Bayesian Quantile Regression using a Mixture of Pólya Tree Prior

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Abstract

1 Introduction

Quantile regression is a powerful way of studying the relationship between response and covariates when one (or several) quantiles are of interest. The dependence between upper or lower quantiles of the response variable and the covariates are expected to vary differentially relative to that of the average. This is often of interest in econometrics, educational studies, biomedical studies, and environment studies (Yu and Moyeed, 2001; Buchinsky, 1994, 1998; He et al., 1998; Koenker and Machado, 1999; Wei et al., 2006; Yu et al., 2003). A comprehensive review of quantile regression was presented by Koenker (2005). Furthermore, mean regression provides less information about the relationship of the average with linear combination of covariates; quantile regression can offer a more complete description of the conditional distribution of the response.

The traditional frequentist approach was proposed by Koenker and Bassett (1978) for a single quantile (τ) with estimators derived by minimizing a loss check function $\sum_{i=1}^{n} \rho_\tau(y_i - \boldsymbol{x}_i'\boldsymbol{\beta})$, where $\rho_\tau(\epsilon) = \epsilon(\tau - \mathrm{I}(\epsilon < 0))$. They do not make any distributional assumptions for residuals and use linear programming techniques for estimation. The popularity of this approach is due to its computational efficiency, well-developed asymptotic properties, and straightforward extensions to simultaneous quantile regression and random effect models. However, asymptotic inference may not be accurate for small sample sizes.

Bayesian approaches offer exact inference. Motivated by the loss check function, Yu and Moyeed (2001) proposed an asymmetric Laplace distribution for the error term, such that maximizing the posterior distribution is equivalent to minimizing the check function. Other than parametric Bayesian approaches, some semiparametric methods have been proposed for median regression. Walker and Mallick (1999) used a diffuse finite Pólya Tree prior for the error term. Kottas and Gelfand (2001) modeled the error by two families of median zero distribution using a mixture Dirichlet process priors, which is very useful for unimodal error distributions. Hanson and Johnson (2002) adopted mixture of Pólya Tree prior on error term to make inference in regression model. They illustrated the implementation on AFT model for the median survival time, which showed robustness of Pólya in terms of multimodality and skewness. Reich et al. (2010) uses an infinite mixture of Gaussian densities on the residual. Other recent approaches include quantile pyramid priors, mixture of Dirichlet process priors of multivariate normal distributions and infinite mixture of Gaussian densities which put quantile constraints on the residuals (Hjort and Petrone, 2007; Hjort and Walker, 2009; Kottas and Krnjajić, 2009).

Like the asymmetric Laplace distribution, all of the above methods are single semiparametric quantile regression methods, which have some limitations. The densities have their restrictive mode at the quantile of interest, which is not appropriate when extreme quantiles are being investigated. Other criticisms include crossed quantile lines, monotonicity constraints and difficulty in making inference for quantile regression parameter for an interval of τs. Joint inference is poor in borrowing information through single quantile regressions. It is not coherent to pool from every individual quantile regression, because the sampling distribution of Y for τ_1 is usually different from that under quantile τ_2 since they are assuming different error distribution under two different quantile regressions (Tokdar and Kadane, 2011).

In order to solve those problems, simultaneous linear quantile regression have been proposed by Tokdar and Kadane (2011). Another popular approach is to assign a nonparametric model for the error term to avoid the monotonicity problem (Scaccia and Green, 2003; Geweke and Keane, 2007; Taddy and Kottas, 2010).

We use a mixture of Pólya Tree (PT) priors in our approach. PT priors were introduced decades ago (Freedman, 1963; Fabius, 1964; Ferguson, 1974) and Lavine (1992, 1994) extended them to Pólya Tree models. The major advantage of Pólya Tree over Dirichlet process is that it can be absolutely continuous with probability 1 and it can be easily tractable. In a regression context, Walker and Mallick (1997, 1999) assigned a finite Pólya Tree prior to the random effects in a generalized linear mixed model. Berger and Guglielmi (2001) used a mixture of Pólya Tree comparing data distribution coming from parametric distribution or mixture of Pólya Tree. They used a Pólya tree process to test the fit of data to a parametric model by embedding the parametric model in a nonparametric alternative and computing the Bayes factor of the parametric model to the nonparametric alternative. As mentioned earlier Hanson and Johnson (2002) modeled the error term as a mixture of Pólya tree prior in the regression model.

Multivariate regression is also possible with Pólya Trees. Paddock (1999, 2002) studied multivariate Pólya Tree in a k-dimensional hypercube. Hanson (2006) constructed a general framework for multivariate random variable with a Pólya Tree distribution. Jara et al. (2009) extended the multivariate mixture of Pólya Tree prior with a directional orthogonal matrix. He also demonstrated how to fit a generalized mixed effect model by modeling multivariate random effects with multivariate mixture of Pólya Tree priors.

In this article, we present a Bayesian approach by adopting a mixture of Pólya Tree prior for the regression error term, and we account for the change of quantile regression parameter via heterogeneity of the error term. As a result, several quantile regression can be fit simultaneously and there is a closed form for posterior quantile regression parameter. Exact inference can be made through Monte Carlo Markov Chain (MCMC) approach, and our method avoids the problem of crossing quantile lines that occurs in the traditional frequentist quantile regressions.

The rest of the paper is organized as follows. In section 2, we introduce the heterogeneity model and derive a closed form for marginalized posterior quantile regression parameter with mixture of Pólya tree prior. In section 3, we conduct some simulation studies and applies our approach on a real data example in section 4. Finally, conclusions and discussions are presented in section 5.

2 Model, Priors, and Computations

2.1 Heterogeneity Model

Let Y be a random variable with CDF F. The τth quantile of Y is defined as

$$Q_Y(\tau) = \inf_y \{y : F(y) \geq \tau\}.$$

If covariates $\boldsymbol{x_1}, \ldots, \boldsymbol{x_n}$ are of interest, then the quantile regression parameter satisfies the following condition:

$$Q_Y(\tau) = \boldsymbol{X'}\boldsymbol{\beta}(\tau),$$

where $\boldsymbol{X}$ is the matrix of covariates including an intercept. If F is continuous, then $F(\boldsymbol{X'}\boldsymbol{\beta}(\tau)) = \tau$, i.e., $\mathrm{p}(Y \leq \boldsymbol{X'}\boldsymbol{\beta}(\tau)) = \tau$.

Now, consider a location shift model,

$$y_i = \boldsymbol{x}_i\beta + \epsilon_i,$$

where $\epsilon_i \overset{\text{i.i.d}}{\sim} F_\epsilon$. Then, the τth quantile regression parameter can be expressed as

$$\boldsymbol{\beta}(\tau) = \boldsymbol{\beta} + F_\epsilon^{-1}(\tau)\boldsymbol{e}_1, \tag{1}$$

where $\boldsymbol{e}_1 = [1, 0, \ldots, 0]^T$, and $F_\epsilon^{-1}(\tau)$ is the τth quantile for error ϵ.

As we can see from equation (1), if the model is homogeneous, i.e., i.i.d case, then for different quantiles τ, the corresponding quantile regression parameters only vary in the first component, the intercept. The rest of the quantile regression parameters stay the same. Therefore, quantile lines for different quantiles are parallel to each other.

Now, consider the heterogeneous linear regression model from He et al. (1998)

$$y_i = \boldsymbol{x}_i'\boldsymbol{\beta} + (\boldsymbol{x}_i'\gamma)\epsilon_i, \tag{2}$$

where $\boldsymbol{x_i'}\gamma$ is positive for all i. Under this model, the τth quantile regression parameter is

$$\boldsymbol{\beta}(\tau) = \boldsymbol{\beta} + F_\epsilon^{-1}(\tau)\gamma, \tag{3}$$

Quantile lines are no longer parallel under the heterogeneous linear model which adds considerably more flexibility in the model.

We use a mixture of Pólya Tree prior for the error term in equation (2) and derive a closed form for posterior quantile regression parameter in (3). Since Pólya tree is a very flexible way to model the unknown distribution, our approach makes fewer assumptions. Exact inference can be made through MCMC using functionals of posterior samples. The next subsection briefly reviews the Pólya tree priors and their relevant properties.

2.2 Pólya Tree

Lavine (1992, 1994) and Mauldin et al. (1992) developed theory for Pólya tress priors as a generalization of the Dirichlet process (Ferguson, 1974). Denote $E = \{0,1\}$ and E^m as the m-fold product of E, $E^0 = \emptyset$, $E^* = \cup_0^\infty E^m$ and Ω be a separable measurable space, $\pi_0 = \Omega$, $\Pi = \{\pi_m : m = 0, 1, \ldots\}$ be a separating binary tree of partitions of Ω. In addition, define $B_\emptyset = \Omega$ and $\forall \epsilon = \epsilon_1 \cdots \epsilon_m \in E^*$, $B_{\epsilon 0}$ and $B_{\epsilon 1}$ are the two partition of B_ϵ.

Definition 2.1. *A random probability measure G on $(\Omega, \mathcal{F})$ is said to have a Pólya tree distribution, or a Pólya tree prior with parameter $(\Pi, \mathcal{A})$, written as $G|\Pi, \mathcal{A} \sim \mathrm{PT}(\Pi, \mathcal{A})$, if there exist nonnegative numbers $\mathcal{A} = \{\alpha_\epsilon, \epsilon \in E^*\}$ and random vectors $\mathcal{Y} = \{Y_\epsilon : \epsilon \in E^*\}$ such that the following hold:*

1. *all the random variables in $\mathcal{Y}$ are independent;*
2. $Y_\epsilon = (Y_{\epsilon 0}, Y_{\epsilon 1}) \sim \mathrm{Dirichlet}(\alpha_{\epsilon 0}, \alpha_{\epsilon 1}), \forall \epsilon \in E^*$;
3. $\forall m = 1, 2, \ldots,$ *and* $\forall \epsilon \in E^*, G(B_{\epsilon_1, \ldots, \epsilon_m}) = \prod_{j=1}^m Y_{\epsilon_1 \cdots \epsilon_j}$.

2.2.1 Pólya Tree Parameters

There are two parameters in the Pólya tree distribution $(\Pi, \mathcal{A})$. A Pólya tree is centered around a pre-specified distribution G_0, which is called the baseline measure. The $\mathcal{A}$ family determines how much G can deviate from G_0. Ferguson (1974) pointed out $\alpha_{\epsilon=1}$ yields a G that is absolutely continuous with probability 1, and $\alpha_{\epsilon_1, \ldots, \epsilon_m} = m^2$ yields G that is absolutely continuous with probability 1. Walker and Mallick (1999) and Paddock (1999) considered $\alpha_{\epsilon_1, \ldots, \epsilon_m} = cm^2$, where $c > 0$. Berger and Guglielmi (2001) considered $\alpha_{\epsilon_1, \ldots, \epsilon_m} = c\rho(m)$. In general, any $\rho(m)$ such that $\sum_{m=1}^\infty \rho(m)^{-1} < \infty$ guarantees G to be absolutely continuous. In our case, we adopt $\alpha_{\epsilon_1, \ldots, \epsilon_m} = cm^2$.

As to the partition parameter Π, the canonical way of constructing a Pólya tree distribution G centering on G_0, a continuous CDF is to choose $B_0 = G_0^{-1}([0, 1/2]), B_1 = G_0^{-1}((1/2, 1])$, such that $G(B_0) = G(B_1) = 1/2$. Furthermore, for all $\epsilon \in E^*$, choose $B_{\epsilon 0}$ and $B_{\epsilon 1}$ to satisfy $G(B_{\epsilon 0}|B_\epsilon) = G(B_{\epsilon 1}|B_\epsilon) = 1/2$, then any choice of $\mathcal{A}$ makes G coincide with G_0. A simple example is to choose $B_{\epsilon 0}$ and $B_{\epsilon 1}$ in level m by setting them as $G_0^{-1}((k/2^m, (k+1)/2^m])$, for $k = 0, \ldots, 2^m - 1$.

2.2.2 Some properties of Pólya Tree

Suppose $G \sim \mathrm{PT}(\Pi, \mathcal{A})$ is a random probability measure and $\epsilon_1, \epsilon_2, \ldots$ are random samples from G.

Definition 2.2 (Expectation of Pólya Tree). *$F = E(G)$ as a probability measure is defined by $F(B) = E(G(B)), \forall B \in \mathcal{B}$. By the definition of Pólya tree, for any $\epsilon \in E^*$,*

$$F(B_\epsilon) = E(G(B_\epsilon)) = \prod_{j=1}^m \frac{\alpha_{\epsilon_1, \ldots, \epsilon_j}}{\alpha_{\epsilon_1, \ldots, \epsilon_{j-1}, 0} + \alpha_{\epsilon_1, \ldots, \epsilon_{j-1}, 1}}.$$

Remark 2.3. *If G is constructed based on baseline measure G_0 and we set $\alpha_{\epsilon_1, \ldots, \epsilon_m} = cm^2$, $\epsilon_{\epsilon_0} = \alpha_{\epsilon_1}$, then $\forall B \in \mathcal{B}, F(B) = G_0(B)$; thus, $F = G_0$, if there is no data.*

Definition 2.4 (Density Function). *Suppose $F = E(G), G|\Pi, \mathcal{A} \sim \mathrm{PT}(\Pi, \mathcal{A})$, where G_0 is the baseline measure. Then, using the canonical construction, $F = G_0$ (as shown above), the density function is*

$$f(y) = \left[\prod_{j=1}^{m} \frac{\alpha_{\epsilon_1,\ldots,\epsilon_j}(y)}{\alpha_{\epsilon_1,\ldots,\epsilon_{j-1},0}(y) + \alpha_{\epsilon_1,\ldots,\epsilon_{j-1},1}(y)}\right] 2^m g_0(y), \tag{4}$$

where g_0 is the pdf of G_0.

Remark 2.5. *When using the canonical construction with no data, $\alpha_{\epsilon_0} = \alpha_{\epsilon_1}$, equation (4) simplifies to*

$$f(y) = g_0(y).$$

Remark 2.6 (Conjugacy). *If $y_1, \ldots, y_n|G \sim G, G|\Pi, \mathcal{A} \sim \mathrm{PT}(\Pi, \mathcal{A})$, then $G|y_1, \ldots, y_n, \Pi, \mathcal{A} \sim \mathrm{PT}(\Pi, \mathcal{A}^*)$, where in $\mathcal{A}^*, \forall \epsilon \in E^*$,*

$$\alpha^*_\epsilon = \alpha_\epsilon + n_\epsilon(y_1, \ldots, y_n),$$

where $n_\epsilon(y_1, \ldots, y_n)$ indicates the count of how many samples of $y_1, \ldots, y_n$ fall in B_ϵ.

2.2.3 Mixture of Pólya Trees

The behavior of a single Pólya tree highly depends on how the partition is specified. A random probability measure G_θ is said to be a mixture of Pólya tree if there exists a random variable θ with distribution h_θ, and Pólya tree parameters $(\Pi^\theta, \mathcal{A}^\theta)$ such that $G_\theta|\theta = \theta \sim \mathrm{PT}(\Pi^\theta, \mathcal{A}^\theta)$.

Example 2.7. *Suppose $G_0 = \mathrm{N}(\mu, \sigma^2)$ is the baseline measure. For $\epsilon \in E^*, \alpha_{\epsilon_m} = cm^2$, $\boldsymbol{\theta} = (\mu, \sigma, c)$ is the mixing index and the distribution on $\Theta = (\mu, \sigma, c)$ is the mixing distribution.*

With the mixture of Pólya tree, the influence of the partition is lessened. Thus, inference will not be affected greatly by a single Pólya tree distribution.

2.2.4 Predictive Error Density, Cumulative Density Function and Quantiles

Suppose G_θ is the baseline measure, $g_0(y)$ is the density function. Π^θ is defined as

$$B^\theta_{\epsilon_1,\ldots,\epsilon_m} = \left(G_\theta^{-1}\left(\frac{k}{2^m}\right), G_\theta^{-1}\left(\frac{k+1}{2^m}\right)\right),$$

where k is the index of partition $\epsilon_1, \ldots, \epsilon_m$ in level m. $\mathcal{A}^c$ is defined as

$$\alpha_{\epsilon_1,\ldots,\epsilon_m} = cm^2.$$

Therefore, the error model is

$$\begin{aligned} y_1, \ldots, y_n|G_\theta &\overset{\text{i.i.d}}{\sim} G, \\ G|\Pi^\theta, \mathcal{A}^c &\sim \mathrm{PT}(\Pi^\theta, \mathcal{A}^c). \end{aligned}$$

The predictive density function of $Y|y_1,\ldots,y_n,\theta$, marginalizing out G, is

$$f_Y^{\theta}(y|y_1,\ldots,y_n) = \lim_{m\to\infty}\left(\prod_{j=2}^{m}\frac{cj^2 + n_{\epsilon_1\cdots\epsilon_j(x)}(y_1,\ldots,y_n)}{2cj^2 + n_{\epsilon_1\cdots\epsilon_{j-1}(x)}(y_1,\ldots,y_n)}\right)2^{m-1}g_0(y), \tag{5}$$

where $n_{\epsilon_1\cdots\epsilon_j(x)}(y_1,\ldots,y_n)$ denotes the number of observations $y_1,\ldots,y_n$ dropping in the bin $\epsilon_1\cdots\epsilon_j$ where y stays in the level j. Notice that, if we restrict the first level weight as $\alpha_0 = \alpha_1 = 1$, then we only need to update levels beyond the first level.

Remark 2.8 (The predictive density for Finite Pólya Tree)**.** *In practice, a finite M level Pólya Tree is usually adopted to approximate the full Pólya tree, in which, only up to M levels are updated. The corresponding predictive density becomes*

$$f_Y^{\theta,M}(y|y_1,\ldots,y_n) = \left(\prod_{j=2}^{M}\frac{cj^2 + n_{\epsilon_1\cdots\epsilon_j(x)}(y_1,\ldots,y_n)}{2cj^2 + n_{\epsilon_1\cdots\epsilon_{j-1}(x)}(y_1,\ldots,y_n)}\right)2^{M-1}g_0(y). \tag{6}$$

The rule of thumb for choosing M is to set $M = \log_2 n$, where n is the sample size (Hanson and Johnson, 2002).

Hanson and Johnson (2002) showed the approximation to (5) given in (6) is exact for M large enough. We now derive the predictive cdf and the predictive quantile(s).

Theorem 2.9. *Based on the predictive density function (6) of a finite Pólya tree distribution, the predictive cumulative density function is*

$$F_Y^{\theta,M}(y|y_1,\ldots,y_n) = \sum_{i=1}^{N-1}P_i + P_N\left(G_\theta(y)2^M - (N-1)\right), \tag{7}$$

where

$$P_i = \frac{1}{2}\left(\prod_{j=2}^{M}\frac{cj^2 + n_{j,\lceil i2^{j-M}\rceil}(y_1,\ldots,y_n)}{2cj^2 + n_{j-1,\lceil i2^{j-1-M}\rceil}(y_1,\ldots,y_n)}\right) \text{ and}$$
$$N = \left\lfloor 2^M G_\theta(y) + 1\right\rfloor,$$

in which $n_{j,\lceil i2^{j-M}\rceil}(y_1,\ldots,y_n)$ denotes the number of observations $y_1,\ldots,y_n$ in the $\lceil i2^{j-M}\rceil$ slot at level j, $\lceil\cdot\rceil$ is the ceiling function, and $\lfloor\cdot\rfloor$ is the floor function.

Proof.

$$
\begin{aligned}
F_Y^{\theta,M}(y|y_1,\ldots,y_n) &= \int_{-\infty}^{y} f_Y^{\theta,M}(y|y_1,\ldots,y_n)dx \\
&= \int_{-\infty}^{y} \left(\prod_{j=2}^{M} \frac{cj^2 + n_{\epsilon_1\cdots\epsilon_j(y)}(y_1,\ldots,y_n)}{2cj^2 + n_{\epsilon_1\cdots\epsilon_{j-1}(y)}(y_1,\ldots,y_n)} \right) 2^{M-1} g_\theta(y)dy \\
&= \sum_{i=1}^{N-1} \left(\prod_{j=2}^{M} \frac{cj^2 + n_{j,\lceil i2^{j-M}\rceil}(y_1,\ldots,y_n)}{2cj^2 + n_{j-1,\lceil i2^{j-1-M}\rceil}(y_1,\ldots,y_n)} 2^{M-1} \int_{\epsilon_{M,i}} g_\theta(y)dy \right) \\
&+ \int_{G_\theta^{-1}((N-1)/2^M)}^{y} \left(\prod_{j=2}^{M} \frac{cj^2 + n_{j,\lceil N2^{j-M}\rceil}(y_1,\ldots,y_n)}{2cj^2 + n_{j-1,\lceil N2^{j-1-M}\rceil}(y_1,\ldots,y_n)} \right) 2^{M-1} g_\theta(y)dy \\
&= \sum_{i=1}^{N-1} P_i + P_N 2^M \left(G_\theta(y) - G_\theta(G_\theta^{-1}\left(\frac{N-1}{2^M}\right)\right) \\
&= \sum_{i=1}^{N-1} P_i + P_N \left(G_\theta(y)2^M - (N-1) \right),
\end{aligned}
$$

where $\epsilon_{M,i}$ is the ith partition in level M. □

Theorem 2.10. *The posterior predictive quantile of finite Pólya tree distribution is*

$$
Q_{Y|y_1,\ldots,y_n}^{\theta,M}(\tau) = G_\theta^{-1}\left(\frac{\tau - \sum_{i=1}^{N} P_i + NP_N}{2^M P_N} \right), \tag{8}
$$

where N satisfies $\sum_{i=1}^{N-1} P_i < \tau \leq \sum_{i=1}^{N} P_i$.

Proof. From equation (7),

$$
\begin{aligned}
\tau = F_Y^{\theta,M}(y|y_1,\ldots,y_n) &= \sum_{i=1}^{N-1} P_i + P_N \left(G_\theta(y)2^M - (N-1) \right) \\
\Rightarrow G_\theta(y) &= \frac{\tau - \sum_{i=1}^{N} P_i + NP_N}{2^M P_N} \\
y &= G_\theta^{-1}\left(\frac{\tau - \sum_{i=1}^{N} P_i + NP_N}{2^M P_N} \right).
\end{aligned}
$$

□

Now the explicit form for quantile regression coefficients in equation (3) becomes:

$$
\boldsymbol{\beta}(\tau) = \boldsymbol{\beta} + \boldsymbol{\gamma} G_\theta^{-1}\left(\frac{\tau - \sum_{i=1}^{N} P_i + NP_N}{2^M P_N} \right), \tag{9}
$$

where P_i and N are the notations in equation (7) and (8). This will greatly facilitate computations.

2.3 Fully Bayesian Quantile Regression Specification with Mixture of Pólya Tree Priors

The full Bayesian specification of quantile regression is given as follows,

$$
\begin{aligned}
y_i &= \boldsymbol{x_i'}\boldsymbol{\beta} + (\boldsymbol{x_i'}\boldsymbol{\gamma})\epsilon_i, i = 1, \ldots, n \\
\epsilon_i | G_\theta &\overset{\text{i.i.d}}{\sim} G_\theta \\
G_\theta | \Pi^\theta, \mathcal{A}^\theta &\sim \text{PT}(\Pi^\theta, \mathcal{A}^\theta) \\
\boldsymbol{\theta} = (\sigma, c) &\sim \pi_{\boldsymbol{\theta}}(\boldsymbol{\theta}) \\
\boldsymbol{\beta} &\sim \pi_{\boldsymbol{\beta}}(\boldsymbol{\beta}) \\
\boldsymbol{\gamma} &\sim \pi_{\gamma}(\boldsymbol{\gamma}).
\end{aligned}
$$

In order to not confound the location parameter, ϵ_i or G is set to have median 0 by fixing $\alpha_0 = \alpha_1 = 1$. For the similar reason, the first component of $\boldsymbol{\gamma}$ is fixed at 1.

The posterior distribution of $(\boldsymbol{\beta}, \boldsymbol{\gamma}, \sigma, c)$ is given as

$$
\begin{aligned}
\text{p}(\boldsymbol{\beta}, \boldsymbol{\gamma}, \sigma, c | \boldsymbol{Y}) &\propto L(\boldsymbol{Y} | \boldsymbol{\beta}, \boldsymbol{\gamma}, \sigma, c) \pi_\beta(\beta) \pi_\gamma(\gamma) \pi_\sigma(\sigma) \pi_c(c) \\
&= \frac{1}{\prod_{i=1}^n (\boldsymbol{x_i'}\boldsymbol{\gamma})} \text{p}\left(\epsilon_1, \ldots, \epsilon_n | \boldsymbol{\beta}, \boldsymbol{\gamma}, \sigma, c\right) \pi_\beta(\beta) \pi_\gamma(\gamma) \pi_\sigma(\sigma) \pi_c(c) \\
&= \frac{1}{\prod_{i=1}^n (\boldsymbol{x_i'}\boldsymbol{\gamma})} \text{p}\left(\epsilon_n | \epsilon_1, \ldots, \epsilon_{n-1}, \boldsymbol{\beta}, \boldsymbol{\gamma}, \sigma, c\right) \cdots \text{p}\left(\epsilon_2 | \epsilon_1, \boldsymbol{\beta}, \boldsymbol{\gamma}, \sigma, c\right) \text{p}\left(\epsilon_1 | \boldsymbol{\beta}, \boldsymbol{\gamma}, \sigma, c\right) \\
&\quad \pi_{\boldsymbol{\beta}}(\boldsymbol{\beta}) \pi_\gamma(\boldsymbol{\gamma}) \pi_\sigma(\sigma) \pi_c(c),
\end{aligned}
\tag{10}
$$

where $\epsilon_i = (y_i - \boldsymbol{x_i'}\boldsymbol{\beta}) / (\boldsymbol{x_i'}\boldsymbol{\gamma})$.

For priors of σ and c, we use gamma distributions with following parameters:

$$
\begin{aligned}
\pi(\sigma) &\sim \Gamma(1/2, 1/2), \\
\pi(c) &\sim \Gamma(1/2, 1/2).
\end{aligned}
$$

Priors for the parameters $(\boldsymbol{\beta}, \boldsymbol{\gamma})$ can be diffuse p-dimensional normal distributions. We specify diffuse gamma distributions for σ and c. For shrinkage model, spike priors could be adopted to shrink the parameter estimates to pre-specified values. In addition, spike priors can also help variable selection in Bayesian model and shrink heterogeneity parameters toward zero to find homogeneous model. Moreover, spike and slab priors can help to accommodate zero-inflated situation and research hypothesis in variable selection.

Here we put continuous spike and slab priors on $(\boldsymbol{\beta}, \boldsymbol{\gamma})$ to shrink them toward zero for each component. The prior for j^{th} component of $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ follows a mixture of spike and slab distributions. The density function of priors for β_j can be written as:

$$
\begin{aligned}
\pi_{\boldsymbol{\beta}}(\beta_j) &= \delta_{\beta_j} \phi(\beta_j; 0, s_j^2 \sigma_{\beta_j}^2) + (1 - \delta_{\beta_j}) \phi(\beta_j; \beta_j^p, \sigma_{\beta_j}^2), \\
\delta_{\beta_j} &\sim \text{Bernoulli}(\pi_{\beta_j}),
\end{aligned}
$$

where $\phi(x; \mu, \sigma^2)$ is the density function of normal distribution at x with mean μ and variance σ^2. $\beta_j^p, \sigma_{\beta_j}^2$ are the mean and variance of the diffuse normal prior for the slab component. δ_{β_j}

is the indicator that β_j comes from spike component or from slab component and π_{β_j} is its probability. $s_j(>0)$ is small enough so that if $\delta_{\beta_j}=1$, it indicates $|\beta_j|<3s_j\sigma_{\beta_j}$ with high probability, thus it can be approximately estimated as 0 and regarded as non-significant and removed from the model; if $\delta_{\beta_j}=0$, it indicates β_j comes from the slab component, thus β_j is believed to come from a diffuse distribution (George and McCulloch, 1993).

We choose $\boldsymbol{\beta}^p$, the mean of normal distribution of slab component, to be least square estimates of $\boldsymbol{Y}$ given covariates matrix $\boldsymbol{X}$, i.e., $(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}$. And let $\sigma^2_{\beta_j}$ be the diagonal component of matrix $\hat{\sigma}^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}$, where $\hat{\sigma}^2=\sum_i^n(y_i-\boldsymbol{x_i}\boldsymbol{\beta}^p)^2/(n-p)$.

The priors for $\boldsymbol{\gamma}$ are similar to priors for $\boldsymbol{\beta}$. But we choose $\boldsymbol{\gamma}^p$ and $\boldsymbol{\sigma}_\gamma$ to be $\mathbf{0}$ and $\mathbf{100}$ to shrink heterogeneity parameters toward 0.

The π_{β_j} and π_{γ_j} control the belief that the corresponding regressors are needed in the model. Large π reflects doubt that regressors should be included, and vice versa. Furthermore, we can put hyper priors on π_{β_j} and π_{γ_j} to get rid of uncertainty about distribution of the components. For example, in this article, we simply assign priors for π_{β_j} and π_{γ_j} to be a beta distribution with parameters $(1,1)$.

2.4 Computational Details

In this section, we describe how to draw posterior samples to make inference in our proposed Bayesian quantile regression model with Pólya tree priors using an MCMC algorithm. Functions are written using Fortran within R (R Core Team, 2013) following R library *DPpackage* (Jara et al., 2011).

We use Metropolis-Hasting within Gibbs sampling algorithm to draw posterior samples. The full conditional distributions of $(\boldsymbol{\beta}|\boldsymbol{\gamma},\sigma,c,\boldsymbol{Y})$, $(\boldsymbol{\gamma}|\boldsymbol{\beta},\sigma,c,\boldsymbol{Y})$, $(\sigma|\boldsymbol{\beta},\boldsymbol{\gamma},c,\boldsymbol{Y})$, and $(c|\boldsymbol{\beta},\boldsymbol{\gamma},\sigma,\boldsymbol{Y})$ are proportional to equation (10).

We use $\beta_j^*\sim N(\beta_j^{l-1},t_{\beta_j}\Sigma_{jj})$ as candidate distribution for β_j in l-th iteration, where Σ_{jj} is the j-th element on the diagonal of matrix $(\boldsymbol{X}'\boldsymbol{X})^{-1}$, t_{β_j} is the tuning parameter for β_j to adjust acceptance rate. Similarly, we use $\gamma_j^*\sim N(\gamma_j^{l-1},t_{\gamma_j}\Sigma_{jj})$ as candidate distribution for γ_j in l-th iteration. For baseline (centering) normal distribution parameter σ (μ is fixed at 0 due to not confound with location parameter $\boldsymbol{\beta}$), we use the lognormal candidate distribution $\sigma^*\sim \mathrm{LN}(\log\sigma^{l-1},t_\sigma)$. The same strategy is applied for Pólya tree weight parameter c, where $c^*\sim\mathrm{LN}(\log c^{l-1},t_c)$.

For good MCMC mixing performance, we adjust the acceptance rate of the adaptive Metropolis-Hasting algorithm to around 0.4 for univariate sampling, 0.2 for multi-dimension sampling. Tuning parameters are increased when current acceptance proportion is larger than target optimal acceptance rate for every 100 iterations during burn-in period; and they are decreased when current acceptance proportion is less than target acceptance rate.

For the quantile regression coefficients, which are functionals of $(\boldsymbol{\beta},\boldsymbol{\gamma},\sigma,c,\boldsymbol{Y})$, we calculate the estimates by equation at each iteration using (9). Exact inference can be made using the posterior samples of the quantile regression coefficients (mean, median, and credible intervals).

3 Simulation Study

We conduct several simulation studies to compare our approach with other existing methods, specifically, the *rq* (RQ) function in the *quantreg* package (Koenker, 2012) in R Core Team (2013) (the standard frequentist quantile regression method) and the flexible Bayesian quantile regression approach by Reich (*FBQR*). We compare the approaches for both homogeneous and heterogeneous models.

3.1 Design

We generated data from the following 6 models,

M1: $y_i = 1 + x_{i1}\beta_1 + x_{i2}\beta_2 + \epsilon_{1i}$,

M2: $y_i = 1 + x_{i1}\beta_1 + x_{i2}\beta_2 + \epsilon_{2i}$,

M3: $y_i = 1 + x_{i1}\beta_1 + x_{i2}\beta_2 + \epsilon_{3i}$,

M4: $y_i = 1 + x_{i1}\beta_1 + x_{i2}\beta_2 + \epsilon_{4i}$,

M1H: $y_i = 1 + x_{i1}\beta_1 + x_{i2}\beta_2 + (1 - 0.5x_{i1} + 0.5x_{i2})\epsilon_{1i}$,

M2H: $y_i = 1 + x_{i1}\beta_1 + x_{i2}\beta_2 + (1 - 0.5x_{i1} + 0.5x_{i2})\epsilon_{2i}$,

M3H: $y_i = 1 + x_{i1}\beta_1 + x_{i2}\beta_2 + (1 - 0.5x_{i1} + 0.5x_{i2})\epsilon_{3i}$,

M4H: $y_i = 1 + x_{i1}\beta_1 + x_{i2}\beta_2 + (1 - 0.5x_{i1} + 0.5x_{i2})\epsilon_{4i}$,

where $x_{i1}, x_{i2} \overset{\text{iid}}{\sim} \mathrm{N}(0,1), \epsilon_{1i} \sim \mathrm{N}(0,1), \epsilon_{2i} \sim t_3, \epsilon_{3i} \overset{\text{iid}}{\sim} 0.5 \times \mathrm{N}(-2,1) + 0.5 \times \mathrm{N}(2,1)$ and $\epsilon_{4i} \sim 0.8N(0,1) + 0.2N(3,3)$. In model 1 (M1), the error distribution coincides with baseline distribution. Model 2 (M2) has a heavier tail distribution, student-t distribution with 3 degrees of freedom. Model 3 (M3) has a bimodal distribution for the error term. Model 4 (M4) uses a skewed mixture of normal distribution error introduced in Reich et al. (2010). Model 1H-4H (M1H-M4H) assume heterogeneous variances such that the quantiles lines are no long parallel to each other.

All covariates and error terms are mutually independent. All coefficients are set to be 1. For each model, we generate 100 data sets with the sample size $n = 200$. The quantiles estimated are 50%, 90%.

Each simulated data set is analyzed using the following four methods: RQ, FBQR, our proposed method using Pólya trees (PT) with normal priors, and our proposed method with spike and slab priors (PTSS). We used the default settings for RQ and FBQR. For PT, we adopt the following prior specifications:

$$\begin{aligned}
\pi(\beta_j) &\sim N(\boldsymbol{\beta}_j^p, \boldsymbol{V}_{jj}), j = 0, 1, 2,\\
\pi(\gamma_j) &\sim N(0, 100), j = 1, 2\\
\pi(\sigma) &\sim \Gamma(a/2, b/2),\\
\pi(c) &\sim \Gamma(a/2, b/2),
\end{aligned}$$

where $\boldsymbol{\beta}^p = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$ is the least square estimator, $\boldsymbol{V} = \hat{\sigma}^2(\boldsymbol{X}'\boldsymbol{X})^{-1}$, $\hat{\sigma}^2 = \sum_{i=1}^n (y_i - \boldsymbol{x_i}\boldsymbol{\beta^p})^2/(n-3)$, $a = b = 1$. For PTSS, we used the same priors for σ and c, but spike-slab priors for $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$:

$$
\begin{aligned}
\pi(\beta_j) &\sim \delta_{\beta_j} N(0, s_j \boldsymbol{V}_{jj}) + (1 - \delta_{\beta_j}) N(\boldsymbol{\beta}_j^p, \boldsymbol{V}_{jj}), j = 0, 1, 2, \\
\pi(\gamma_j) &\sim \delta_{\gamma_j} N(0, 100 s_j) + (1 - \delta_{\gamma_j}) N(0, 100), j = 1, 2 \\
\delta_{\beta_j} &\sim \text{Bernoulli}(\pi_{\beta_j}), \pi_{\beta_j} \sim \text{Beta}(1, 1), \\
\delta_{\gamma_j} &\sim \text{Bernoulli}(\pi_{\gamma_j}), \pi_{\gamma_j} \sim \text{Beta}(1, 1).
\end{aligned}
$$

And we choose $s_j = 1/1000$ from George and McCulloch (1993).

A partial Pólya tree with $M = 6$ levels was adopted in the model. For Monte Carlo Markov chain parameter, 40,000 iterations of a single Markov chain were used, during which, 20,000 samples were saved after a burn-in period of 20,000 samples. It takes around 100 seconds for one simulation for PT under R version 2.15.3 (2013-03-01) and platform: x86_64-apple-darwin9.8.0/x86_64 (64-bit). Acceptance rates were set to approach 25% for $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ candidates during the adaptive Metropolis-Hastings algorithm. We also tested the method proposed by Reich (FBQR), which conducts a single τ quantile regression for linear model and assigns an infinite mixture of Gaussian densities for the error term and the standard frequentist quantile regression approach, *rq* function in the *quantreg* package (Koenker, 2012) in R Core Team (2013) (RQ).

Methods are evaluated based on mean squared error:

$$
\text{MSE} = \frac{1}{N} \sum_{i=1}^{N} (\hat{\beta}_j(\tau) - \beta_j(\tau))^2,
$$

where N is the number of simulations, $\beta_j(\tau)$ is the j^{th} component of the true quantile regression parameters. $\hat{\beta}_j(\tau)$ is the j^{th} component of estimated quantile regression parameters. And we use the posterior mean as estimated parameters.

Table 1: Mean squared error (reported as 100*average) and standard error (reported as 100*standard error) for each quantile regression method. The three columns (RQ, FBQR, PT) stand for frequentist method *rq* function from *quantreg* R package, flexible Bayesian method by Reich, and our Bayesian approach using Pólya tree separately.

	RQ	BQR	PT	PTSS	RQ	BQR	PT	PTSS	RQ	BQR	PT	PTSS	RQ	BQR	PT	PTSS
M1 50%					M2 50%				M3 50%				M4 50%			
β_0	0.73	0.82	0.65	0.65	0.83	0.74	1.36	1.37	36.36	17.42	6.50	11.76	1.13	1.10	11.13	11.13
β_1	-1.13	-0.93	-0.78	-0.78	0.92	0.83	1.48	1.48	25.86	4.24	4.08	4.95	1.47	0.95	1.41	1.41
β_2	1.42	0.96	0.93	0.93	1.29	1.03	1.66	1.67	20.12	3.19	4.30	5.41	1.43	0.98	1.64	1.63
M1 90%					M2 90%				M3 90%				M4 90%			
β_0	-1.66	0.78	-1.53	-1.78	3.95	3.47	6.55	6.36	6.10	4.68	4.53	5.92	14.95	12.42	18.08	17.18
β_1	-1.75	-1.30	-0.64	-0.65	4.66	2.30	3.36	2.53	3.82	2.76	5.39	5.60	16.66	5.94	8.42	5.88
β_2	-0.34	1.33	1.50	1.31	4.43	2.68	3.82	2.95	5.63	3.63	6.30	6.58	13.62	4.56	7.74	5.67
M1H 50%					M2H 50%				M3H 50%				M4H 50%			
β_0	4.72	3.10	3.57	3.74	6.11	5.42	8.12	9.21	94.92	21.20	14.71	23.63	11.28	8.36	18.17	21.54
β_1	8.42	5.06	5.69	6.89	9.90	8.62	13.61	17.47	150.79	22.02	20.91	29.31	13.76	10.46	22.66	32.82
β_2	10.03	5.39	6.72	8.13	10.35	7.89	14.95	20.85	204.72	20.28	17.64	33.30	17.99	13.44	18.53	36.25
M1H 90%					M2H 90%				M3H 90%				M4H 90%			
β_0	10.50	8.14	7.42	8.56	32.61	15.41	28.54	26.90	16.10	11.31	15.48	23.81	110.08	41.07	62.97	81.63
β_1	16.54	11.34	10.39	23.18	45.61	21.58	45.96	63.43	26.47	15.55	27.82	61.66	177.03	52.48	79.16	112.10
β_2	17.81	14.85	16.20	32.15	53.44	17.36	39.98	63.70	23.27	17.30	23.41	87.85	182.33	63.00	96.33	215.79

3.2 Results

The simulation results are shown in Table 1. The proposed Bayesian quantile regression method with Pólya tree prior (PT) does well (in terms of MSE) relative to Reich's method (FBQR) and traditional frequentist approach (rq). The differences becomes quite large in the non-unimodal case (M2) and heterogeneous model (M3).

In Model 2 and Model 3 with $\tau = 0.5$, where the error is distributed as a bimodal distribution (mixture of normal distributions), the *rq* method performs poorly in terms of MSE since the mode of the error is no longer the quantile of interest. In contrast, our method (PT) is not impacted by lack of unimodality and heterogeneity and provides more information for the relationship between responses and covariates. In Model 3 with $\tau = 0.9$, Reich's method (FBQR) outperforms our approach (PT), since the error is assigned an infinite mixture of normal distribution with mode at $\tau = 0.9$ in his model, which is very close to the true distribution. Less information is available from our approach to detect the shape at a particular quantile of the distribution since there are few observations at extreme quantiles.

4 Analysis of the Tours Data

In this section, we apply our Bayesian quantile regression approach to examine the quantiles of 6 month weight loss from a recent weight management study (Perri et al., 2008). This trial was designed to test whether a lifestyle modification program could effectively help people to manage their weights in the long term. In particular, we are interested in the effects of age and race. The response of interest is the weight loss from baseline to 6 months later. The age of the subjects ranged from 50 to 75, and there were 43 people with race classified as black and 181 people as white. Our goal is to determine how the percentiles of weight change are affected by their age and race. "Age" covariates are scaled to 0 to 5 with every increment representing 5 years age increase.

We fitted regression models for quantiles (10%, 30%, 50%, 70%, 90%). And we used Bayesian posterior samples to build 95% credible intervals.

Results appear in Table 2. Whites generally lose more weight than blacks. The difference is not significant for the least successful weight loss (10 % percentile) shown by RQ, but is reported as significant by FBQR, PT and PTSS. The differential becomes larger when comparing more successful weight losers (30% - 90% percentile). For example, whites lose 6.08 kg more than blacks among people losing most weights (90%) reported from method RQ (4.30 kg from FBQR, 5.01 kg and 4.27 kg from PT and PTSS).

The effect of age on the weight loss is tiny and not significant in most cases (only significant in 90% quantile regression by RQ and 10% - 70% by PT). The trend is negative showing that elder people tend to lose less weight. For example, people lose 0.57 kg less weight for every 5 years older reported by PT.

PTSS tends to shrink coefficients toward zero. For example, coefficients of AGE were shrunk toward zero, thus was not significant for all quantiles. It can help to select variables in Bayesian models. For example, we can exclude AGE out of the regressors or conclude the variance is homogeneous on the AGE covariates.

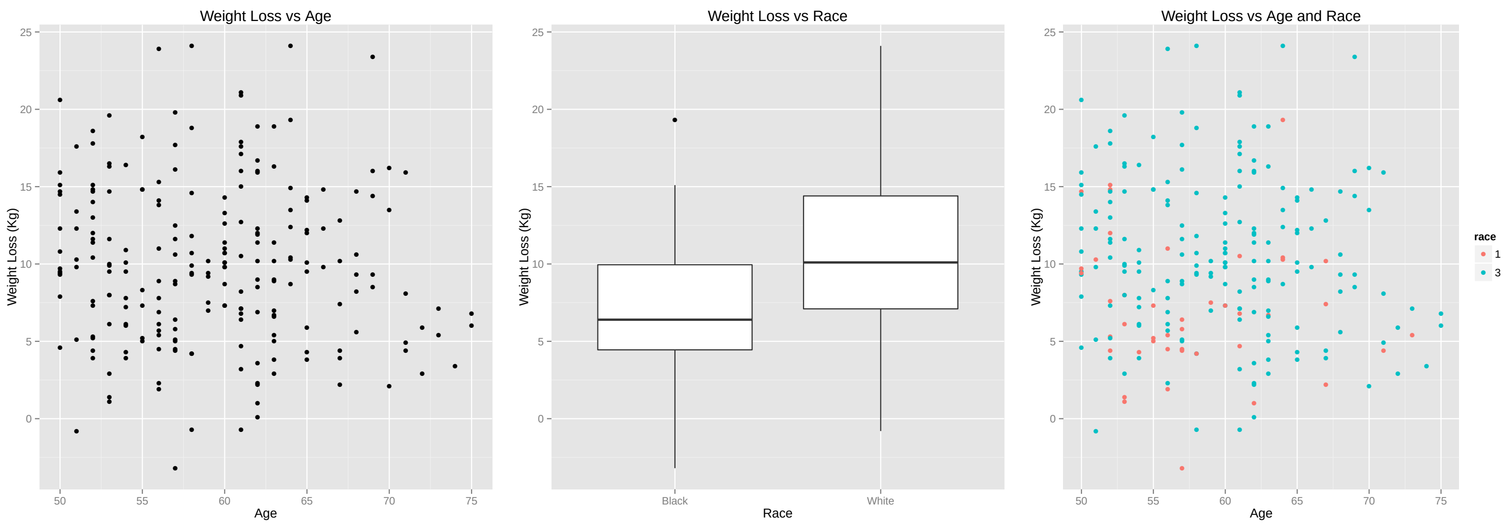

Figure 1: Scatterplots of weight loss vs age and Boxplots of weight loss for each race. The boxplots use the default settings: (0.75, 0.5, 0.25) quantile for box and $Q1 - 1.5IQR$ for lower whisker and $Q3 + 1.5IQR$ for upper whisker.

5 Discussion

This paper introduced a Bayesian approach for simultaneous linear quantile regression by introducing mixture of Pólya tree priors and estimating heterogeneity parameters. By marginalizing the predictive density function of the Pólya tree distribution, quantiles of interest can be obtained in closed form by inverting the predictive cumulative distribution. Exact posterior inference can be made via MCMC. Here, quantile lines cannot cross since quantiles are estimated through density estimation. **The simulations show our method performs better than the frequentist approach especially when the error is multimodal and highly skewed.** We also applied and illustrated our approach on the Tours data exploring the relationship between quantiles of weight loss and age and race.

Further research includes quantile regression for correlated data by modelling error as a mixture of multivariate Pólya tree distribution and shrinking the heterogeneity coefficients to zero for increased efficiency. Our approach allows for quantile regression with missing data under ignorability by adding a data augmentation step. We are exploring extending our approach to allow for nonignorable missingness.

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Table 2: 95% credible (confidence) intervals for quantile regression parameters for tours dataset. RQ stands for the traditional frequentist approach from quantreg package (Koenker, 2012), FBQR stands for method introduced in Reich et al. (2010), PT is our proposed Pólya trees approach with normal priors and PTSS stands for Pólya trees approach with spike-slab priors .

Term	RQ	FBQR	PT	PTSS
10%				
Intercept	2.20 (1.39, 4.63)	2.16 (0.11, 4.07)	2.72 (1.21, 4.17)	1.44 (0.15, 2.59)
Age	-0.25 (-0.73, 0.16)	-0.43 (-1.17, 0.24)	-0.63 (-1.16, -0.15)	-0.12 (-0.53, 0.24)
Race	2.40 (-0.23, 3.92)	2.88 (0.99, 5.34)	2.70 (1.25, 4.28)	3.19 (1.98, 4.54)
30%				
Intercept	5.56 (4.83, 6.52)	5.22 (3.62, 6.79)	5.68 (4.75, 6.63)	4.84 (3.99, 5.66)
Age	-0.66 (-1.28, 0.05)	-0.46 (-1.00, 0.09)	-0.53 (-0.78, -0.30)	-0.04 (-0.20, 0.09)
Race	3.74 (2.04, 4.42)	3.56 (1.98, 5.24)	3.37 (2.34, 4.50)	3.51 (2.48, 4.53)
50%				
Intercept	7.83 (5.42, 9.09)	7.65 (5.99, 9.23)	7.51 (6.55, 8.44)	6.90 (6.01, 7.80)
Age	-0.57 (-1.04, 0.14)	-0.51 (-1.06, 0.03)	-0.46 (-0.60, -0.32)	-0.00 (-0.00, 0.00)
Race	3.53 (2.52, 5.46)	3.86 (2.36, 5.46)	3.79 (2.88, 4.84)	3.70 (2.62, 4.63)
70%				
Intercept	9.70 (7.95, 12.39)	9.89 (8.23, 11.70)	9.86 (8.79, 11.07)	9.60 (8.72, 10.58)
Age	-0.69 (-1.12, 0.20)	-0.54 (-1.13, 0.07)	-0.37 (-0.65, -0.11)	0.06 (-0.12, 0.26)
Race	4.80 (2.11, 6.61)	4.30 (2.46, 5.87)	4.32 (3.20, 5.52)	3.96 (2.73, 4.92)
90%				
Intercept	12.61 (11.48, 15.27)	14.07 (11.75, 17.45)	12.90 (11.33, 14.67)	12.91 (11.72, 14.37)
Age	-0.71 (-1.59, -0.05)	-0.55 (-1.36, 0.30)	-0.25 (-0.81, 0.28)	0.13 (-0.26, 0.60)
Race	6.08 (2.48, 6.85)	4.30 (1.21, 6.74)	5.01 (3.33, 6.71)	4.27 (2.73, 5.44)

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