

We now describe the update of the m^{th} regression tree $(T_m^{(j)}, \boldsymbol{\mu}_m^{(j)})$ in the ensemble \mathcal{E}_j used to approximate β_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 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 $\mathbf{X}_i(T)$ 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 $\mathbf{r}_i = \mathbf{R}_i + \mathbf{X}_i(T_m^{(j)})\boldsymbol{\mu}_m^{(j)}$ 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.

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

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

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

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

Observe that the (ℓ, ℓ') 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^{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

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

From our computation above, we know that

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

We further have

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

Hence

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

We conclude that

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

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

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

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

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