We now describe the update of the mth regression tree $(T_m^{(j)}, \boldsymbol{\mu}_m^{(j)})$ in the ensemble $\mathcal{E}_j$ used to approximate β_j. Let $\boldsymbol{\mathcal{E}}^-$ denote the collection of all remaining $M(p+1) - 1$ regression trees, where, for notational compactness, we have suppressed the dependence of this collection on the indices j and m. Additionally, let $\boldsymbol{r}_i = (r_{i1}, \ldots, r_{in_i})^\top$ be the vector of subject i's *partial residuals* where

$$r_{it} = R_{it} + x_{itj} g(\boldsymbol{z}_{it}; T_m^{(j)}, \boldsymbol{\mu}_m^{(j)}),$$

where we have again suppressed the dependence of r_{it} on j and m for brevity.

Before describing the update of the tree, we require some additional notation. For an arbitrary decision tree T with $L(T)$ leaves, for each $i = 1, \ldots, n$, let $I_i(\ell; T)$ be the set of indices t such that $\boldsymbol{z}_{it}$ is contained in leaf ℓ of tree t. In other words, $I_i(\ell; T)$ records which observations from subject i are mapped to leaf ℓ in tree T. Further, let $\boldsymbol{X}_i(T)$ be the $n_i \times L(T)$ matrix whose (t, ℓ) entry is equal to x_{itj} if $t \in I_i(\ell, T)$ and is zero otherwise. With this additional notation, we have $\boldsymbol{r}_i = \boldsymbol{R}_i + \boldsymbol{X}_i(T_m^{(j)}) \boldsymbol{\mu}_m^{(j)}$ for each $i = 1, \ldots, n$.

Marginal likelihood of $T_m^{(-j)}$, conditional on $\boldsymbol{\mathcal{E}}^-$

The conditional conjugacy allows us to marginalize out $\boldsymbol{\mu}$ and compute $p(\boldsymbol{Y}|T, \boldsymbol{\mathcal{E}}^-, \sigma^2)$. To this end, observe that

$$
\begin{aligned}
p(\boldsymbol{Y}|T, \boldsymbol{\mu}, \boldsymbol{\mathcal{E}}^-, \sigma^2) &= \prod_{i=1}^n p(\boldsymbol{y}_i|T, \boldsymbol{\mu}, \boldsymbol{\mathcal{E}}^-, \sigma^2) \\
&= \prod_{i=1}^n (2\pi\sigma^2)^{-\frac{n_i}{2}} |\Omega_i|^{\frac{1}{2}} \exp\left\{ -\frac{1}{2\sigma^2} (\boldsymbol{r}_i - \boldsymbol{X}_i(T)\boldsymbol{\mu})^\top \Omega_i (\boldsymbol{r}_i - \boldsymbol{X}_i(T)\boldsymbol{\mu}) \right\}
\end{aligned}
$$

We additionally have

$$p(\boldsymbol{\mu}|T) = (2\pi\tau^2)^{-\frac{L(T)}{2}} \exp\left\{ -\frac{(\boldsymbol{\mu} - \mu_0 \boldsymbol{1}_{L(T)})^\top (\boldsymbol{\mu} - \mu_0 \boldsymbol{1}_{L(T)})}{2\tau^2} \right\}$$

We therefore compute

$$
\begin{aligned}
p(\boldsymbol{Y}, \boldsymbol{\mu} | T, \boldsymbol{\mathcal{E}}^-, \sigma^2) &= \left(2\pi\sigma^2\right)^{-\frac{N}{2}} \times \left(\prod_{i=1}^{N} |\Omega_i|\right)^{\frac{1}{2}} \times \left(2\pi\tau^2\right)^{-\frac{L(T)}{2}} \times \exp\left\{-\frac{\tau^{-2}(\boldsymbol{\mu} - \mu_0 \mathbf{1}_{L(T)})^\top (\boldsymbol{\mu} - \mu_0 \mathbf{1}_{L(T)})}{2\tau^2}\right\} \\
&\quad \times \exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(\boldsymbol{r}_i - \boldsymbol{X}_i(T)\boldsymbol{\mu})^\top \Omega_i (\boldsymbol{r}_i - \boldsymbol{X}_i(T))\right\}
\end{aligned}
$$

$$
\begin{aligned}
&= \left(2\pi\sigma^2\right)^{-\frac{N}{2}} \times \left(\prod_{i=1}^{n} |\Omega_i|\right)^{\frac{1}{2}} \times \exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^{n} \boldsymbol{r}_i^\top \Omega_i \boldsymbol{r}_i\right\} \\
&\quad \times \left(2\pi\tau^2\right)^{-\frac{L(T)}{2}} \exp\left\{-\frac{1}{2}\left[\boldsymbol{\mu}^\top P(T)\boldsymbol{\mu} - 2\boldsymbol{\mu}\Theta(T) + \tau^{-2}\mu_0^2 L(T)\right]\right\}
\end{aligned}
\tag{1}
$$

where

$$
P(T) = \tau^{-2} I_{L(T)} + \sigma^{-2} \sum_{i=1}^{n} \boldsymbol{X}_i(T)^\top \Omega_i \boldsymbol{X}_i(T)
$$

$$
\Theta(T) = \tau^{-2} \mu_0 \mathbf{1}_{L(T)} + \sigma^{-2} \sum_{i=1}^{n} \boldsymbol{X}_i(T)^\top \Omega_i \boldsymbol{r}_i.
$$

Observe that the terms in the first line of Equation (1) do not depend on T or μ. We will collect these terms into a constant C, where we suppress the dependence on $\sigma^2, \boldsymbol{\Omega}$ and the $\boldsymbol{r}_i$'s from the notation.

Integrating out $\boldsymbol{\mu}$ from Equation (1), we obtain

$$
p(\boldsymbol{Y} | T, \boldsymbol{\mathcal{E}}^{-1}, \sigma^2) = C \times \tau^{-L(T)} \times \exp\left\{\frac{\Theta(T)^\top P(T)^{-1}\Theta(T) + L\mu_0^2 \tau^{-2}}{2}\right\}
$$

Computing $P(T)$ in the general case. Recall that

$$
P(T) = \tau^{-2} I_{L(T)} + \sigma^{-2} \sum_{i=1}^{n} \boldsymbol{X}_i(T)^\top \Omega_i \boldsymbol{X}_i(T).
$$

2

Observe that the (ℓ, ℓ') entry of $\boldsymbol{X}_i^\top \Omega_i \boldsymbol{X}_i(T)$ is given by

$$(\boldsymbol{X}_i^\top \Omega_i \boldsymbol{X}_i(T))_{\ell,\ell'} = \sum_{t=1}^{n_i} \sum_{t'=1}^{n_i} \omega_{t,t'} (\boldsymbol{X}_i(T))_{\ell,t} (\boldsymbol{X}_i(T))_{\ell',t'}$$

$$= \sum_{t=1}^{n_i} \sum_{t'=1}^{n_i} \omega_{itt'} x_{itj} x_{it'j} \mathbb{1}(t \in I_i(\ell;T), t' \in I_i(\ell';T))$$

$$= \sum_{t \in I_i(\ell;T)} \sum_{t' \in I_i(\ell';T)} \omega_{itt'} x_{itj} x_{it'j}$$

Computing $P(T)$ for independent errors. Suppose first that $\Omega_i = I_{n_i}$ for each $i = 1, \ldots, n$. For $\ell \neq \ell'$, since $\omega_{itt'} = \mathbb{1}(t = t')$ we have

$$(\boldsymbol{X}_i(T)^\top \Omega_i \boldsymbol{X}_i(T))_{\ell,\ell'} = \sum_{t=1}^{n_i} \sum_{t'=1}^{n_i} \omega_{itt'} x_{itj} x_{it'j} \mathbb{1}(t \in I_i(\ell;T), t' \in I_i(\ell';T))$$

$$= \sum_{t=1}^{n_i} x_{itj}^2 \mathbb{1}(t \in I_i(\ell;T), t \in I_i(\ell';T))$$

Since the tth observation for subject i can be associated to only one leaf in the tree T, we conclude that $P(T)$ is diagonal with diagonal entries

$$(P(T))_{\ell,\ell} = \tau^{-2} I_{L(T)} + \sigma^{-2} \sum_{i=1}^{n} \sum_{t \in I_i(\ell;T)} x_{itj}^2.$$

Computing $P(T)$ for compound symmetry. Suppose that for each $i = 1, \ldots, n$

$$\Omega_i^{-1} = (1 - \rho) I_{n_i} + \rho \times \boldsymbol{1}_{n_i} \boldsymbol{1}_{n_i}^\top.$$

It is not difficult to verify that in fact

$$\Omega_i^{-1} = \frac{1}{1 - \rho} I_{n_i} - \frac{\rho}{(1 - \rho)^2 + n_i \rho (1 - \rho)} \boldsymbol{1}_{n_i} \boldsymbol{1}_{n_i}^\top.$$

We therefore have

$$\boldsymbol{X}_i(T)^\top \Omega_i \boldsymbol{X}_i(T) = \frac{1}{1 - \rho} \boldsymbol{X}_i(T)^\top \boldsymbol{X}_i(T) - \frac{\rho}{(1 - \rho)^2 + n_i \rho (1 - \rho)} \boldsymbol{X}_i(T)^\top \boldsymbol{1}_{n_i} \boldsymbol{1}_{n_i}^\top \boldsymbol{X}_i(T)$$

3

From our computation above, we know that

$$(\boldsymbol{X}_i(T)^\top \boldsymbol{X}_i(T))_{\ell,\ell'} = \sum_{t=1}^{n_i} x_{itj}^2 \mathbb{1}(t \in I_i(\ell;T), t \in I_i(\ell';T))$$

$$= \mathbb{1}(\ell = \ell') \times \sum_{t \in I_i(\ell)} x_{ijt}^2$$

We further have

$$(\boldsymbol{1}_{L(T)}^\top \boldsymbol{X}_i(T))_\ell = \sum_{t \in I_i(\ell;T)} x_{itj}$$

Hence

$$(\boldsymbol{X}_i(T)^\top \boldsymbol{1}_{L(T)} \boldsymbol{1}_{L(T)}^\top \boldsymbol{X}_i(T))_{\ell,\ell'} = \left(\sum_{t \in I_i(\ell;T)} x_{itj} \right) \times \left(\sum_{t' \in I_i(\ell';T)} x_{it'j} \right)$$