since some of its technical details are specific for genetic applications, which are not our main use case. A comparison between RETCO and RE-EM algorithm is presented in Appendix D. As expected, RETCO’s performance is uniformly superior to both algorithms due to its use of prediction error estimates for splitting and the careful consideration of correlation structures in splitting and prediction.
5.2 Real Data Analysis

This section presents real data analyses comparing the performance of the standard regression tree and RF algorithms to their RETCO versions for six different data sets with various correlation structures. The data sets and the prediction problems are briefly described in Section 5.2.1, additional technical information can be found in Appendix D.

Table 2 summarizes the results. As can be seen, for all the six analyses the test errors of the standard regression tree and RF algorithms are greater than the test errors of their RETCO versions (negative error difference [%]), moreover in several analyses the improvement of RETCO over the standard algorithm is very large.

5.2.1 Prediction Problems Description

- **FIFA** – This data set contains football players’ market-values. The data set has a clustered correlation structure, where the cluster variable is the player’s club, such that market-values of players from the same club are correlated but from different clubs are not correlated. The prediction goal is to predict the market-values of new players from new clubs. In order to satisfy this prediction goal, the training set contains the observations of players from 20 clubs that were randomly sampled (548 observations), and the test set contains the observations of the other clubs (17,939 observations). Since the covariate values of the prediction set are not the same as the covariate values of the training set, CV-type loss function is used in the algorithms’ splitting criterion – CV for RETCO and CV for the standard regression tree/RF algorithms. The prediction error is estimated by the average squared errors of the test set. The data set is publicly available on Kaggle.

- **Communities and Crime** – This data set presents the number of violent crimes per population size in US communities. The data set has a clustered correlation structure, where the clusters are the US states (each state contains many communities). The training set contains 15 clusters that were randomly sampled (790 observations), where the test set contains the other clusters (1,204 observations). For the same reason as in the FIFA data set, CV-type loss function is used in the algorithms’ splitting criterion. The data set was introduced by Redmond and Baveja (2002), and is publicly available on the UCI repository.

| Correlation Structure | Data Set Name      | Regression Tree | RF     |
|-----------------------|--------------------|----------------|--------|
| Clusters              | FIFA               | −4.9%          | −7.1%  |
|                       | Crimes             | −8.1%          | −4.4%  |
| Spatial               | Korea Temperature  | −14.5%         | −13.6% |
|                       | California Housing | −14.2%         | −3.3%  |
| Longitudinal          | Parkinson’s Disease| −32.9%         | −35.4% |
|                       | Wages              | −20.1%         | −7.9%  |

Table 2: Error difference [%] between RETCO and standard regression tree, and between RETCO and standard RF.
- **South Korea Temperature** (*bias correction of numerical prediction model temperature forecast*) – This data set contains daily maximal temperature measurements (collected in August between the years 2013 – 2017) at several sites in South Korea. The prediction goal is to predict the maximal temperature of new days. Measurements of the first two years were selected (575 observations) in order to predict the maximal temperature of the same set of days in the next years (2,325 observations). Due to the spatial correlation structure, exponential kernel covariance function was used for modeling. Since all the records are measured at the same sites, in-sample error type is used in the algorithms’ splitting criterion ($C_p$ for RETCO and squared error loss for the standard regression tree/RF). The data set was introduced by Cho et al. (2020), and is publicly available on UCI repository.

- **California Housing Prices** – This data set contains the median house value within a block for different blocks in California. Some of the blocks belong to the same clusters (same coordinate values), therefore the data set has a clustered-spatial correlation structure, which can be represented by the following kernel covariance function:

$$\text{Cov}(y_i, y_j) = K(|z_i - z_j|) + \sigma_b^2 I_{\text{cluster}(i) = \text{cluster}(j)} + \sigma^2 I_{i = j},$$

where $K(\cdot)$ is the exponential kernel covariance function, $z_i, z_j$ are the coordinates and $\text{cluster}(i), \text{cluster}(j)$ are the clusters of $y_i, y_j$. The prediction goal is to predict the median house value of new blocks from new clusters. Therefore, 100 clusters are randomly sampled (279 observations) for the training set and the other clusters are used as the test set (12,124 observations). Since the prediction goal is to predict median house values from new clusters, then $b^* \neq b$. However, due to the spatial correlation, the prediction set median house values are correlated with the training set median house values, and therefore this setting satisfies the $b^* \neq b \cap b^* \not\perp b$ scenario (see Section 2.2.1). CV-type loss function is used in the algorithms’ splitting criterion since the covariate points of the training set and the prediction set are different. The data set was introduced by Pace and Barry (1997), and is publicly available on Kaggle.

- **Parkinson’s Disease Telemonitoring** – This longitudinal data set contains Parkinson’s disease symptom scores of 42 individuals along six-months trial. The clustered-temporal correlation structure, where the clusters refer to the individuals, can be modeled by LMM with random intercept for the cluster and random slope for the time variable. The prediction goal is predicting the score of new individuals, therefore five individuals were randomly sampled (742 observations) for the training set and the others were designated as the test set (5,179 observations). The covariates in this data set are biomedical voice measurements and their values are approximately the same for all the individuals. Therefore, $C_p$ and squared error loss loss functions are used in the splitting criterion for RETCO and standard regression tree/RF, respectively. The data set was introduced by Tsanas et al. (2009), and is publicly available on the UCI repository.

- **Wages** – This longitudinal data set presents the average hourly wages by year of 888 employees. As in the Parkinson’s Disease Telemonitoring data set, this data set can be modeled by LMM with random intercept and random slope, where the employee is
the cluster variable. The prediction goal is to predict the average hourly wage of new employees. 50 individuals were randomly sampled (331 observations) for the training set and the other are used as the test set (6,071 observations). Since the covariate values of the training set and the prediction set are different, CV-type loss function is used in the algorithms’ splitting criterion. The data set was introduced by Singer et al. (2003), and is publicly available in brogar package in R software.

6. Conclusions

This paper presents a new algorithm, RETCO, for fitting regression trees-based models for correlated data. Analyzing various settings with different correlation structures lead to the conclusion that RETCO substantially improves prediction performance in settings involving correlated data.

Unlike standard regression trees-based models, which ignore the correlation structure of the data, RETCO accounts for the correlation structure in various ways, such as using prediction error estimates for correlated data as the loss function in the splitting criterion. As discussed and demonstrated, using prediction error estimators for correlated data instead of training error neutralizes the tendency to fit a tree that divides the training set based on its correlation structure, as is likely to happen in standard regression trees-based models.

Extensive data analysis, including analysis of six different real data sets, shows the superiority of RETCO over standard regression trees-based model, as well as its generality that enables to implement it under various settings.

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Appendix A. Theoretical Background

This appendix extends the theoretical background that is given in Section 2.

A.1 Regression Tree, Random Forest and Gradient Boosting

Algorithm 2 presents a typical regression tree algorithm.

**Algorithm 2 A typical tree-based algorithm**

**Input:** y, X.
**Output:** f(·).

**High-level setting:** select a training error loss function and define stopping rules

**Initialization:** $S = \{g_1, \mu_1\}$, where $g_1 = \mathbb{R}^p$, $\mu_1 = \frac{1}{n} \sum_{i=1}^{n} y_i / n$.

**repeat**

1. Given the predefined stopping rules, for each node $s \in S$ solve the following optimization problem:

   $$c_s, j_s = \text{argmin}_{c \in \mathbb{R}, j \in J_s} \left\{ \frac{1}{|I_s|} \sum_{i \in I_s} \text{Loss}(y_i, I(x_{i,j} \leq c) \mu_s^I(c) + I(x_{i,j} > c) \mu_s^R(c)) \right\},$$

   where $J_s$ is the set of available covariates for splitting node $s$, $I_s = \{i | x_i \in g_s\}$, $\mu_s^I(c)$ and $\mu_s^R(c)$ are the mean estimators of $\{y_i | x_i \in g_s \cap x_{i,j} \leq c\}$ and $\{y_i | x_i \in g_s \cap x_{i,j} > c\}$ respectively.

2. Update $S$ by replacing $(g_s, \mu_s)$ by the new two nodes: $(g_s \cap x_{j_s} \leq c_s, \mu_s^I(c_s))$, $(g_s \cap x_{j_s} > c_s, \mu_s^R(c_s))$, where $x_{j_s}$ is the covariate $j_s$ and $\mu_s^I(c_s), \mu_s^R(c_s)$ are the related mean predictors.

**until** Stopping rules are satisfied $\forall s \in S$

Random forest (RF) and gradient boosting (GB) predictor are based on averaging an ensemble of trees:

$$f(x^*) = \sum_{t=1}^{T} \lambda_t \sum_{s=1}^{S_t} I(x^* \in g_{t,s}) \mu_{t,s},$$

where $T$ is the number of trees and $\lambda_t \in (0, 1]$ is the learning rate (for RF $\lambda_t = 1/T$, $\forall t$).

The regression trees in RF and GB are fitted in different ways than in a standard regression tree. In RF, the training set of each tree is sampled from the original sample (e.g., sampling with replacement of size $n$, half-sample), and the set of the potential covariates of each split is a random sample of $J_s$. In GB the trees are dependent and created consecutively, where the dependent variable of each tree is the residual of the previous tree. Also, there are many techniques for reducing over-fitting and model variance which are relevant for RF and GB, but not relevant for standard regression tree model. For more information about RF and GB see Freund et al. (1999); Friedman (2001); Breiman (2001); Hastie et al. (2009).

Note, unlike in regression tree model, which tends to over-fit and therefore suffers from high variance, RF has relatively low variance due to the averaging over the $T$ trees. This property affects the optimal structure of trees in RF. While the tree depth in regression tree model should be restricted in order to avoid over-fitting, the trees in RF can be large
whenever $T$ is respectively large (Criminisi et al., 2011). Since the trees in RF are correlated, the RF variance decreases in a smaller rate than $T$. Commonly the trees’ depth in RF is also restricted for various reasons, such as computational cost that RF with deep trees (and consequently large $T$) requires.

## A.2 Prediction Error Estimation and Model Selection for Correlated Data

### A.2.1 Cp

The original Cp, when $\text{Cov}(\mathbf{y}, \mathbf{y}) = \sigma^2 \times \mathbf{I}_n$ and $\text{Cov}(\mathbf{y}^*, \mathbf{y}) = 0$, was introduced by Mallows (1973) is:

$$Cp = \frac{1}{n} \| \mathbf{y} - \hat{\mathbf{y}} \|_2^2 + \frac{2\sigma^2}{n} p.$$  

### A.2.2 AIC

The standard AIC under normality and i.i.d assumptions, that was introduced by Akaike (1974) is:

$$AIC = - \frac{2\ell(\mathbf{y}; \hat{\mathbf{E}}(\mathbf{y}|X), \sigma^2)}{n} + \frac{2p}{n},$$

where $\ell(\mathbf{y}; \hat{\mathbf{E}}(\mathbf{y}|X), \sigma^2)$ is the log-likelihood of $\mathbf{y}$.

## Appendix B. Estimating Variance Components for Clustered Data

When $\mathbf{y}$ has a clustered correlation structure, i.e., its covariance matrix follows:

$$\text{Cov}[i, j] = \begin{cases} 
\sigma^2_{\epsilon} + \sigma^2_{b}, & \text{when } i = j \\
\sigma^2_{b}, & \text{when } i \neq j \text{ but } c(i) = c(j), \\
0, & \text{o.w}
\end{cases},$$

where $c(i)$ is the cluster that observation $i$ belongs to and $\sigma_{\epsilon}$, $\sigma_b$ are in $R^+$, then $\sigma^2_{\epsilon}$ and $\sigma^2_b$ can be estimated in a closed-form way. In order to simplify the equations let us assume $\mathbb{E}\mathbf{y} = 0$. In this case:

$$\hat{\sigma}^2_{\epsilon} = \frac{\sum_{i=1}^{n} (y_i - \bar{y}(i))^2}{(n - C)},$$

where $\bar{y}(i)$ is the average of the cluster that $y_i$ belongs to, and $C$ is the number of clusters,

$$\hat{\sigma}^2_{b} = \left( \frac{\sum_{i=1}^{n} (\bar{y}(i) - \bar{y})^2}{C - 1} - \hat{\sigma}^2_{\epsilon} \right) \times \frac{C - 1}{n - \sum_{j=1}^{C} n_j^2/n},$$

where $\bar{y}$ is the average of $\mathbf{y}$ and $n_j$ is the number of observations in cluster $j$. When $\mathbb{E}(\mathbf{y}) \neq 0$, the variance parameters should be calculated for the residual, $\mathbf{y} - \hat{\mathbf{E}}\mathbf{y}$.
Algorithm 3 RE-EM Algorithm

Input: \( y, X, Z \).
Output: \( f(\cdot), \hat{b} \).
Initialization: \( \hat{b}^{(0)} = 0 \).
repeat
1. Using the fixed effects covariates, fit CART algorithm (Breiman et al., 1984) for \((y - Z\hat{b}^{(k-1)})\) and extract \( \{g^{(k)}_s\}_{s=1}^S \) from the fitted tree.
2. Estimate \( \{\mu_s\}_{s=1}^S \), \( G \) and \( \sigma^2 \) using the following LMM model:

\[
y_i = \sum_{s=1}^S I(x_i \in g^{(k)}_s)\mu_s + z_i b + \epsilon_i,
\]

where \( b \sim N_q(0, G) \), \( \epsilon_i \sim N(0, \sigma^2) \).
3. Given \( \{\mu^{(k)}_s\}_{s=1}^S \), \( \hat{G}^{(k)} \) and \( \hat{V}^{(k)} = Z\hat{G}^{(k)}Z' + \hat{\sigma}^2^{(k)}I_n \): estimate \( \hat{b}^{(k)} \) using the BLUP formula.
until Convergence of \( \hat{b}^{(k)} \).

Appendix C. Comparison with Other Methods

Algorithm 3 presents the RE-EM algorithm, which was proposed by Sela and Simonoff (2012). Algorithm 4 presents MRF algorithm for a single tree, that was proposed by Stephan et al. (2015). For MRF, in order to simplify notations, denote \( y, X, Z \) as the bootstrap sample and ignore the features sampling at each split.

Appendix D. Numerical Results

This appendix presents additional results that are related to Section 5.1, as well as detailed information relating the settings in Section 5.2.

D.1 Regression Tree - New Random Effects \((b^* \perp b)\)

D.1.1 In-Sample Error Setting:

Given the simulation setting that is described in Section 5.1.1, Figure 4, left panel, presents the effect of the cluster size \((n_c)\), on the performance of RETCO. As can be seen in the figure, for larger block size \((n_c = 150)\) the average error difference[%] is smaller. Figure 4, middle panel, presents the effect of the sample size on the performance of RETCO. As can be seen, RETCO performs better for all the settings. Also, as expected, the error difference[%] variance is smaller for larger sample sizes. The variance depends on the maximal depth of the tree, which was set to three. Tree with three levels has potentially eight predictors, which is a large amount of predictors when \( n = 100 \), but small when \( n = 1000 \).

2. Stephan et al. (2015) do not supply an organized algorithm, Algorithm 4 tries to formalize their approach as given in their supplementary material.
Algorithm 4 Mixed Random Forest (algorithm for fitting a single tree)

Input: $y, X, Z.$
Output: $f(\cdot), \hat{\sigma}_b^2, \hat{\sigma}^2.$
Initialization: $g_1 = \{0, 1\}^J$. Also, estimate $\hat{\delta} = \sigma^2/\sigma_b^2$.

repeat
1. Given the predefined stopping rules, for each node $s \in \mathcal{S}$, find the following parameters:
   $$\tilde{j}_s, \tilde{\sigma}^2 = \arg\max_{j_s \in J_s, \sigma^2 \in \mathbb{R}^+} \ell(y; \sigma^2, \mu_s^l, \mu_s^r, \{\mu_l\}_{l \in \mathcal{S}/s}, \{g_l\}_{l \in \mathcal{S}/s}),$$
   where $\mu_s^l, \mu_s^r$ and $\{\mu_l\}_{l \in \mathcal{S}/s}$ are the GLS estimators for $\{y_i| x_i \in g_s \cap (x_{i,j_s} = 0)\}$, $\{y_i| x_i \in g_s \cap (x_{i,j_s} = 1)\}$, and $\{y_i| x_i \in g_l\}_{l \in \mathcal{S}/s}$ subsets respectively.

2. Update $f(\cdot)$: replace each node $s \in \mathcal{S}$ by $\{g_s \cap (x_{j_s} = 0), \mu_s^l\}$ and $\{g_s \cap (x_{j_s} = 1), \mu_s^r\}$.
until Stopping rules are satisfied $\forall s \in \mathcal{S}$.

Figure 4: Boxplots of the error difference[\%]. Left: In-sample error setting, $b^* \perp b$, $n = 300$, $\sigma_b^2 = 1$ and different $n_c$. The means are $-9.9$, $-8.0$ and $-4.3$. Middle: In-sample error setting, $b^* \perp b$, $\sigma_b^2 = 1$ $n_c = 50$ and different $n$. The means are $-2.9$, $-9.9$ and $-5.0$. Right: Generalization error setting, $b^* \perp b$, $n = 300$, $n_c = 50$ and different $\sigma_b^2$. The means are $-2.8$, $-11.0$ and $-7.3$.

Therefore, when $n = 100$ the trees are noisy for both algorithms, and their relative difference is noisy as well.

D.1.2 Generalization Prediction Error Setting:
In order to analyze RETCO performance in generalization prediction error setting, the test set setting was changed such that the prediction set covariates are nonidentical to the training sample covariates (but are sampled from the same distribution). As was described in the paper, $CV_c$ loss function estimates the generalization error unbiasedly by correcting the standard CV error. Therefore, $CV_c$ loss function is used in RETCO and CV loss function is used for the standard regression tree algorithm. Figure 4, right panel, presents the error difference[\%] for different $\sigma_b^2$.  

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D.2 Comparison With RE-EM

Figure 5, left figure, presents the error difference between RETCO and RE-EM for the scenario when $b^* \perp b$. All the other setting details are the same as in Section 5.1.1. Similarly, Figure 5, right figure, presents the error difference between RETCO and RE-EM for the scenario when $b^* = b$. All the other setting details are the same as in Section 5.1.2. As can be seen in Figure 5, RETCO performs better than RE-EM.

D.3 Real Data Analysis

Detailed information about the settings of the real data analyses is given below.

General information:

- The number of covariates that were sampled at each split in the RF implementations is $\text{round}(\log_2(p))$.
- The number of trees that are used for the RF is not fixed. The fitting process was stopped once the overall RF error was converged in both algorithms, RETCO and the standard regression tree.

Specific information for each data set analysis:

- **FIFA**
  - Dependent variable: Player’s market values
  - Cluster variable: Player’s club
  - Loss function type: CV
  - Number of covariates: 11
  - Regression tree depth: 5
  - Minimum number of observations in a node: 3
  - Number of trees for RF: 60
  - Comments: The covariates that are used in this analysis are: ‘Age’, ‘Overall’, ‘Potential’, ‘Wage’, ‘Special’, ‘Preferred Foot’, ‘International Reputation’, ‘Weak Foot’, ‘Skill Moves’, ‘Height’, ‘Weight’. Other variables have many missing values or are irrelevant.
• *Crimes (Communities and Crime in US)*
  – Dependent variable: Violent crimes in US communities per population size
  – Cluster variable: State
  – Loss function type: CV
  – Number of covariates: 100 (all the available covariates were used)
  – Regression tree depth: 5
  – Minimum number of observations in a node: 3
  – Number of trees for RF: 55
  – Comments: -

• *Korea Temperature* (*bias correction of numerical prediction model temperature forecast*)
  – Dependent variable: Daily maximum temperature at several sites in South Korea
  – Cluster variable: Day
  – Loss function type: Cp (since training and test set measurements are sampled from the same sites)
  – Number of covariates: 4
  – Regression tree depth: 5
  – Minimum number of observations in a node: 3
  – Number of trees for RF: 70
  – Comments:
    * The covariates that are used in this analysis are: 'Present_Tmin', 'DEM', 'Slope', 'Solar radiation'. Other variables in this data set are models’s scores of the data set supplier, which are based on previous dependent variable measurements (and therefore cannot be used in LMM framework)
    * Exponential kernel covariance function was used. Maximal temperature of different days are assumed to be uncorrelated.
    * The original data set contains records from July and August. Due to many missing values in July along the years, only records from August are analyzed. Also, sites with missing values along the years were omitted.

• *California Housing*
  – Dependent variable: Values of houses in California
  – Cluster variable: Block’s cluster (blocks with the same coordinate values)
  – Loss function type: CV
  – Number of covariates: 6 (all the available covariates were used)
  – Regression tree depth: 5
  – Minimum number of observations in a node: 3
  – Number of trees for RF: 50
  – Comments: -
• Parkinson’s Disease Telemonitoring
  – Dependent variable: Total UPDRS score, which is a score of Parkinson’s Disease progression
  – Cluster variable: Patient
  – Loss function type: Cp (all the individuals receive approximately the same covariate values)
  – Number of covariates: 18
  – Regression tree depth: 5
  – Minimum number of observations in a node: 3
  – Number of trees for RF: 80
  – Comments: All the supplied covariates were used except the motor_UPDRS (which its relation with the dependent variable is not fully clear to us)

• Wages
  – Dependent variable: Average hourly wages
  – Cluster variable: Employee
  – Loss function type: CV
  – Number of covariates: 6 (all the available covariates were used)
  – Regression tree depth: 4
  – Minimum number of observations in a node: 3
  – Number of trees for RF: 80
  – Comments: -

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