

We now describe the update of the  $m^{\text{th}}$  regression tree  $(T_m^{(j)}, \boldsymbol{\mu}_m^{(j)})$  in the ensemble  $\mathcal{E}_j$  used to approximate  $\beta_j$ . Let  $\mathcal{E}^-$  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  $\mathbf{r}_i = (r_{i1}, \dots, r_{in_i})^\top$  be the vector of subject  $i$ 's *partial residuals* where

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

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

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

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

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

We additionally have

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

We therefore compute

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

where

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

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

That is, we have

$$\begin{aligned}
p(\mathbf{Y}, \boldsymbol{\mu} | T, \boldsymbol{\mathcal{E}}^{-1}, \sigma^2) &= C \times \tau^{-L(T)} \times \exp \left\{ -\frac{1}{2} \left[ (\boldsymbol{\mu} - P^{-1}(T)\Theta(T))^\top P(T) (\boldsymbol{\mu} - P^{-1}(T)\Theta(T)) \right] \right\} \\
&\quad \times \exp \left\{ \frac{1}{2} \left[ \Theta(T)^\top P^{-1}(T) \Theta(T) - L\mu_0^2 \tau^{-2} \right] \right\}
\end{aligned} \tag{2}$$

Equation (2) shows that

$$\boldsymbol{\mu} | T, \mathbf{Y}, \boldsymbol{\mathcal{E}}^{-1}, \sigma^2 \sim \mathcal{N}(P^{-1}(T)\Theta(T), P^{-1}(T)).$$

Further, by integrating out  $\boldsymbol{\mu}$  from the right-hand side of Equation (2), we compute

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

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

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

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

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

**The independent error case.** Suppose first that  $\Omega_i = I_{n_i}$  for each  $i = 1, \dots, n$ . For  $\ell \neq \ell'$ , since  $\omega_{itt'} = \mathbb{1}(t = t')$  we have

$$\begin{aligned} (\mathbf{X}_i(T)^\top \Omega_i \mathbf{X}_i(T))_{\ell, \ell'} &= \sum_{t=1}^{n_i} \sum_{t'=1}^{n_i} \omega_{itt'} x_{itj} x_{it'j} \mathbb{1}(t \in I_i(\ell; T), t' \in I_i(\ell'; T)) \\ &= \sum_{t=1}^{n_i} x_{itj}^2 \mathbb{1}(t \in I_i(\ell; T), t \in I_i(\ell'; T)) \end{aligned}$$

Since the  $t^{\text{th}}$  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

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

Recall further that

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

When each  $\Omega_i = I_{n_i}$  we have for each  $i = 1, \dots, n$ ,

$$\begin{aligned} (\mathbf{X}_i(T)^\top \Omega_i \mathbf{r}_i)_\ell &= \sum_{t=1}^{n_i} x_{itj} r_{it} \mathbb{1}(t \in I_i(\ell)) \\ &= \sum_{t \in I_i(\ell; T)} x_{itj} r_{it} \end{aligned}$$

Hence

$$(\Theta(t))_\ell = \tau^{-2}\mu_0 + \sigma^{-2} \sum_{i=1}^n \sum_{t \in I_i(\ell; T)} x_{itj} r_{it}$$

**The compound symmetry case.** Suppose that for each  $i = 1, \dots, n$

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

It is not difficult to verify that in fact

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

We therefore have

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

Observe that

$$\begin{aligned} (\mathbf{X}_i(T)^\top \mathbf{X}_i(T))_{\ell, \ell'} &= \sum_{t=1}^{n_i} x_{itj}^2 \mathbb{1}(t \in I_i(\ell; T), t \in I_i(\ell'; T)) \\ &= \mathbb{1}(\ell = \ell') \times \sum_{t \in I_i(\ell; T)} x_{itj}^2 \end{aligned}$$

We further have

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

Hence

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

We conclude that

$$\begin{aligned} (P(T))_{\ell, \ell'} &= \mathbb{1}(\ell = \ell') \times \left[ \tau^{-2} + \frac{\sigma^{-2}}{1 - \rho} \times \sum_{i=1}^n \sum_{t \in I_i(\ell)} x_{itj}^2 \right] \\ &\quad - \frac{\rho}{1 - \rho} \times \sum_{i=1}^n \frac{1}{1 - \rho + n_i \rho} \times \left( \sum_{t \in I_i(\ell; T)} x_{itj} \right) \left( \sum_{t' \in I_i(\ell'; T)} x_{it'j} \right) \end{aligned}$$

Turning our attention to  $\Theta(T)$ , have

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

Notice that

$$(\mathbf{X}_i(T)^\top \mathbf{r}_i)_\ell = \sum_{t=1}^{n_i} x_{itj} r_{it} \times \mathbb{1}(t \in I_i(\ell; T)) = \sum_{t \in I_i(\ell; T)} x_{itj} r_{it}$$

and

$$(\mathbf{X}_i^\top \mathbf{1}_{n_i} \mathbf{1}_{n_i}^\top \mathbf{r}_i)_\ell = \left( \mathbf{1}_{n_i}^\top \mathbf{r}_i \right) \times \sum_{t \in I_i(\ell; T)} x_{itj}$$

We conclude that

$$\Theta(T)_\ell = \tau^{-2} \mu_0 + \frac{\sigma^{-2}}{1-\rho} \times \sum_{i=1}^n \sum_{t \in I_i(\ell; T)} \left[ x_{itj} r_{it} - \frac{\rho \times \mathbf{1}_{n_i}^\top \mathbf{r}_i}{1-\rho+n_i\rho} x_{itj} \right]$$