Continuous-Time Birth-Death MCMC for Bayesian Regression Tree Models

Reza Mohammadi,
University of Amsterdam,
a.mohammadi@uva.nl

Matthew Pratola,
The Ohio State University,
mpratola@stat.osu.edu

Maurits Kaptein,
University of Tilburg,
m.c.kaptein@uvt.nl

Abstract

Decision trees are flexible models that are well suited for many statistical regression problems. In a Bayesian framework for regression trees, Markov Chain Monte Carlo (MCMC) search algorithms are required to generate samples of tree models according to their posterior probabilities. The critical component of such an MCMC algorithm is to construct good Metropolis-Hastings steps for updating the tree topology. However, such algorithms frequently suffer from local mode stickiness and poor mixing. As a result, the algorithms are slow to converge. Hitherto, authors have primarily used discrete-time birth/death mechanisms for Bayesian (sums of) regression tree models to explore the model space. These algorithms are efficient only if the acceptance rate is high which is not always the case. Here we overcome this issue by developing a new search algorithm which is based on a continuous-time birth-death Markov process. This search algorithm explores the model space by jumping between parameter spaces corresponding to different tree structures. In the proposed algorithm, the moves between models are always accepted which can dramatically improve the convergence and mixing properties of the MCMC algorithm. We provide theoretical support of the algorithm for Bayesian regression tree models and demonstrate its performance.

Keywords: Bayesian Regression Trees, Decision trees, Continuous-time MCMC, Bayesian structure learning, Birth-death process, Bayesian model selection.

1 Introduction

Classification and regression trees (Breiman et al., 1984) provide a flexible modeling approach using a binary decision tree with regard to some splitting rules based on a set of predictor variables. Tree models often perform well on benchmark datasets, and they are, at least conceptually, easy to understand (De’ath and Fabricius, 2000). Tree-based models, and their extensions such as ensembles of trees (Prasad et al., 2006) and sums of trees (Chipman et al., 2010) are an active research area and arguably some of the most popular machine learning tools (Biau, 2012; Biau et al., 2008; Chipman et al., 1998; Denison et al.)
Much contemporary research work has focussed on Bayesian formulations of regression trees (see, e.g., Denison et al., 1998, Chipman et al., 2010). The Bayesian paradigm provides, next to a good predictive performance, a principled method for quantifying uncertainty (Robert, 2007). This Bayesian formulation can, amongst other uses, be extremely valuable in sequential decision problems (Robbins, 1985, Gittins et al., 2011) and active learning (Cohn et al., 1996) in which for popular approaches such as Thompson sampling (Thompson, 1933, Agrawal and Goyal, 2012) it is vital to know not merely the expected values (or some other point estimate) of the modeled outcome, but rather to obtain a quantitative formulation of the associated uncertainty (Eckles and Kaptein, 2014). This is exactly what Bayesian methods readily provide (Robert, 2007).

Recent Bayesian formulations of regression trees have already found their way into many applications (Gramacy and Lee, 2008), but computationally efficient sampling algorithms for tree models and sum-of-tree models have proven non-trivial: the model space of possible trees grows rapidly as a function of the number of features and efficient exploration of this space has proven cumbersome (Pratola, 2016). Numerous methods have been proposed to address this problem; indeed, the popular sums-of-trees model specification proposed by Chipman et al. (2010) is itself an attempt to reduce the tree depth and thereby partly mitigate the problem. Other recent approaches have focussed on efficiently generating Metropolis-Hasting (MH) proposals in the Markov Chain Monte Carlo (MCMC) algorithm (see Pratola, 2016, Wu et al., 2007, for examples), or alternatives to the MH sampler such as sequential MCMC (Taddy et al., 2011) and particle based approaches (Lakshminarayanan et al., 2013).

To the best of our knowledge, the most effective search algorithm known at this point in time is provided by Pratola (2016), who nicely integrates earlier advances and adds a number of novel methods to generate tree proposals. Pratola (2016) implements these methods using an algorithm that is known as reversible jump MCMC (RJ-MCMC) (Green, 1995): a sampling scheme based on an ergodic, discrete-time Markov chain. In this article we make a significant contribution to this literature by proposing a novel continuous-time search algorithm (CT-MCMC) that has proven extremely efficient in the field of (Gaussian) graphical models (Mohammadi and Wit, 2015, Mohammadi et al., 2017). In this paper we analyze and evaluate this novel approach to efficient posterior sampling for Bayesian regression trees, classification trees, and sum of trees models and we demonstrate that our proposed scheme converges to the desired target distribution.

This paper is structured as follows: in the next Section we introduce the tree and sums of tree models more formally and introduce the sampling challenges associated with this model in more detail. Next, in Section 3 we detail our suggested alternative birth-death approach and provide both an efficient algorithm and the theoretical justification for our proposal. Subsequently, we extend this proposal to also include the rotation moves suggested by Pratola (2016). In Section 4 we compare the performance of our method—in terms of both it statistical properties and its computation time—to the current state of the art (Pratola, 2016) using a simple, well-known, example that is notoriously challenging for tree models (Wu et al., 2007). Finally, in Section 5 we discuss the limitations of our contribution and provide pointers for future work.
2 Sampling from the sum of trees model

In this work we consider binary regression or classification trees and sum of trees models. Given a feature vector $x$ of length $d$, and a scalar output of interest $y$ we can denote the tree model as follows:

$$y = g(x; T, \theta_T) + \epsilon$$

where $T$ denotes the interior nodes of the tree, $\theta_T$ denotes a set of maps associated with the terminal nodes, and $\epsilon$ denotes the error (for regression models $\epsilon \sim \mathcal{N}(0, \sigma^2)$). Effectively, $T$ encodes all the (binary) split rules that jointly generate the tree structure. This is often expressed using a list of tuples $\{(\nu_1, c_1), (\nu_2, c_2), \ldots\}$ where $\nu_i \in \{1, \ldots, d\}$ indicates which element of the feature vector to split on, and $c_i$ denotes the associated value of the split (see, e.g., Pratola, 2016). This way of expressing the tree is however limited since it does not encode the actual topology $\tau$ of the tree, which encodes the number of nodes in a tree, whether a node is internal and terminal, parent/child edges, and node depths. Hence, more precisely $\tau$ and $\{(\nu_1, c_1), (\nu_2, c_2), \ldots\}$ jointly make up the full tree structure $T$. Figure 1 illustrates our notation at this point in the paper; in Section 3 we will gradually introduce some additional notation necessary for our theoretical justification.

Given the number of terminal nodes, $n_t$, the maps $\theta_T = \{\mu_1, \mu_2, \ldots, \mu_{n_t}\}$ take as input a feature vector $x$ and produce a response $\mu_j(x)$. In typical linear regression models the maps are constants; $\mu_j(x) = \mu_j$. Taken together, $T$ represents a partitioning of the feature space and a mapping from an input feature $x$ to a response value encoded in $\theta_T$. Note that the popular sum-of-trees model (Chipman et al., 2010) provides a conceptually straightforward extension of the above specified single tree model:

$$y = \sum_{m=1}^{M} g(x; T_m, \theta_m) + \epsilon$$

where the sum runs over $M$ distinct trees whose outputs are added.

The Bayesian formulation of the tree model is completed by using priors of the form

$$\pi(T, \theta_T, \sigma^2) = \pi(\theta_T|T, \sigma^2)\pi(T)\pi(\sigma^2)$$

and in the case of the sum-of-trees model we have

$$\pi(T, \theta_T, \sigma^2) = \prod_{m=1}^{M} \pi(\theta_{T_m}|T_m, \sigma^2)\pi(T_m)\pi(\sigma^2)$$

(see Pratola, 2016 for details).

For a single tree—which is easily extended to the sum-of-tree case—sampling from the posterior of the model is conceptually carried out by iterating the following steps:

1. Draw a new topology $\tau|y, \sigma^2, \{(\nu_i, c_i)\}$ using some method of generating new topologies such as a birth/death or rotation and subsequently accepting or rejecting the proposal.
\[
T = \{ \tau, (\nu_1, c_1), (\nu_2, c_2) \}
\]
\[
\theta_T = \{ \mu_1, \mu_2, \mu_3 \}
\]

\[\eta_1 \nu_1 > c_1 \nu_2 > c_2 \eta_2 \mu_1 \mu_2 \mu_3\]

Figure 1: A simple example of our main notation for a tree model which has 2 interior nodes \( \eta_1, \eta_2 \). \( T \) encodes both the split rules \( \{ (\nu_1, c_1), (\nu_2, c_2), \ldots \} \) as well as the topology \( \tau \). The set of maps \( \theta_T = \{ \mu_1, \mu_2, \ldots, \mu_n \} \) determines the values of the terminal nodes.

2. draw the split rules \( (\nu_i, c_i) | y, \tau, \sigma^2, \{ (\nu_i, c_i) \} \), \( \forall i \) using perturb or perturb within change-of-variable proposals,

3. draw \( \mu_j | y, \tau, \sigma^2, \{ (\nu_i, c_i) \} \) using (conjugate) Gibbs sampling, and finally,

4. draw \( \sigma^2 | y, \tau, \{ \mu_j \}, \{ (\nu_i, c_i) \} \) also using Gibbs.

The above algorithm has been implemented successfully in earlier work (see Pratola, 2016). For the sampling of \( \tau | y, \sigma^2, \{ (\nu_i, c_i) \} \) (i.e., in step 1 above) the current state-of-the-art is to use a RJ-MCMC approach. In practice this performs well only if the acceptance rate is high (the computation of which is detailed in Equation 4 of Pratola, 2016). When the acceptance rate is low, the mixing of the chain is poor and the exploration of the full model space is notoriously slow.

3 Continuous-time birth-death MCMC algorithm

The issue of a low acceptance rate in step 1 of the algorithm mentioned in the previous section is surprisingly common: as the tree space is extremely large, proposals with a low likelihood are frequent. This specific issue can however be overcome by adopting a continuous-time Markov process—or a CT-MCMC approach—as an alternative to RJ-MCMC. In this sampling scheme the algorithm explores the model space by either jumping to a larger dimension (birth) or lower dimension (death) as in step 1 above, but this time each of these events is modeled as an independent Poisson process. The change events thus occur in continuous time and their rates determine the stationary distribution of the process; see Figure 2 for a graphical overview of possible birth and deaths from a given tree. In CT-MCMC the moves between models are always accepted making the algorithm more efficient.

Cappé et al. (2003) have shown, on appropriate rescaling of time, that the RJ-MCMC converges to a continuous time birth-death chain. One advantage of CT-MCMC is its ability to transit to low probability regions that can form a kind of “springboard” for the algorithm to flexibly move from one mode to another. The CT-MCMC algorithm has already been used in the context of graphical
models (Mohammadi and Wit, 2015, Mohammadi et al., 2017, Mohammadi and Wit, 2019) and mixture distributions (Stephens, 2000, Mohammadi et al., 2013).

\[
\eta_1 \nu_1 > c_1 \nu_2 > c_2 \eta_2 \mu_2 \mu_3 \mu_1 \eta_1 \nu_1 > c_1 \nu_2 > c_2 \eta_2 \mu_2 \mu_3 \nu_j > c_k \eta_i \mu_i^! \mu_i^!#
\]

Our strategy is to view each component of the terminal nodes of the tree as a point in parameter space, and construct a Markov chain with the posterior distribution of the parameters as its stationary distribution. For given tree \((T, \theta_T)\) and our data \(D\), our target posterior distribution is \(Pr(T, \theta_T | D) \propto L(T, \theta_T) \pi(T, \theta_T)\) where \(L(T, \theta_T)\) is the likelihood. We take advantage of the theory on general classes of Markov birth-death processes from Preston (1977, Section 7 and 8). This class of Markov jump processes evolve in jumps which occur a finite number of times in any finite time interval. These jumps are of two types: (i) birth in which a single point is added, and the process jumps to a state that contains the additional point; and (ii) death in which one of the points in the current state is deleted, and the process jumps to a state with one less point. Preston (1977) shows that this process converges to a unique stationary distribution provided that the detailed balance conditions hold.

To properly define the birth and death events in our case we need to introduce some additional notation identifying the different nodes in the tree and their respective variables and cut-points. Let \((T, \theta_T)\) define our tree model as before, but additionally let \(n_t\) be the number of terminal nodes, \(n_v\) the number of variables, and \(n_c\) the number of cut-points. Given the current state \((T, \theta_T)\):

- A birth event goes to state \((T^{b_{ijk}}, \theta_T^{b_{ijk}}) = (T \cup (\eta_i, \nu_{ij}, c_{ijk}), \theta_T \cup (\mu'_i, \mu'_r)) \setminus \mu_i)\) with birth rate \(B_{ijk}(T, \theta_T)\) where \(i \in 1, ..., n_t, j \in 1, ..., n_v, k \in 1, ..., n_c\).
Furthermore, we define $B(T, \theta_T) = \sum_{i=1}^{n_t} \sum_{j=1}^{n_v} \sum_{k=1}^{n_c} B_{ijk}(T, \theta_T)$. Hence, a birth event changes the topology $\tau$ of the current tree $T$ by adding node $i$. However, to complete the specification of the new tree $(T_{bijk}, \theta_{T_{bijk}})$ we also need to add variable $\nu_j$ and cut-point $c_k$ as well as the new terminal maps $(\mu_l^i, \mu_r^i)$. This process is illustrated in Figure 2 on the (bottom) right where a birth occurs at map $\mu_1$.

- A death event goes to state $(T_d, \theta_{T_d}) = (T \setminus (\eta_i, \nu_i, c_i), \theta_T \setminus (\mu_l^i, \mu_r^i) \cup \mu_i)$ with death rate $D_i(T, \theta_T)$ where $i \in 1, ..., n_d$ and $n_d$ is the number of possible deaths. Furthermore we define $D(T, \theta_T) = \sum_{i=1}^{n_d} D_i(T, \theta_T)$. Hence, a death event changes the topology $\tau$ by removing node $i$, including its associated variable and cut-point, $(\nu_i, c_i)$ and their respective maps $(\mu_l^i, \mu_r^i)$. However, to complete the specification of the tree, we need to add a new map $\mu_i$. This process is illustrated in Figure 2 on the left where a death occurs at node $\eta_2$.

Since birth and death events are independent Poisson processes, the time between two consecutive events has an exponential distribution with mean $1/(B(T, \theta_T) + D(T, \theta_T))$. Thus, the birth and death probabilities are

\[
\Pr(\text{birth at node } \eta_i \text{ for variable } \nu_j \text{ and cut-point } c_k) = \frac{B_{ijk}(T, \theta_T)}{B(T, \theta_T) + D(T, \theta_T)},
\]

\[
\Pr(\text{death at node } \eta_i) = \frac{D_i(T, \theta_T)}{B(T, \theta_T) + D(T, \theta_T)}.
\]

The corresponding Markov process converges to our target posterior distribution $Pr(T, \theta_T | D)$ given sufficient conditions that are provided in the following theorem.

**Theorem 3.1** The birth-death process defined by the birth and death probabilities (2) and (3) has stationary distribution $Pr(T, \theta_T | D)$ if

\[
B_{ijk}(T, \theta_T) = \min \left\{ 1, \frac{Pr(T_{bijk}, \theta_{T_{bijk}} | D) Pr(\mu_i)}{Pr(T, \theta_T | D) Pr(\mu_l^i) Pr(\mu_r^i)} \right\}
\]

and

\[
D_i(T, \theta_T) = \min \left\{ 1, \frac{Pr(T_{di}, \theta_{T_{di}} | D) Pr(\mu_i)}{Pr(T, \theta_T | D) Pr(\mu_l^i) Pr(\mu_r^i)} \right\}.
\]

**Proof.** See Appendix A.

Given the results provided above for step 1, our proposed algorithm for the posterior sampling from a sums of tree model is presented in Algorithm 1.

### 3.1 Computational improvements and further additions

While Algorithm 1 is feasible, in practice, it can be improved by a) exploiting conjugacy, and b) including rotation proposals (as initially suggested by Pratola, 2016, for the RJ-MCMC case). Below we detail each in turn.

Conjugate priors on the terminal node parameters $\mu_j \in \Theta_T$, $j = 1, ..., n_t$ can simplify the CT-MCMC algorithm. In our example below we are interested in modeling a continuous response which leads to i.i.d. priors $\pi(\mu_j) \sim N(0, \tau^2)$.
Algorithm 1. Given a tree \((T, \theta_T)\) iterate the following steps:

**Step 1.** Draw new topology \(\tau\) (including possible new \(\nu_j, c_k\)) using CT-MCMC:

1.1. Calculate the birth rates \(B_{ijk}\) according to \((4)\) for \(i \in 1, \ldots, n_t, \ j \in 1, \ldots, n_\nu, \ k \in 1, \ldots, n_c\).

1.2. Calculate the death rates \(D_i\) according to \((5)\) for \(i \in 1, \ldots, n_d\).

1.3. Jump to a new topology \(\tau\) with probabilities given by \((2)\) and \((3)\).

**Step 2.** Draw the new split rules \((\nu_i, c_i)\) \(\forall i\).

**Step 3.** Draw new \(\mu_j\)'s using (conjugate) Gibbs sampling.

**Step 4.** Draw \(\sigma^2\) also using Gibbs sampling.

(Chipman et al., 2010). Marginalizing out a single terminal node parameter \(\mu_i\), the integrated likelihood is given by

\[
Pr(T_{bijk}, \theta_{T_{bijk}} | D) = \int_{\mu_i} Pr(T_{bijk}, \theta_{T_{bijk}} | \mu_i) \pi(\mu_i) d\mu_i \]

which is available in closed form for conjugate priors (similarly for integrating two terminal node parameters). Applying this marginalization to equations \((4)\) and \((5)\) the updated birth and death rates for CT-MCMC search algorithm are

\[
B_{ijk}(T, \theta_T) = \min \left\{ 1, \frac{Pr(T_{bijk}, \theta_{T_{bijk}} | D)}{Pr(T, \theta_T | D)} \right\} \tag{6}
\]

and

\[
D_i(T, \theta_T) = \min \left\{ 1, \frac{Pr(T_{dij}, \theta_{T_{dij}} | D)}{Pr(T, \theta_T | D)} \right\}. \tag{7}
\]

The proposed search algorithm for sampling the tree model using \((6)\) and \((7)\) can then be combined with conjugate Gibbs updates of the continuous parameters, similar to the Metropolis-within-Gibbs algorithm; see for example Stephens (2000).

Finally, while above we have introduced our main results focusing merely on birth-death moves for simplicity, building on recent work by Pratola (2016) we can extend our sampling approach to so-called rotate proposals: rotate proposals can be thought of as a multivariate generalization of the simple univariate rotation mechanism found in the binary search tree literature (see, e.g., Sleator et al., 1988) and implemented in Gramacy and Lee (2008). This generalization allows dimension-changing proposals to occur at any interior node of a tree, and directly moves between modes of high likelihood and is described in detail in Pratola (2016). In appendix B we demonstrate the correctness of this approach once added to the proposed birth-death mechanism in the CT-MCMC case, and we present an efficient way of implementing rotate proposals within algorithm \((7)\) using marginalization.

### 4 Empirical evaluation of our sampling approach

We examine here the performance of our proposed CT-MCMC search algorithm based on a simulation scenario that is often used in the regression tree literature
as it serves as a simple demonstration where proper mixing of the regression trees topological structure is important (Wu et al., 2007). The synthetic dataset consists of \( d = 3 \) covariates and the response \( y \) is calculated for \( n = 300 \) datapoints as:

\[
y = \begin{cases} 
1 + \mathcal{N}(0, \sigma^2) & \text{if } x_1 \leq 0.5, x_2 \leq 0.5 \\
3 + \mathcal{N}(0, \sigma^2) & \text{if } x_1 \leq 0.5, x_2 > 0.5 \\
5 + \mathcal{N}(0, \sigma^2) & \text{if } x_1 > 0.5 
\end{cases}
\] (8)

Note that, following [Wu et al. 2007], we generate covariates such that \( x_1 \) and \( x_3 \) are confounded (see the supplementary materials of [Pratola 2016] for details) which makes this simple data generating scheme particularly challenging.

Following [Pratola 2016] we fit a single tree model (thus \( M = 1 \) in Eq. 1) to this data using the following approaches:

- **RJ-A**: Here we use a straightforward RJ-MCMC algorithm which is based on discrete time birth-death proposals as described in [Pratola 2016].
- **RJ-B**: Here we use discrete time RJ-MCMC algorithm to which we add the rotation proposals as described in [Pratola 2016].
- **RJ-C**: Here we use discrete time RJ-MCMC algorithm including rotation proposals and perturbation. The latter addition concerns the second step of the sampling procedure as outlined in Section 2 which concerns the sampling of the split rules \((\nu_i, c_i)\). This is not the main focus of this paper, however, we want to see whether this additional mechanism is also useful for the CT-MCMC approach (see [Pratola 2016] for detail).
- **CT-A**: Here we use our proposed CT-MCMC algorithm which is based on continuous time birth-death approach; see Algorithm 3.
- **CT-B**: Here we add rotation proposals to the CT-MCMC algorithm described in Algorithm 3 for details we refer to appendix B.
- **CT-C**: Here we use both birth-death and rotation proposals and we add perturbation proposals to the second step of Algorithm 3.

For each of the above sampling approaches we examine the prediction error, the sampling efficiency, the exploration behavior, and the computation time. Table 1 presents our results for \( \sigma^2 = 1 \) which presents a relatively challenging, high-noise, scenario. On average, over 100 replications, the prediction error of each of the models is similar, and hence, as expected, the different sampling methods do not differentiate in terms of predictive performance. However, in terms of computational efficiency, measured as the effective sample size computed based on the posterior draws, it is clear that the CT-MCMC methods perform better than the RJ-MCMC approaches across the board. Our most elaborate proposal—combining CT-MCMC with both rotation proposals and perturbation proposals—provides the best performance. This is especially prominent when looking at the exploration behavior of the different sampling methods: In this synthetic example it is possible to derive the variable activity analytically which should be approximately 0.3, 0.4, and 0.3 respectively. Finally, it is clear that the computational computation time of our newly proposed
methods is on par, or faster, than the current state-of-art methods. To summarize, across the board we find a good empirical performance of our suggested CT-MCMC method(s). Appendix C provides additional simulation results for the cases $\sigma \in (0.01, 0.1)$ showing that in both of these cases our suggested method again outperforms the RJ methods and that in these lower noise scenarios the RJ methods fail to properly explore the parameters space while our suggested CT method maintains proper variable activity.

| Method | Error $\sigma^2$ | Efficiency | Exploration | Time $\sigma^2$ |
|--------|-----------------|------------|-------------|----------------|
| RJ-A   | 0.34 48691.69   | 8213.17    | 9962.27     | 8043.08       |
| RJ-B   | 0.34 48924.93   | 292.62     | 4488.81     | 293.59        |
| RJ-C   | 0.34 49393.92   | 2075.90    | 5046.14     | 1590.71       |
| CT-A   | 0.34 48639.18   | 4469.34    | 15918.11    | 5168.80       |
| CT-B   | 0.34 48965.62   | 8755.03    | 17833.03    | 6167.75       |
| CT-C   | 0.34 48861.64   | 11014.10   | 19728.24    | 6167.75       |

Table 1: Overview of the performance measures of different sampling methods for simulation example for the case $\sigma^2 = 1$ in (8). The table reports the average over 100 replications of the prediction error, the sampling efficiency, the exploration behavior, and the computation time.

5 Discussion

In this paper we introduced a continuous time MCMC search algorithm for posterior sampling from Bayesian regression trees and sums of trees (BART). Our work is inspired by earlier work in this space demonstrating the efficiency of continuous time MCMC search algorithms (see, e.g., Mohammadi and Wit [2015], Mohammadi et al. [2017]). Using the general theory described by Preston (1977) we have shown analytically that our proposed sampling approach converges to our desired target posterior distribution $\Pr(T, \theta_T | D)$ in the case of birth-death proposals. Next, we extended this result to also include the novel rotate proposals initially proposed by Pratola (2016). Jointly, these suggestions lead to an efficient sampling mechanism for Bayesian (additive) regression trees; a model that is gaining popularity in applied studies (see, e.g., Logan et al. [2017]) and hence effective sampling methods are sought after.

Our current work provides theoretical guarantees regarding the convergence of our CT-MCMC search algorithm. There is still room for additional computational improvements: while our marginalizing approach, combined with our mixture approach to include rotation proposals (see Appendix B), provide important steps in providing a computationally feasible CT-MCMC method, we believe additional gains might be possible. For example, in our current implementation we do not use the weights—provided by the waiting times—in our computation of the models predictions: doing so might lead to equally accurate predictions for even smaller numbers of posterior draws but is complicated due to the extremely large set of possible models. Furthermore, while our current implementation parallelizes parts of the sampling process, additional gains might be achieved here. Our current implementation of the methods prosed in this paper are available at https://bitbucket.org/mpratola/openbt, and will shortly be submitted to CRAN.
We hope our current results improve the practical usability of Bayesian regression tree models for applied researchers by speeding up, and improving the accuracy, of the sampling process. Our methods seem to work well for reasonably sized problems (e.g., thousands of observations, tens of variables); we think their actual performance on big datasets needs to be further investigated.

Appendix A: Proof of Theorem 3.1

Our proof here is based on the theory of general continuous time Markov birth-death processes derived by Preston (1977). We use the notation defined in the body of this paper. Assume that at a given time, the process is in a tree state \((T, \theta_T)\). The process is characterized by the birth rates \(B_{ijk}(T, \theta_T)\), the death rates \(D_i(T, \theta_T)\), and the birth and death transition kernels \(K_B((T, \theta_T) \to (T^*, \theta_{T^*}))\) and \(K_D((T, \theta_T) \to (T^*, \theta_{T^*}))\).

Birth and death events occur as independent Poisson processes with rates \(B_{ijk}(T, \theta_T)\) and \(D_i(T, \theta_T)\) respectively. Given that a specific birth occurs, the probability that the following jump leads to a point in \(H \subset \Omega_{T^{b_{ijk}}}\) (where \(\Omega_{T^{b_{ijk}}}\) is the space of \(\theta_{T^{b_{ijk}}}\)) is

\[
K_B((T, \theta_T) \to (T^{b_{ijk}}, H)) = Pr(T \to T^{b_{ijk}}) \times Pr(\theta_{T^{b_{ijk}}} \to H | T \to T^{b_{ijk}})
\]

\[
= \frac{B_{ijk}(T, \theta_T)}{B(T, \theta_T)} \int I(\theta_{T^{b_{ijk}}} \in H) Pr(\mu_{n_i}) Pr(\mu_{n_r}) d\mu_{n_i} d\mu_{n_r},
\]

in which \(B(T, \theta_T) = \sum_{ijk} B_{ijk}(T, \theta_T)\) and \(Pr(\cdot)\) is a proposal distribution for \(\mu\)’s.

Similarly, given a specific death occurs, the probability that the following jump leads to a point in \(F \subset \Omega_{T^{d_i}}\) (where \(\Omega_{T^{d_i}}\) is the space of \(\theta_{T^{d_i}}\)) is

\[
K_D((T, \theta_T) \to (T^{d_i}, F)) = Pr(T \to T^{d_i}) \times Pr(\theta_{T^{d_i}} \to F | T \to T^{d_i})
\]

\[
= \frac{D_i(T, \theta_T)}{D(T, \theta_T)} \int I(\theta_{T^{d_i}} \in F) Pr(\mu_i) d\mu_i,
\]

in which \(D(T, \theta_T) = \sum_i D_i(T, \theta_T)\) and \(Pr(\cdot)\) is a proposal distribution for \(\mu\)’s.

This birth-death process satisfies the detailed balance conditions if

\[
\int_H B(T, \theta_T) Pr(T, \theta_T | D) d\theta_T = \sum_{ijk} \int_{\theta_{T^{b_{ijk}}}} D(T^{b_{ijk}}, \theta_{T^{b_{ijk}}}) K_D((T^{b_{ijk}}, \theta_{T^{b_{ijk}}}) \to (T, F)) Pr(T^{b_{ijk}}, \theta_{T^{b_{ijk}}} | D) d\theta_{T^{b_{ijk}}},
\]

and

\[
\int_F D(T, \theta_T) Pr(T, \theta_T | D) d\theta_T = \sum_i \int_{\theta_{T^{d_i}}} B(T^{d_i}, \theta_{T^{d_i}}) K_B((T^{d_i}, \theta_{T^{d_i}}) \to (T, F)) Pr(T^{d_i}, \theta_{T^{d_i}} | D) d\theta_{T^{d_i}}.
\]
We check the first part of the detailed balance conditions \([10]\) as follows. For the left hand side (LHS) we have:

\[
LHS = \int \int B(T, \theta_T) \Pr(T, \theta_T | D) d\theta_T
\]

\[
= \int \theta_T \in F \Pr(T, \theta_T | D) d\theta_T
\]

\[
= \int \theta_T \in F \left( \sum_{ijk} B_{ijk}(T, \theta_T) \Pr(T, \theta_T | D) \right) d\theta_T
\]

\[
= \sum_{ijk} \int \theta_T \in F B_{ijk}(T, \theta_T) \Pr(T, \theta_T | D) \left( \int \Pr(\mu_i^a) \Pr(\mu_r^b) d\mu_i^a d\mu_r^b \right) d\theta_T
\]

\[\text{[Pr(.) must integrate to 1]}\]

\[
= \sum_{ijk} \int \theta_T \in F B_{ijk}(T, \theta_T) \Pr(T, \theta_T | D) \Pr(\mu_i^a) \Pr(\mu_r^b) d\mu_i^a d\mu_r^b d\theta_T.
\]

Furthermore, for the right hand side (RHS) of \([10]\), by using \([9]\) we have

\[
RHS = \sum_{ijk} \int \int D(T^{b_{ijk}}, \theta_{T^{b_{ijk}}}) K_D((T^{b_{ijk}}, \theta_{T^{b_{ijk}}}); (T, F)) \Pr(T^{b_{ijk}}, \theta_{T^{b_{ijk}}}| D) d\theta_{T^{b_{ijk}}}
\]

\[\text{[equation (9)\]}\]

\[
= \sum_{ijk} \int \mu_i \in \mu_i \left( \int \Pr(\mu_i) d\mu_i \right) \Pr(T^{b_{ijk}}, \theta_{T^{b_{ijk}}}| D) d\theta_{T^{b_{ijk}}}
\]

\[
= \sum_{ijk} \int \theta_T \in F \left( \Pr(T^{b_{ijk}}, \theta_{T^{b_{ijk}}} | D) \Pr(\mu_i) \Pr(T^{b_{ijk}}, \theta_{T^{b_{ijk}}}| D) d\mu_i d\theta_{T^{b_{ijk}}}.\right.
\]

Note that the number of terminal nodes \(n_t\) for performing a birth in the original tree \(T\) equals the number of possible death nodes \(n_d\) in the new tree \(T^{b_{ijk}}\).

It follows that we have \(LHS=RHS\) provided that

\[
B_{ijk}(T, \theta_T) \Pr(T, \theta_T | D) \Pr(\mu_i^a) \Pr(\mu_r^b) = D_i(T^{b_{ijk}}, \theta_{T^{b_{ijk}}}) \Pr(\mu_i) \Pr(T^{b_{ijk}}, \theta_{T^{b_{ijk}}}| D),
\]

which is satisfied if we define our birth and death rates as

\[
B_{ijk}(T, \theta_T) = \min \left\{ 1, \frac{\Pr(T^{b_{ijk}}, \theta_{T^{b_{ijk}}}| D) \Pr(\mu_i)}{\Pr(T, \theta_T | D) \Pr(\mu_i^a) \Pr(\mu_r^b)} \right\}
\]

and

\[
D_i(T, \theta_T) = \min \left\{ 1, \frac{\Pr(T^{d_i}, \theta_{T^{d_i}} | D) \Pr(\mu_i)}{\Pr(T, \theta_T | D) \Pr(\mu_i^a)} \right\}.
\]
Appendix B: Extending of CT-MCMC algorithm to rotate mechanism

Here we consider extending the CT-MCMC algorithm to include the rotate mechanism. Following the construction of Preston (1977), let the state space be $$\Omega = \bigcup_{n=0}^{\infty} \Omega_n$$ where $$\Omega_n$$ is made up of all states of cardinality $$n$$ and are disjoint. Further, let $$\Omega^{b(n)}$$ be the states from which a birth into $$\Omega_n$$ originates, let $$\Omega^{d(n)}$$ be the states from which a death into $$\Omega_n$$ originates and let $$\Omega^{r(n)}$$ be the states from which a rotate into $$\Omega_n$$ originates. Then these are disjoint and the overal transition kernel is given by (Preston, 1977)

$$K^{(n)}_{\Omega \times F} = K^{b(n)}_{\Omega \times F} + K^{d(n)}_{\Omega \times F} + K^{r(n)}_{\Omega \times F}$$

where $$K^{b(n)}_{\Omega \times F}$$ is the birth transition kernel, $$K^{d(n)}_{\Omega \times F}$$ is the death transition kernel, and $$K^{r(n)}_{\Omega \times F}$$ is the rotate transition kernel.

Let $$\mathcal{F}_n$$ be the $$\sigma$$-field of subsets of $$\Omega_n$$ and let $$\mathcal{F}$$ be the $$\sigma$$-field on $$\Omega$$ generated by the $$\mathcal{F}_n$$. We consider a jump process that can jump from state $$x \in \Omega_n$$ to a point in one of $$\Omega^{b(n)}, \Omega^{d(n)}, \Omega^{r(n)}$$. Let $$\mu$$ denote a measure on $$(\Omega, \mathcal{F})$$ and $$\mu_n$$ denote $$\mu$$ restricted to $$\Omega_n$$. Let $$B, D, R : \Omega \rightarrow \mathbb{R}^+$$ be $$\mathcal{F}$$-measurable with $$D(x) = R(x) = 0$$ for $$x \in \Omega_0$$ and let $$\alpha = B + D + R$$. For $$n \geq 1$$ we define the transition probability kernels

$$K^{(n)}_{B} : \Omega_n \times \mathcal{F}_n \rightarrow \mathbb{R}^+, \quad K^{(n)}_{D} : \Omega_n \times \mathcal{F}_n \rightarrow \mathbb{R}^+, \quad K^{(n)}_{R} : \Omega_n \times \mathcal{F}_n \rightarrow \mathbb{R}^+$$

and

$$K^{(n)}_{\Omega \times \mathcal{F}} = K^{(n)}_{B} + K^{(n)}_{D} + K^{(n)}_{R}$$

Then the overall transition kernel is given by (Preston, 1977)

$$K(x, F) = \frac{B(x)}{\alpha(x)} K^{(n)}_{B}(x, F) + \frac{D(x)}{\alpha(x)} K^{(n)}_{D}(x, F) + \frac{R(X)}{\alpha(x)} K^{(n)}_{R}(x, F)$$

for $$x \in \Omega_n, n \geq 1$$ and let $$\frac{B(x)}{\alpha(x)} = \frac{D(x)}{\alpha(x)} = \frac{R(X)}{\alpha(x)} = \frac{1}{2}$$ if $$\alpha(x) = 0$$, and

$$K(x, F) = K^{(0)}_{\Omega}(x, F)$$

if $$x \in \Omega_0$$.

A rotate event goes to state $$(T^{r_i}, \theta_r, i)$$ with rotate rate $$R_{ij}(T, \theta_T)$$ where $$i \in 1, \ldots, n$$ and $$n_r$$ is the number of possible rotatable nodes (see Pratola, 2016, for details) and $$j \in 1, \ldots, n_i$$ is the number of possible outcomes from a rotate at the $$i$$'th rotatable node. Furthermore we define $$R(T, \theta_T) = \sum_{i=1}^{n_r} \sum_{j=1}^{n_i} R_{ij}(T, \theta_T)$$. Hence, a rotate event changes the topology $$\tau$$ by rearranging internal nodes according to the rules described in Pratola (2016).

In total, we consider the overall number of topological changes to the tree to occur via birth and death moves (as defined earlier) and rotate moves which occur with respective rates $$B_{ijk}(T, \theta_T), D_i(T, \theta_T)$$ and $$R_{ijk}(T, \theta_T)$$ given the tree is in state $$(T, \theta_T)$$. With rotate, we do not know how many of the $$j$$ possible outcomes of a rotate at node $$i$$ will increase the dimension of $$\theta_T$$ thereby creating a new $$\mu$$ parameter. So, to make things easier—and since this is what we do in practice—we integrate out all of these parameters and work directly with the marginal likelihood. In this case, the birth/death transition kernels from above become:

$$K_B(T \rightarrow T^{b_{ijk}}) = \frac{B_{ijk}(T)}{B(T)}$$

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\[ K_D(T \rightarrow T^{d_i}) = \frac{D_i(T)}{D(T)}, \]

and

\[ K_R(T \rightarrow T^{r_{ij}}) = \frac{R_{ij}(T)}{R(T)}. \]

One of the things we need is that birth is inverse of death, death is inverse of birth and rotate is inverse of rotate. This means that in this case our detailed balance condition will consist of 3 equations, essentially the birth/death balances from earlier as well as a rotate balance condition:

\[ B(T) \Pr(T \mid D) = \sum_{ijk} D(T^{b_{ij}}) K_D((T^{b_{ij}}) \rightarrow T) \Pr(T^{b_{ij}} \mid D), \]

\[ D(T) \Pr(T \mid D) = \sum_i B(T^{d_i}) K_B((T^{d_i}) \rightarrow T) \Pr(T^{d_i} \mid D), \]

and

\[ R(T) \Pr(T \mid D) = \sum_{ij} R(T^{r_{ij}}) K_R((T^{r_{ij}}) \rightarrow T) \Pr(T^{r_{ij}} \mid D), \]

where \( T^{r_{ij}} \) is the tree state generated from previously choosing the \( j \)’th rotate generated at rotatable node \( i \) and \( \Pr(T \mid D) = \int_{\theta_T} \Pr(T; \theta_T \mid D) \) is the marginal posterior.

For the rotate balance, we have

\[ \sum_{ij} R_{ij}(T) \Pr(T \mid D) = \sum_{ij} R_{ij}(T^{r_{ij}}) \Pr(T^{r_{ij}} \mid D) \]

which is satisfied if

\[ R_{ij}(T) \Pr(T \mid D) = R_{ij}(T^{r_{ij}}) \Pr(T^{r_{ij}} \mid D). \]

Thus, the corresponding rate for the rotate move is

\[ R_{ij}(T) = \min \left\{ 1, \frac{\Pr(T^{r_{ij}} \mid D)}{\Pr(T \mid D)} \right\}, \]

and similarly working with the integrated posterior, the corresponding rates for the birth/death moves become

\[ B_{ijk}(T) = \min \left\{ 1, \frac{\Pr(T^{b_{ijk}} \mid D)}{\Pr(T \mid D)} \right\}, \]

and

\[ D_i(T) = \min \left\{ 1, \frac{\Pr(T^{d_i} \mid D)}{\Pr(T \mid D)} \right\}. \]
Given this construction, the probability of birth, death and rotate moves occur with probabilities given by

\[ \Pr(\text{birth at node } \eta_i \text{ for variable } \nu_j \text{ and cut-point } c_k) = \frac{B_{ijk}(T)}{B(T) + D(T) + R(T)}, \]

\[ \Pr(\text{death at node } \eta_i) = \frac{D_i(T)}{B(T) + D(T) + R(T)}, \]

and

\[ \Pr(\text{rotate } j \text{ at node } \eta_i) = \frac{R_{ij}(T)}{B(T) + D(T) + R(T)}. \]

Note that in practice this approach is too expensive because we have to calculate \( B(T) + D(T) + R(T) \) at each iteration. To address this problem we split this move into two moves: a birth/death part and a rotate part can be performed separately to reduce computational burden. To do so, we introduce parameter \( \alpha \). The idea is that with probability \( \alpha \) we perform a birth/death move via CTMCMC, and with probability \( 1 - \alpha \) we perform a rotate move via CTMCMC. That is, our move corresponds to the mixture distribution

\[ \alpha \left[ \frac{B_{ijk}(T)}{B(T) + D(T)} + \frac{D_i(T)}{B(T) + D(T)} \right] + (1 - \alpha) \frac{R_{ij}(T)}{R(T)} \]

for some fixed, known \( \alpha \). Note that if \( \alpha = \frac{B(T) + D(T)}{B(T) + D(T) + R(T)} \), then this mixture distribution corresponds exactly to the distribution for the full CTMCMC algorithm.

## Appendix C: Additional simulation results.

Here we present a number of additional simulation results for the simulation scenario in the Section 4 and described in the main text for \( \sigma \in (0.1, 0.01) \). Tables 2 and 3 demonstrate that also in these cases our proposed CT-MCMC method performs well.

| Method | Error | Efficiency | Exploration | Time |
|--------|-------|------------|-------------|------|
| RJ-A  | 0.34  | 491.39.97  | 9764.68     | 11121.61 | 9787.23 | 0.31 | 0.39 | 0.29 | 10423.52 |
| RJ-B  | 0.34  | 493.22.50  | 268.78      | 5100.31  | 271.50  | 0.28 | 0.44 | 0.28 | 12945.54 |
| RJ-C  | 0.34  | 490.47.38  | 2086.35     | 5166.18  | 1485.15 | 0.15 | 0.44 | 0.41 | 11301.24 |
| CT-A  | 0.34  | 489.70.91  | 4558.35     | 15736.32 | 5273.00 | 0.29 | 0.37 | 0.35 | 5043.35  |
| CT-B  | 0.34  | 491.82.14  | 12612.75    | 18490.68 | 7816.40 | 0.32 | 0.38 | 0.30 | 4299.14  |
| CT-C  | 0.34  | 491.48.75  | 15528.82    | 20861.04 | 7816.40 | 0.32 | 0.38 | 0.31 | 4415.88  |

Table 2: Overview of the performance measures of different sampling methods for simulation example for the case \( \sigma^2 = 0.1 \) in [8]. The table reports the average over 100 replications of the prediction error, the sampling efficiency, the exploration behavior, and the computation time.

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Table 3: Overview of the performance measures of different sampling methods for simulation example for the case $\sigma^2 = 0.01$ in (8). The table reports the average over 100 replications of the prediction error, the sampling efficiency, the exploration behavior, and the computation time.

| Method | Error $\sigma^2$ | Efficiency $x_1$ | Exploration $x_2$ | Time $x_3$ | Time $\sigma^2$ |
|--------|------------------|------------------|-------------------|------------|----------------|
| RJ-A   | 0.33 49996.84    | 9547.09          | 10870.28          | 9687.82    | 0.32 0.39 0.29 11692.32 |
| RJ-B   | 0.33 49115.34    | 271.84           | 5163.61           | 274.84     | 0.28 0.44 0.28 13992.97 |
| RJ-C   | 0.33 49126.91    | 4568.60          | 15578.86          | 5277.27    | 0.29 0.37 0.35 5128.07 |
| CT-A   | 0.33 49316.73    | 13400.68         | 18345.99          | 8097.88    | 0.32 0.38 0.30 4442.95 |
| CT-B   | 0.33 49017.75    | 16117.32         | 20068.37          | 8097.88    | 0.32 0.38 0.31 4431.98 |

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