urBART MCMC updates

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1 Updating trees

Suppose there are n observations in a terminal node and suppose that the (partial) residuals in this terminal node are denoted by vectors $R_1, \ldots, R_n$. The prior distribution for these residuals is:

$$R_1, \ldots, R_n | \mu, \Psi \sim N(\mu, \Psi^{-1})$$

Furthermore the prior on μ is:

$$\mu \sim N(0, \tau_\mu^{-1} I)$$

Using π to denote a probability distribution, we want to find:

$$\begin{aligned}
\pi(R_1, \ldots, R_n | \sigma) &= \int \pi(R_1, \ldots, R_n | \mu, \tau) \pi(\mu) \partial\mu \\
&\propto \int \prod_{i=1}^{n} \tau^{1/2} e^{-\frac{\tau}{2}(R_i - \mu)^2} \tau_\mu^{1/2} e^{-\frac{\tau_\mu}{2}\mu^2} \partial\mu \\
&= \int \tau^{n/2} e^{-\frac{\tau}{2}\sum(R_i - \mu)^2} \tau_\mu^{1/2} e^{-\frac{\tau_\mu}{2}\mu^2} \partial\mu \\
&= \int \tau^{n/2} \tau_\mu^{1/2} e^{-\frac{1}{2}\left[\tau\left\{\sum R_i^2 + n\mu^2 - 2\mu n \bar{R}\right\} + \tau_\mu \mu^2\right]} \partial\mu \\
&= \tau^{n/2} \tau_\mu^{1/2} e^{-\frac{1}{2}\left[\tau \sum R_i^2\right]} \int e^{-\frac{1}{2}Q} \partial\mu
\end{aligned}$$

where

$$
\begin{aligned}
Q &= \tau n \mu^2 - 2\tau n \mu \bar{R} + \tau_\mu \mu^2 \\
&= (\tau_\mu + n\tau)\mu^2 - 2\tau n \mu \bar{R} \\
&= (\tau_\mu + n\tau) \left[\mu^2 - \frac{2\tau n \mu \bar{R}}{\tau_\mu + n\tau} \right] \\
&= (\tau_\mu + n\tau) \left[\left(\mu - \frac{2\tau n \bar{R}}{\tau_\mu + n\tau} \right)^2 - \left(\frac{\tau n \bar{R}}{\tau_\mu + n\tau} \right)^2 \right] \\
&= (\tau_\mu + n\tau) \left(\mu - \frac{2\tau n \bar{R}}{\tau_\mu + n\tau} \right)^2 - \frac{(n\tau\bar{R})^2}{\tau_\mu + n\tau}
\end{aligned}
$$

so therefore:

$$
\begin{aligned}
\int e^{-\frac{1}{2}Q} \partial\mu &= \int \exp\left[-\frac{\tau_\mu + n\tau}{2} \left(\mu - \frac{2\tau n \bar{R}}{\tau_\mu + n\tau} \right)^2 + \frac{(n\tau\bar{R})^2}{2(\tau_\mu + n\tau)} \right] \partial\mu \\
&\propto \exp\left[\frac{1}{2} \frac{(\tau n \bar{R})^2}{\tau_\mu + n\tau} \right] (\tau_\mu + n\tau)^{-1/2}
\end{aligned}
$$

And finally:

$$
\begin{aligned}
\pi(R_1, \ldots, R_n | \tau) \propto & (\tau_\mu + n\tau)^{-1/2} \tau^{n/2} \tau_\mu^{1/2} \exp\left[\frac{1}{2} \frac{(\tau n \bar{R})^2}{\tau_\mu + n\tau} \right] \exp\left[-\frac{\tau}{2} \sum R_i^2 \right] \\
&= \tau^{n/2} \left(\frac{\tau_\mu}{\tau_\mu + n\tau} \right)^{1/2} \exp\left[-\frac{\tau}{2} \left\{ \sum R_i^2 - \frac{\tau (n\bar{R})^2}{\tau_\mu + n\tau} \right\} \right]
\end{aligned}
$$

Including multiple terminal nodes

When we put back in terminal nodes we write R_{ji} where j is the terminal node and i is still the observation, so in terminal node j we have partial residuals $R_{j1}, \ldots, R_{jn_j}$. When we have $j = 1, \ldots, b$ terminal nodes the full conditional distribution is then:

$$
\prod_{j=1}^{b} \pi(R_{j1}, \ldots, R_{jn_j} | \tau) \propto \prod_{j=1}^{b} \left\{ \tau^{n_j/2} \left(\frac{\tau_\mu}{\tau_\mu + n_j\tau} \right)^{1/2} \exp\left[-\frac{\tau}{2} \left\{ \sum_{i=1}^{n_j} R_{ji}^2 - \frac{\tau (n_j \bar{R}_j)^2}{\tau_\mu + n_j\tau} \right\} \right] \right\}
$$

which on the log scale gives:

$$\sum_{j=1}^{b}\left\{\frac{n_j}{2}\log(\tau)+\frac{1}{2}\log\left(\frac{\tau_\mu}{\tau_\mu+n_j\tau}\right)-\frac{\tau}{2}\left[\sum_{i=1}^{n_j}R_{ji}^2-\frac{\tau(n_j\bar{R}_j)^2}{\tau_\mu+n_j\tau}\right]\right\}$$

This can be simplified further to give:

$$\frac{n}{2}\log(\tau)+\frac{1}{2}\sum_{j=1}^{b}\log\left(\frac{\tau_\mu}{\tau_\mu+n_j\tau}\right)-\frac{\tau}{2}\sum_{j=1}^{b}\sum_{i=1}^{n_j}R_{ji}^2+\frac{\tau^2}{2}\sum_{j=1}^{b}\frac{S_j^2}{\tau_\mu+n_j\tau}$$

where $S_j=\sum_{i=1}^{n_j}R_{ji}$

Updating μ

The full conditional for μ_j (the terminal node parameters for node j) is similar to the above but without the integration:

$$\begin{aligned}
\pi(\mu_j|\ldots) &\propto \prod_{i=1}^{n_j}\tau^{1/2}e^{-\frac{\tau}{2}(R_{ji}-\mu_j)^2}\tau_\mu^{1/2}e^{-\frac{\tau_\mu}{2}\mu_j^2}\\
&\propto e^{-\frac{\tau}{2}\sum_{i=1}^{n_j}(R_{ji}-\mu_j)^2}e^{-\frac{\tau_\mu}{2}\mu_j^2}\\
&\propto e^{-\frac{\tau}{2}\left[n_j\mu_j^2-2\mu_j\sum_{i=1}^{n_j}R_{ji}\right]-\frac{\tau_\mu}{2}\mu_j^2}\\
&\propto e^{-\frac{Q}{2}}
\end{aligned}$$

Now:

$$\begin{aligned}
Q &= n_j\tau\mu_j^2-2\mu_j\tau S_j+\tau_\mu\mu_j^2\\
&= (n_j\tau+\tau_\mu)\mu_j^2-2\tau\mu_j S_j\\
&= (n_j\tau+\tau_\mu)\left[\mu_j^2-\frac{2\tau\mu_j S_j}{n_j\tau+\tau_\mu}\right]\\
&\propto (n_j\tau+\tau_\mu)\left[\mu_j-\frac{\tau\mu_j S_j}{n_j\tau+\tau_\mu}\right]^2
\end{aligned}$$

so therefore:

$$\mu_j|\ldots\sim N\left(\frac{\tau S_j}{n_j\tau+\tau_\mu},(n_j\tau+\tau_\mu)^2\right)$$

Update for τ

I am using the shape/rate parameterisation of the gamma with prior $\tau \sim Ga(\nu/2, \nu\lambda/2)$. Letting μ_i be the prediction of the ith observation we get:

$$\pi(\tau|\ldots) \propto \prod_{i=1}^{n} \tau^{1/2} e^{-\frac{\tau}{2}(y_i-\mu_i)^2} \tau^{\nu/2} e^{-\tau\nu\lambda/2}$$

Letting $S = \sum_{i=1}^{n}(y_i - \mu_i)^2$ we get:

$$\begin{aligned}\pi(\tau|\ldots) &\propto \tau^{n/2} e^{-\frac{\tau}{2}S} \tau^{\nu/2} e^{-\tau\nu\lambda/2} \\ &= \tau^{(n+\nu)/2} e^{-\frac{\tau}{2}(S+\nu\lambda)}\end{aligned}$$

so

$$\tau|\ldots \sim Ga\left(\frac{n+\nu}{2}, \frac{S+\nu\lambda}{2}\right)$$

Tree prior

The tree prior used by BARTMachine says that the probability of a node being non-terminal is:

$$P(\text{node is non-terminal}) = \alpha(1+d)^{-\beta}$$

So the probability of a node being terminal is 1 minus this. A stump just has probability 1 - α. For Bart Machine $\alpha = 0.95$ and $\beta = 2$

Thus for a tree with k non-terminal nodes and b terminal nodes we have:

$$P = \prod_{i=1}^{b} \left[1 - \alpha(1+d_i^t)^{-\beta}\right] \prod_{i=1}^{k} \left[\alpha(1+d_i^{nt})^{-\beta}\right]$$

where d_i^t is the depth of the ith terminal node and d_i^{nt} is the depth of the ith non-terminal node. On the log scale this gives:

$$\log P = \sum_{i=1}^{b} \left[\log\left(1 - \alpha(1 + d_i^t)^{-\beta}\right)\right] + \sum_{i=1}^{k} \left[\log(\alpha) - \beta\log(1 + d_i^{nt})\right]$$