Variational Inference for Quantile Regression

Bufei Guo
Washington University in St. Louis

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Variational Inference for Quantile Regression

by

Bufei Guo

A thesis presented to
The Graduate School
of Washington University in
partial fulfillment of the
requirements for the degree
of Master of Arts

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Bufei Guo

Washington University in St. Louis

May 2019
Dedicated to My Parents.
Quantile regression (QR) (Koenker and Bassett, 1978), is an alternative to classic linear regression with extensive applications in many fields. This thesis studies Bayesian quantile regression (Yu and Moyeed, 2001) using variational inference, which is one of the alternative methods to the Markov chain Monte Carlo (MCMC) in approximating intractable posterior distributions. The lasso regularization is shown to be effective in improving the accuracy of quantile regression (Li and Zhu, 2008). This thesis developed variational inference for quantile regression and regularized quantile regression with the lasso penalty. Simulation results show that variational inference is a computationally more efficient alternative to the MCMC, while providing a comparable accuracy.
1. Introduction

Regression is a technique used to explain the relationship between explanatory variable $X = [x_1, \ldots, x_n]$ and a response variable $y$. Least square estimation (LSE) is one of the widely used methods, that targets the conditional expectation $\mathbb{E}(y|X = [x_1, \ldots, x_n])$. When heterogeneity is present in the random error, it provides an inadequate description of the distribution of response variable $y$ as only the average relationship between $X$ and $y$ is considered. Quantile regression (QR) was first introduced by Koenker and Bassett (1978), which provides an alternative to least square estimator, especially for the linear model with non-Gaussian errors. QR is able to provide a more complete description of the relationship between the explanatory variables and the response by modeling the conditional distribution $y|X = [x_1, \ldots, x_n]$ at different quantiles. Oftentimes, QR gives comparable estimation accuracy as the least square method under Gaussian errors and provides a more robust alternative when the “outliers” in the model are difficult to identify. QR has a broad application in many fields like survival analysis (Koenker and Geling, 2001), financial economics (Bassett and Chen, 2001) and environmental modeling (Pandey and Nguyen, 1999).
1.1 Bayesian quantile regression

Consider $X = [x_1, \ldots, x_k]$, where $x_i = (x_{i,1}, \ldots, x_{i,n})'$ is the explanatory variable and $y = (y_1, \ldots, y_n)'$ is the response variable. The $p$th ($0 < p < 1$) conditional quantile of $y_i$ given $x_i$ is defined as

$$Q_p(y_i|x_i) = x'_i\beta_p,$$

where $\beta_p \in \mathbb{R}^k$ is the vector of coefficients. The $p$th ($0 < p < 1$) quantile regression estimator of $\beta$ is the solution to the quantile regression minimization problem given by

$$\min_{\beta} \sum_{i=1}^{n} \rho_p(y_i - x'_i\beta),$$

(1.1)

where $\rho_p(\cdot)$ is an asymmetrix loss function,

$$\rho_p(u) = u(p - I(u < 0)),$$

(1.2)

and $I(\cdot)$ is the indicator function. Equivalently, we can write (1.2) as

$$\rho_p(u) = \frac{|u| + (2p - 1)u}{2}.$$  

Figure 1.1 shows the loss functions at three different quantiles, namely $p = 0.25$, 0.50 and 0.75.
Regularization, e.g. lasso (Tibshirani, 1996), is also adapted in QR to prevent over-fitting and improve prediction when the explanatory variables are high-dimensional (Li et al., 2010). This problem can be modified as an optimization over the quantile functions $f_i = x_i \beta_i$, $i = 1, \ldots, n$ for

$$\sum_{i=1}^{n} \rho_p(y_i - f_i) + \lambda ||f||_q,$$

where $f = (f_1, \ldots, f_n)$ and $|| \cdot ||_q$ is the $q$th norm (Abeywardana and Ramos, 2015). For example, when $q = 1$, this is the lasso penalty.

In Bayesian quantile regression, the coefficient $\beta_p$ is sampled from its posterior distribution using the random walk Metropolis-Hastings algorithm (Yu and Moyeed, 2001) or Gibbs samplers (Tsionas, 2003). Li et al. (2010) studied Bayesian regularized quantile regression with the group lasso and elastic net penalty. Yu and Moyeed (2001) proposed that QR can be incorporated into Bayesian inference framework by assuming the error

![Figure 1.1. Loss function in (1.2) at different quantiles](image)

Figure 1.1. Loss function in (1.2) at different quantiles
terms follow the asymmetric Laplace distribution (ALD). Based on the ALD distributed error assumption, the likelihood function of $\beta$ can be constructed, then its posterior distribution can be derived using Bayes’ theorem.

**Asymmetric Laplace distribution**

The probability density function (pdf) of an asymmetric Laplace distribution (ALD) is defined as

$$f(x; \mu, \sigma, p) = \frac{p(1-p)}{\sigma} \exp \left( -\frac{(x-\mu)}{\sigma} [p - I(x \leq \mu)] \right), \quad x \in (-\infty, \infty), \quad (1.3)$$

where $0 < p < 1$ is the skewness parameter, $\sigma > 0$ is the scale parameter, and $\mu \in \mathbb{R}$ is the location parameter. The distribution ALD $(x; \mu, \sigma, p)$ has mean $E(x) = \frac{1-2p}{p(1-p)}$ and variance $\text{Var}(x) = \frac{1-2p+2p^2}{p^2(1-p)^2}$. The corresponding CDF and quantile function are, respectively,

$$F(x; \mu, \sigma, p) = \begin{cases} 
p \exp \left( \frac{1-p}{\sigma} (x - \mu) \right), & x \leq \mu, \\
1 - (1-p) \exp \left( -\frac{p}{\sigma} (x - \mu) \right), & x > \mu, \end{cases} \quad (1.4)$$

and

$$F^{-1}(x; \mu, \sigma, p) = \begin{cases} 
\mu \exp \left( \frac{\sigma}{1-p} \log \left( \frac{x}{p} \right) \right), & 0 \leq x < p, \\
\mu - \frac{2}{p} \log \left( \frac{1-x}{1-p} \right), & p < x \leq 1. \end{cases} \quad (1.5)$$

As the $p$th quantile of the ALD distribution equals to the location parameter $\mu$, i.e. $F^{-1}(x; \mu, \sigma, p)|_{x=p} = \mu$, the ALD is used as the error distribution in quantile regression models (Yu and Moyeed, 2001).
The ALD can also be represented as a the mixture of an exponential and a normal distribution (Reed and Yu, 2009). If a variable $\epsilon$ follows the ALD in (1.3), we can represent $\epsilon$ as a location-scale mixture of normal distributions given by

$$
\epsilon = \theta z + \tau \sqrt{z} u,
$$

where

$$
\theta = \frac{1 - 2p}{p(1 - p)} \text{ and } \tau^2 = \frac{2}{p(1 - p)}.
$$

1.1.1 Quantile regression under the asymmetric Laplace distributed error

Consider the model

$$
y_i = x_i' \beta_p + \epsilon_i, \ i = 1, \ldots, n
$$

(1.7)
where \( y_i \in \mathbb{R} \) is the response variable, \( x_i \in \mathbb{R}^k \) is the explanatory variable, \( \beta_p \in \mathbb{R}^k \) is the regression parameter for the \( p \)th quantile and \( \epsilon_i \sim \text{ALD}(0, \sigma, p) \) is the error term. By representing \( \epsilon_i \) as in (1.6), Equation (1.7) can be rewritten as

\[
y_i = x_i' \beta_p + \theta z_i + \tau \sqrt{\sigma} z_i u_i, \quad i = 1, \ldots, n,
\]

where \( u_i \sim \text{N}(0, 1) \) and \( z_i \) follows the exponential distribution with rate \( \sigma \), e.g., \( \exp(\sigma) \).

Both \( \theta \) and \( \tau \) are constants with

\[
\theta = \frac{1 - 2p}{p(1 - p)} \quad \text{and} \quad \tau^2 = \frac{2}{p(1 - p)}.
\]

From (1.8), \( y_i \) also follows an asymmetric Laplace distribution with location parameter \( x_i \beta_p \), scale parameter \( \sigma \) and asymmetry parameter \( p \), e.g., \( \text{ALD}(x_i' \beta_p, \sigma, p) \). The conditional distribution of \( y_i \) given \( z_i \) is a normal distribution with mean \( x_i \beta_p - \theta z_i \) and variance \( \tau^2 z_i \). The conditional density of \( y = (y_1, \ldots, y_n)' \) given \( z = (z_1, \ldots, z_n)' \) and \( \beta_p \) is

\[
f(y|\beta_p, z) \propto (\Pi_{i=1}^n z_i^{-\frac{3}{2}}) \exp \left( -\Pi_{i=1}^n \frac{(y_i - x_i' \beta_p - \theta z_i)^2}{2 \tau^2 z_i} \right).
\]

Connection with Gibbs sampling

The conditional distribution \( p(z_j|z_{-j}, \beta_p, y) \) is known as the full conditional in MCMC (Casella and George, 1992). The approximating density function in quantile regression can be derived from the full conditional distribution of variables in Gibbs sampling. We will first review quantile regression using Gibbs sampling which iteratively samples from the full conditional distributions.
Gibbs sampling for quantile regression

We first consider the model in (1.8). First we consider the quantile regression with the scale parameter $\sigma$ fixed at $\sigma = 1$. Let the prior distribution be

$$\beta_p \sim N(\mu_{p0}, \Sigma_{p0}), \quad z_i \sim \exp(1).$$

(1.10)

The full conditional density of $\beta_p$ can be shown as (Kozumi and Kobayashi, 2011)

$$\beta_p|y, z \sim N(\mu_p, \Sigma_p),$$

(1.11)

where

$$\Sigma^{-1}_p = \sum_{i=1}^{n} \frac{x_i x_i'}{\tau^2 z_i} + \Sigma^{-1}_{p0},$$

(1.12)

$$\mu_p = \sum_{i=1}^{n} \frac{x_i (y_i - \theta z_i)}{\tau^2 z_i} + \Sigma^{-1}_{p0} \mu_{p0}.$$  

(1.13)

The full conditional density of $z_i, i = 1, ..., n$ is a generalized inverse Gaussian distribution (Kozumi and Kobayashi, 2011)

$$z_i|y, \beta_p \sim GIG\left(\frac{1}{2}, a_i, b_i\right),$$

(1.14)

where

$$a_i = 2 + \frac{\theta^2}{\tau^2} \quad \text{and} \quad b_i = \frac{(y_i - x_i' \beta_p)^2}{\tau^2}.$$  

(1.15)

The pdf of a generalized inverse Gaussian distribution is given by

$$f(p, a, b) = \frac{(a/b)^{p/2}}{2K_p(\sqrt{ab})} x^{p-1} \exp(-\frac{1}{2}(ax + b/x)), a > 0, b > 0, p \in \mathbb{R},$$

(1.16)

where $K_p(\cdot)$ is the Bessel function of the third type. Next we extend our discussion to the more general case by treating $\sigma$ as an unknown variable and a prior is assigned to $\sigma$. The prior distribution for $\beta_p$ is the same as (1.11)

$$\beta_p \sim N(\mu_{p0}, \Sigma_{p0}),$$

(1.17)
and a prior was given to $\sigma$ 

$$\sigma \sim IG(m_0, n_0), \quad (1.18)$$

where $IG(\cdot)$ is the inverse gamma distribution. Similar to the previous situation, the posterior for $\beta_p$ and $z$ is the same as (1.11) and (1.14) respectively. The full conditional density for $\sigma$ is then given by 

$$\sigma|y, \beta_p, z \sim IG(m_p, n_p), \quad (1.19)$$

where 

$$m_p = 3n + m_0 
\quad n_p = n_0 + \sum_{i=1}^{n} (z_i + \frac{(y_i - x_i'\beta_p - \theta z_i)^2}{2\tau^2 z_i})$$

Then the algorithm of Gibbs sampler iterates between the full conditional distribution of $\beta_p$ given $y$, $z$, $\sigma$, the full conditional distribution of $z_i$ given $y$, $\beta_p$, $\sigma$, and the full conditional distribution of $\sigma$ given $y$, $\beta_p$, $z$. But this process can be time consuming when the parameter space is high dimensional and the data set is large.

**Gibbs Sampling for quantile regression with the lasso penalty**

The lasso regularization on quantile regression is brought up in Li and Zhu (2008), where the $L_1$-norm penalty (lasso) is added to the minimization problem 

$$\min_{\beta} \sum_{i=1}^{n} \rho_p(y_i - x_i'\beta) + \lambda \sum_{i=1}^{k} |\beta_i|,$$

Li et al. (2010) proposed an equivalent Bayesian formulation to the problem by putting a Laplace prior with mean zero and scale $\frac{\sigma}{\lambda_j}$, $j = 1, \ldots, m$ on $\beta$

$$p(\beta_p|\sigma, \lambda) = \prod_{j=1}^{k} \frac{\lambda_j}{\sigma} \exp\left(-\frac{\lambda_j}{\sigma} |\beta_j| \right), \quad (1.20)$$
which leads to the posterior distribution

$$p(\beta_p|y, \sigma, z) \propto \exp\left(-\frac{1}{\sigma} \sum_{i=1}^{n} \rho_p(y_i - x'_i\beta_p) - \frac{\lambda_j}{\sigma} \sum_{j=1}^{k} |\beta_j|\right), \quad (1.21)$$

where \(\lambda_j\)'s are the regularization parameter for corresponding regression coefficients \(\beta_j\).

We put an inverse gamma prior on \(\sigma\) and a gamma prior on \(\eta_j = \frac{\lambda_j}{\sigma}, \ j = 1, \ldots, m\). Let \(s = (s_1, \ldots, s_k)\) and the prior of \(\beta_p\) can be further written as

$$p(\beta_p|\sigma, \lambda) = \prod_{j=1}^{k} \frac{\lambda_j}{\sigma} \exp\left(-\frac{\lambda_j}{\sigma} |\beta_j|\right)$$

$$= \prod_{j=1}^{k} \int_{0}^{\infty} \frac{1}{\sqrt{a\pi s_j}} \exp\left(-\beta_j^2 \frac{\eta_j^2}{2s_j}\right) \frac{\eta_j^2}{2} \exp\left(-\frac{\eta_j^2 s_j}{2}\right) ds_j. \quad (1.22)$$

Then the full conditional distribution of \(\beta_j\) is \(N(\tilde{\mu}_j, \tilde{\omega_j}^2)\), with

$$\tilde{\mu}_j = \tilde{\omega_j}^2 \frac{1}{\sigma \tau^2} \sum_{i=1}^{n} y_{i,j} x_{i,j} z_i^{-1}, \quad (1.23)$$

and

$$\tilde{\omega_j}^{-2} = \frac{1}{\sigma \tau^2} \sum_{i=1}^{n} x_{i,j}^2 z_i^{-1} + s_j^{-1}, \quad (1.24)$$

where

$$y_{i,j} = y_i - \theta z_i - \sum_{l=1, l\neq j}^{k} x_{i,l} \beta_l. \quad (1.25)$$

The full conditional distribution of \(z_i\) follows the same distribution as the previous case in (1.14), which is \(GIG(\frac{1}{2}, \tilde{a}_i, \tilde{b}_i)\), with

$$\tilde{a}_i = \frac{\theta^2}{\sigma \tau^2} + \frac{2}{\sigma}, \quad (1.26)$$

and

$$\tilde{b}_j = \frac{(y_i - x'_i \beta_p)^2}{\sigma \tau^2}. \quad (1.27)$$
The full conditional distribution for $s_j$ is given by

$$p(s_j|y, z, \beta_p, s_{-j}, \tau, \eta^2) \propto p(\beta_j|s_j)p(s_j|\eta^2)$$

$$\propto s_k^{-1/2} \exp\{-\frac{1}{2}(\eta^2 s_j + \beta_j^2 s_j^{-1})\},$$

which is $GIG(\frac{1}{2}, \eta_j^2, \beta_j^2)$. The full conditional distribution for $\sigma^2$ is also an inverse gamma distribution $IG(\tilde{m}, \tilde{n})$, with

$$\tilde{m} = 3n + m_0,$$

and

$$\tilde{n} = n_0 + \sum_{i=1}^{n} (z_i + \left(y_i - x_i' \beta_p - \theta z_i\right)^2).$$

The full conditional distribution of $\eta^2$ follows a gamma distribution with shape parameter $c + 1$ and rate parameter $\frac{1}{2} \sum_{j=1}^{k} s_k + d$, which is given by

$$p(\eta^2|y, z, \beta_p, s, \sigma) \propto p(s|\eta^2)p(\eta^2)$$

$$\propto (\eta^2)^{k+c-1} \exp\left\{-\eta^2 \left(\frac{\sum_{j=1}^{k} s_k}{2} + d\right)\right\},$$

where $c$ and $d$ are constants given in the joint prior distribution of $\tau$ and $\eta^2$

$$\tau, \eta^2 \sim \tau^{\psi-1} \exp(-\xi \tau)(\eta^2)^{\psi-1} \exp(-d \eta^2).$$

### 1.1.2 Variational inference

Variational inference is one of the popular methods to approximate intractable or difficult-to-compute posterior distributions $p(y|\cdot)$ with an approximate posterior distribution $q(y)$. Compared with MCMC such as Gibbs sampling, variational inference tends to be faster while achieves comparable prediction especially when dealing with large-scale data sets (Blei et al., 2016).
The idea of variational inference is to approximate the conditional density of latent variables given observed variables using optimization. Let \( \mathbf{x} = (x_1, \ldots, x_n) \) be the set of observed variables and \( \mathbf{z} = (z_1, \ldots, z_m) \) be the set of latent variables. The joint density of \( \mathbf{x} \) and \( \mathbf{z} \) is \( p(\mathbf{x}, \mathbf{z}) \). In the case that the conditional distribution \( p(\mathbf{z}|\mathbf{x}) \) is not directly tractable, variational inference provides an alternative approach by approximating the conditional distribution \( p(\mathbf{z}|\mathbf{x}) \) using a tractable distribution \( q^*(\mathbf{z}) \in \Theta \), where \( \Theta \) is the family of densities over the latent variables. All density functions \( q(\mathbf{z}) \in \Theta \) are candidate approximations to \( p(\mathbf{z}|\mathbf{x}) \). By solving the optimization problem, one can try to find the member in \( \Theta \) that is the closest to \( p(\mathbf{z}|\mathbf{x}) \) in the Kullback-Leibler (KL) distance (Blei et al., 2016)

\[
q^*(\mathbf{z}) = \arg\min_{q(\mathbf{z}) \in Q} \text{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x})),
\]  

(1.33)

where \( \text{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x})) \) is the Kullback-Leiber distance between the posterior distribution \( p(\mathbf{z}|\mathbf{x}) \) and the candidate distribution \( q(\mathbf{z}) \) in the family \( \Theta \). It is defined as

\[
\text{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x})) = \mathbb{E}(\log q(\mathbf{z})) - \mathbb{E}(\log p(\mathbf{z}|\mathbf{x})),
\]  

(1.34)

which is always non-negative (van Erven and Harremos, 2014). Wang and Blei (2018) gave the asymptotic properties of variational inference by proving that the posterior density given by variational inference converges to the KL minimizer of a normal distribution centered at the truth. Zhang and Gao (2017) proved that the upper bound of the convergence rate, at which the variational posterior \( q^*(\mathbf{z}) \) converges to the true posterior \( p(\mathbf{z}|\mathbf{x}) \) is given by

\[
\epsilon_n^2 + \frac{1}{n} \inf_{q(\mathbf{z}) \in \Theta} p_n^{(n)} \text{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x})),
\]  

(1.35)
where $\epsilon_n^2$ is the rate of convergence of the posterior distribution $p(z|x)$. The second term is the variational approximation error with respect to $\Theta$ under $p_0^{(n)}$, where $p_0^{(n)}$ is the process that generates all the $x_i$'s. If $q(z)$ equals to the exact posterior distribution $p(z|x)$, the second term will be zero. The convergence rate will be the convergence rate of the posterior distribution given by MCMC. In general, the second term in (1.35)

$$\frac{1}{n} \inf_{q(z) \in \Theta} p_0^{(n)} KL(q(z)||p(z|x))$$

is dominated by the first term $\epsilon_n^2$ in (1.35). Variational inference does not require the sampling process required in MCMC and Gibbs sampling. Hence, it provides computational advantages without violating the asymptotic property of estimators in large-scale data set situations.
2. Variational inference for quantile regression

2.1 Algorithm of variational Bayes

Numerical implementation of the variational inference, the CAVI (coordinate ascent variational inference) algorithm in Blei et al. (2016), is closely related to Gibbs sampling. In each iteration, CAVI optimizes every parameter sequentially, while keep others fixed. Finally, a local optimum is reached. Consider the model with parameter vector (latent variable) $\theta$ and observed variable $y$. Bayesian inference is based on the posterior density function

$$p(\theta|y) = \frac{p(y, \theta)}{p(y)}.$$  \hspace{1cm} (2.1)

Let $q(\cdot)$ be an arbitrary density function over the density family $\Theta$. The logarithm of the marginal likelihood function satisfies

$$\log p(y) = \log p(y) \int q(\theta)d\theta$$

$$= \int q(\beta_p, z) \log \left\{ \frac{p(y, \beta_p, z)/q(\beta_p, z)}{p(\beta_p, z|y)/q(\beta_p, z)} \right\} d\beta_p dz$$

$$= \int q(\beta_p, z) \log \left\{ \frac{p(y, \beta_p, z)}{q(\beta_p, z)} \right\} d\beta_p dz + \int q(\beta_p, z) \log \left\{ \frac{q(\beta_p, z)}{p(\beta_p, z|y)} \right\} d\beta_p dz$$

$$\geq \int q(\beta_p, z) \log \left\{ \frac{p(y, \beta_p, z)}{q(\beta_p, z)} \right\} d\beta_p dz.$$  \hspace{1cm} (2.2)
where $\theta = (\beta_p, z)$ and $q(\cdot) \in \Theta$ is the candidate distribution used to approximate $p(\cdot)$.

The above inequality holds because the second integral in (2.2)

$$
\int q(\beta_p, z) \log \left\{ \frac{q(\beta_p, z)}{p(\beta_p, z|y)} \right\} d\beta_p dz, \tag{2.3}
$$

is the KL distance between $q(\beta_p, z)$ and $p(\beta_p, z|y)$, which is always non-negative by definition (Kullback and Leibler, 1951). The equality holds if and only if $q(\beta_p, z) = p(\beta_p, z|y)$. Under this special case, the estimation of variational inference will coincide with the estimation given by Gibbs sampling. Recall from Equation (1.33), that the goal of variational inference is to find the distribution $q(\cdot)$ that is closest to the conditional distribution $p(\theta|y)$ in KL distance. According to (2.2), minimizing the KL distance in (2.3) between $q(\beta_p, z)$ and $p(\beta_p, z|y)$ is equivalent to maximizing the lower bound

$$
L = \int q(\beta_p, z) \log \left\{ \frac{p(y, \beta_p, z)}{q(\beta_p, z)} \right\} d\beta_p dz. \tag{2.4}
$$

In variational inference, the assumption of the complexity of the density family $\Theta$ determines the complexity of optimization problem. In the mean-filed variational family (a.k.a. naive mean approach) (Blei et al., 2016), where the latent variables $\theta$ are assumed to be mutually independent and governed by distinct factors in the variational density $q(\theta_i)$, is used to approximate the conditional distribution $p(\theta_i|y, \theta_{-i})$. e.g.

$$
q(\theta) = \prod_{i=1}^{n} q(\theta_i),
$$

where each latent variable $\theta_i$ is governed by its own variational factor. One can also use other approximations such as generalized mean field (Blei et al., 2016), in which the
parameters of interest are divided into groups and the parameters inside each group are allowed to be dependent. e.g.

\[ q(\theta) = \prod_{i=1}^{n} q(\theta_{i_1}, \ldots, \theta_{i_m}). \]

In this thesis, we adopt the mean-field variational family approach, by assuming independence between latent variables \( \beta_p \) and \( z \). Then the log-likelihood function can be written as

\[
\int q(\beta_p, z) \log \{ \frac{p(y, \beta_p, z)}{q(\beta_p, z)} \} d\beta_p dz = \int q(\beta_p) q(z) \log \{ \frac{p(y|\beta_p, z)p(\beta_p)p(z)}{q(\beta_p)q(z)} \} d\beta_p dz \\
= \int q(\beta_p) q(z) \log \{ p(y|\beta_p, z) \} d\beta_p dz \\
+ \int q(\beta_p) \log \{ \frac{p(\beta_p)}{q(\beta_p)} \} d\beta_p \\
+ \int q(z) \log \{ \frac{p(z)}{q(z)} \} dz,
\]

where \( q(\cdot) \) is the candidate density from the density family \( \Theta \). Consider the jth variable \( z_j \) in the latent variable \( z \). The conditional density of \( z_j \) conditioning on all other latent variables and observed variables is

\[ p(z_j|z_{-j}, \beta_p, y), \]

where \( z_{-j} = (z_1, \ldots, z_{j-1}, z_{j+1}, \ldots, z_n) \). Then one can fix all other variational factors in \( z_{-j} \), and maximize the lower bound of this conditional distribution with respect to the density of \( z_j \). The optimal \( q_{j}^*(z_j) \in \Theta_j \) is proportional to the exponential of the expected log conditional density (Blei et al., 2016)

\[ q^*(z_j) \propto \exp(\mathbb{E}_{-j}(\log p(z_j|y, z_{-j}))). \]  \hspace{1cm} (2.6)

The latent variables are updated successively using (2.6). The iteration stops when the difference between two sequential lower bound is negligible. i.e., smaller than a pre-speci-
ified tolerance level.

Algorithm: (CAVI)

---

Step 1 Initialize $q(\theta)$

Step 2 Update $q(z_j^*)$, $j = 1, \ldots, n$ and $q(\beta_p)$ by

$$q^*(z_j) \propto \exp(\mathbb{E}_{-j}(\log p(z_j|y, z_{-j}))),$$

$$\vdots$$

$$q(\beta_p) \propto \exp(\mathbb{E}_z(\log p(\beta_p|y, z)))$$

Step 3 Update the lower bound $L$, repeat step 2 and 3 until the change in $L$ is negligible.

---

2.2 Variational inference for quantile regression without regularization

We start from the simplest case, where the scale parameter is fixed at $\sigma = 1$. Then only $\beta_p$ and $z$ need to be updated in the iterations of variational inference.

The optimal approximation density function $q^*(\beta_p)$ is given by

$$q(\beta_p) \propto \exp(\mathbb{E}_z(\log p(\beta_p|y, z)))$$
with

$$\log p(\beta_p | y, z) = -\frac{1}{2} \left( \log(2\pi) + \log \left( \det \left( \sum_{i=1}^{n} \frac{x_i x_i'}{\tau^2 z_i} + \Sigma_{p0}^{-1} \right) \right) \right)$$

$$- \frac{1}{2} (\beta_p - \mu_{p0})' \left( \sum_{i=1}^{n} \frac{x_i x_i'}{\tau^2 z_i} + \Sigma_{p0}^{-1} \right) (\beta_p - \mu_{p0})$$

$$= -\frac{1}{2} \log \left( \det \left( \sum_{i=1}^{n} \frac{x_i x_i'}{\tau^2 z_i} + \Sigma_{p0}^{-1} \right) \right)$$

$$- \frac{1}{2} \beta_p' \left( \sum_{i=1}^{n} \frac{x_i x_i'}{\tau^2 z_i} + \Sigma_{p0}^{-1} \right) \beta_p$$

$$+ \beta_p' \left( \sum_{i=1}^{n} \frac{x_i (y_i - \theta z_i)}{\tau^2 z_i} + \Sigma_{p0}^{-1} \mu_{p0} \right)$$

$$- \frac{1}{2} \left( \sum_{i=1}^{n} \frac{x_i (y_i - \theta z_i)}{\tau^2 z_i} + \Sigma_{p0}^{-1} \mu_{p0} \right)' \left( \sum_{i=1}^{n} \frac{x_i x_i'}{\tau^2 z_i} + \Sigma_{p0}^{-1} \right)^{-1} \left( \sum_{i=1}^{n} \frac{x_i (y_i - \theta z_i)}{\tau^2 z_i} + \Sigma_{p0}^{-1} \mu_{p0} \right)$$

$$+ \text{const.}$$

(2.7)

The expectation of \(\log p(\beta_p | y, z)\) is with respect to \(z_i\), where \(z_i\) follows the generalized inverse Gaussian distribution \(\text{GIG}(\frac{1}{2}, a_q, b_q)\), with

$$\mathbb{E}(z_i) = \frac{\sqrt{b_q} K_{3/2}(\sqrt{a_q b_q})}{\sqrt{a_q} K_{1/2}(\sqrt{a_q b_q})},$$

$$\mathbb{E}(\frac{1}{z_i}) = \frac{\sqrt{a_q} K_{3/2}(\sqrt{a_q b_q})}{\sqrt{b_q} K_{1/2}(\sqrt{a_q b_q})} - \frac{1}{b_q},$$

and

$$\mathbb{E}(\ln z_i) = \ln \frac{\sqrt{b_q}}{\sqrt{a_q}} + \frac{\partial}{\partial p} \ln K_p(\sqrt{a_q b_q}),$$

where \(K_p(\cdot)\) is the Bessel function with order \(p\). The approximation of the expectations could be used for simplicity in some situations (Abeywardana and Ramos, 2015), with

$$\mathbb{E}(z_i) = \frac{\sqrt{b_q}}{a_q},$$

(2.8)
and
\[ E\left(\frac{1}{z_i}\right) = \sqrt{\frac{a_{q_i}}{b_{q_i}}} - \frac{1}{b_{q_i}}. \] (2.9)

In general the exact values of these expectations are preferred, as the approximated value might cause convergence problems, e.g., the value of the lower bound sometimes diverges if the approximated values are used. The expectation of the logarithm of the full conditional density \( \log p(\beta_p|y, z) \) is

\[
\mathbb{E}_q(\log p(\beta_p|y, z)) = \beta'_p \left( \sum_{i=1}^{n} \frac{x_i y_i}{\tau^2} \mathbb{E}\left(\frac{1}{z_i}\right) - \sum_{i=1}^{n} \frac{\theta}{\tau^2} x_i + \Sigma_{\mu_0}^{-1} \mu_0 \right)
- \frac{1}{2}\beta'_p \left( \sum_{i=1}^{n} \frac{x_i x'_i}{\tau^2} \mathbb{E}\left(\frac{1}{z_i}\right) + \Sigma_{\mu_0}^{-1} \right) \beta_p + \text{const.} \tag{2.10}\]

Taking exponential of the expectation \( \mathbb{E}_q(\log p(\beta_p|y, z)) \), we then see that the density function of \( q(\beta_p) \) is for the multivariate normal distribution \( N(\mu_q, \Sigma_q) \), with

\[ \Sigma_q = \left( \sum_{i=1}^{n} \frac{x_i x'_i}{\tau^2} \mathbb{E}\left(\frac{1}{z_i}\right) + \Sigma_{\mu_0}^{-1} \right)^{-1} \tag{2.11}\]

and

\[ \mu_q = \Sigma_q \left( \sum_{i=1}^{n} \frac{x_i y_i}{\tau^2} \mathbb{E}\left(\frac{1}{z_i}\right) - \sum_{i=1}^{n} \frac{\theta}{\tau^2} x_i + \Sigma_{\mu_0}^{-1} \mu_0 \right). \tag{2.12}\]

The pdf of \( q(z_i)'s \) are calculated in a similar manner as

\[ q(z_i) \propto \exp(\mathbb{E}_{\beta_p}(\log p(z_i|y, \beta_p))), \tag{2.13}\]

where

\[ \log p(z_i|y, \beta_p) = -\frac{1}{2} \log(z_i) - \frac{1}{2}(a_i z_i + b_i/z_i) + \text{const.} \tag{2.14}\]
The expectation of the log conditional density \( \log p(z_i|y, \beta_p) \) with respect to \( \beta_p \) follows the GIG distribution

\[
q(z_i) \sim GIG\left(\frac{1}{2}, a_{q_i}, b_{q_i}\right),
\]

with

\[
a_{q_i} = 2 + \theta^2, \tag{2.16}
\]

and

\[
b_{q_i} = \frac{y_i^2 - 2y_i x_i' \mu_q + x_i' (\mu_q \mu_q' + \Sigma_q) x_i}{\tau^2}. \tag{2.17}
\]

The \( \mu_q \) and \( \Sigma_q \) in (2.17) are the mean and variance of \( q(\beta_p) \), which are given in (2.11) and (2.12). From (2.4), the lower bound is given by

\[
\mathbb{E}(\log p(y|\theta)) + \mathbb{E}(\log(p(\theta))) - \mathbb{E}(\log(q(\theta))), \tag{2.18}
\]

with \( \theta = (z, \beta_p) \). Then the lower bound \( l \) is

\[
l = \int q(z)q(\beta_p) \log(p(y|z, \beta_p)) dz d\beta_p + \int q(z) \log(p(z)/q(z)) dz
+ \int q(\beta_p) \log(p(\beta_p)/q(\beta_p)) d\beta_p
= \mathbb{E}_{q(z),q(\beta_p)} \log \left( (y|z, \beta_p) \right) + \mathbb{E}_{q(z)} \log(p(z)) - \mathbb{E}_{q(\beta_p)} \log(q(\beta_p))
+ \mathbb{E}_{q(\beta_p)} \log(p(\beta_p)) - \mathbb{E}_{q(\beta_p)} \log(q(\beta_p)). \tag{2.19}
\]

The variational inference algorithm when \( \sigma = 1 \) is

**Algorithm 1:**

---

**Step 1** Initialize mean \( \mu_q \) and covariance matrix \( \Sigma_q \).

**Step 2** Repeat Steps 3-5 if the absolute change in lower bound \( l \geq t \), where \( t \) is the tolerance given, e.g. \( t = 10^{-5} \).
Step3 Update parameters in $q(z)$. $q(z_i) \sim GIG(\frac{1}{2}, a_{q_i}, b_{q_i})$, where

$$
a_{q_i} = 2 + \frac{\theta_2}{\tau^2},
$$

$$
b_{q_i} = \frac{y_i^2 - 2y_i x'_i \mu_q + x'_i (\mu_q \mu'_q + \Sigma_q) x_i}{\tau^2}.
$$

Step4 Update parameters in $q(\beta_p)$. $q(\beta_p) \sim N(\mu_q, \Sigma_q)$, where

$$
\Sigma_q = \left( \sum_{i=1}^{n} \frac{x_i x'_i}{\tau^2} E \left( \frac{1}{z_i} \right) + \Sigma_{p0}^{-1} \right)^{-1}
$$

$$
\mu_q = \Sigma_q \left( \sum_{i=1}^{n} \frac{x_i y_i}{\tau^2} E \left( \frac{1}{z_i} \right) - \sum_{i=1}^{n} \frac{\theta}{\tau^2} x_i + \Sigma_{p0}^{-1} \mu_{p0} \right).
$$

Step5 Update lower bound $l$

$$
l = \mathbb{E}_{q(x), q(\beta_p)}(y|z, \beta_p) + \mathbb{E}_{q(x)} \log(p(z)) - \mathbb{E}_{q(x)} \log(q(z))
$$

$$
+ \mathbb{E}_{q(\beta_p)} \log(p(\beta_p)) - \mathbb{E}_{q(\beta_p)} \log(q(\beta_p)).
$$

When the scale parameter $\sigma$ is taken into account, similar as the case in Gibbs sampling, a prior distribution of $\sigma$ is assumed and we update the value of $\beta_p$, $z$ and $\sigma$ successively in the iteration of variational inference. The approximation distribution of $\beta_p$, $z$ and $\sigma$ are given by

$$
q(\beta_p) \sim N(\mu_q, \Sigma_q),
$$

$$
q(z_i) \sim GIG(a_{q_i}, b_{q_i}),
$$

and

$$
q(\sigma) \sim IG(m_q, n_q),
$$

\begin{align*}
\text{(2.20)} \\
\text{(2.21)} \\
\text{(2.22)}
\end{align*}
with

\[ \Sigma_q = \left( \sum_{i=1}^{n} \frac{x_i x_i'}{\tau^2} \mathbb{E} \left( \frac{1}{z_i} \right) \mathbb{E} \left( \frac{1}{\sigma} \right) + \Sigma_{p0}^{-1} \right)^{-1}, \quad (2.23) \]

\[ \mu_q = \Sigma_q \left( Q \mathbb{E} \left( \frac{1}{\sigma} \right) + \Sigma_{p0}^{-1} \mu_{p0} \right), \quad (2.24) \]

\[ a_{qi} = \left( 2 + \frac{\theta^2}{\tau^2} \right) \mathbb{E} \left( \frac{1}{\sigma} \right), \quad (2.25) \]

\[ b_{qi} = \frac{M}{\tau^2} \mathbb{E} \left( \frac{1}{\sigma} \right), \quad (2.26) \]

\[ m_q = 3n + m_0, \quad (2.27) \]

and

\[ n_q = n_0 + \sum_{i=1}^{n} \mathbb{E}(z_i) + N. \quad (2.28) \]

The \( Q \) in Equation (2.24) is given by

\[ Q = \left( \sum_{i=1}^{n} \frac{x_i y_i}{\tau^2} \mathbb{E} \left( \frac{1}{z_i} \right) - \sum_{i=1}^{n} \frac{\theta}{\tau^2} x_i \right). \quad (2.29) \]

The \( M \) is Equation (2.26) is given by

\[ M = y_i^2 - 2y_i x_i' \mu_q + x_i' (\mu_q \mu_q' + \Sigma_q) x_i. \quad (2.30) \]

The \( N \) in Equation (2.28) is given by

\[ N = \sum_{i=1}^{n} \frac{M}{2\tau^2} \mathbb{E} \left( \frac{1}{z_i} \right) - \frac{\theta(y_i - x_i' \mu_p)}{\tau^2} + \frac{\theta^2}{2\tau^2} \mathbb{E}(z_i). \quad (2.31) \]

Algorithm 2:

---

Step1 Initialize mean \( \mu_q \) and covariance matrix \( \Sigma_q \).

Step2 while absolute change in lower bound \( l \geq t \), \( t \) is the tolerance given, e.g. \( t = 10^{-5} \).
Step 3 Update parameters in $q(z)$, using $q(z_i) \sim GIG(\frac{1}{2}, a_{q_i}, b_{q_i})$.

Step 4 Update parameters in $q(\beta_p)$, using $q(\beta_p) \sim N(\mu_q, \Sigma_q)$.

Step 5 Update parameters in $q(\sigma)$, using $q(\sigma) \sim IG(m_q, n_q)$.

Step 6 Update the lower bound $l$

### 2.3 Variational inference for quantile regression with the lasso penalty

The approximation density function $q(\cdot)$ is calculated using the same method given in Section (2.2)

\begin{equation}
q(\theta_i) \propto \exp(\mathbb{E}_{\theta_{-i}}(\log p(\theta_i|\theta_{-i}))),
\end{equation}

where $\theta_{-i}$ is the vector of variables without the $i$th variable $\theta_i$. The density function of $q(\beta_j)$ follows the normal distribution

\begin{equation}
N(\mu_{q_j}, \omega_{q_j}),
\end{equation}

with

\begin{equation}
\omega_{q_j}^{-2} = \frac{\mathbb{E}(1/\sigma)}{\tau^2} \sum_{i=1}^{n} x_{i,j}^2 \mathbb{E}(1/z_i) + \mathbb{E}(1/s_j),
\end{equation}

and

\begin{equation}
\mu_{q_j} = \omega_{q_j}^2 \left( \frac{\mathbb{E}(1/\sigma)}{\tau^2} \sum_{i=1}^{n} x_{i,j} \left( y_i \mathbb{E} \left( \frac{1}{z_i} \right) - \theta - \sum_{l=1,l \neq j}^{k} x_{i,l} \mu_{q_l} \mathbb{E} \left( \frac{1}{z_i} \right) \right) \right),
\end{equation}

where $\mathbb{E}(1/\sigma) = \frac{m_q}{n_q}$ with $m_q$ and $n_q$ given in (2.44) and (2.45). The density function of $q(z_i)$ follows the generalized inverse Gaussian

\begin{equation}
GIG(\frac{1}{2}, \tilde{a}_{q_i}, \tilde{b}_{q_i}),
\end{equation}
with
\[ a_{q_i} = \left( \frac{\theta^2}{\tau^2} + 2 \right) \mathbb{E} \left( \frac{1}{\sigma} \right), \quad (2.37) \]
and
\[ b_{q_i} = \frac{(y_i^2 - 2y_i \mathbf{x}'_i \mathbf{\mu}_q + \mathbf{x}'_i \mathbb{E}(\mathbf{\beta}'_j \mathbf{\beta}'_p) \mathbf{x}_i) \mathbb{E}(\frac{1}{\sigma})}{\tau^2}. \quad (2.38) \]

The density functions of \( q(s_j) \) and \( q(\eta^2) \) follow the generalized inverse Gaussian
\[ GIG\left(\frac{1}{2}, \eta_{q_j}^2, \beta_{q_j}^2\right), \quad (2.39) \]
and the Gamma distribution
\[ \text{Gamma} \left( k + c, \sum_{j=1}^{k} \frac{\mathbb{E}(s_j)}{2} + d \right), \quad (2.40) \]
respectively, with
\[ \eta_{q_j}^2 = \mathbb{E}(\eta^2) = \frac{k + c}{\sum_{j=1}^{k} \frac{\mathbb{E}(s_j)}{2} + d}, \quad (2.41) \]
and
\[ \beta_{q_j}^2 = \mathbb{E}(\beta^2_j) = \mu_{q_j}^2 + \omega_{q_j}^2. \quad (2.42) \]
The density function of \( q(\sigma) \) follows the inverse Gamma distribution
\[ IG(m_q, n_q), \quad (2.43) \]
with
\[ m_q = 3n + m_0, \quad (2.44) \]
and
\[ n_q = n_0 + \sum_{i=1}^{n} \left\{ \left( 1 + \frac{\theta^2}{2\tau^2} \right) \mathbb{E}(z_i) + \frac{\mathbb{E}(y_i - \mathbf{x}_i \mathbf{\beta}_j)^2}{2\tau^2} \mathbb{E} \left( \frac{1}{z_i} \right) - \frac{\mathbb{E}(y_i - \mathbf{x}_i \mathbf{\beta})}{\tau^2} \theta \right\}. \quad (2.45) \]
Algorithm 3:

Step 1. Initialize parameters in the prior distribution, including \( m_0, n_0, c \) and \( d \).

Step 2. Initialize mean \( \mu_q \) and covariance matrix \( \Sigma_q \).

Step 3. Update parameters in \( q(\sigma) \), using \( q(\sigma) \sim IG(m_q, n_q) \).

Step 4. Update parameters in \( q(s_j) \), using \( q(s_j) \sim GIG(\frac{1}{2}, \eta_{q_j}^2, \beta_{q_j}^2) \).

Step 5. Update parameters in \( q(\eta^2) \), using \( q(\eta^2) \sim Gamma(k + c, \sum_{j=1}^k \frac{E(s_j)}{2} + d) \).

Step 6. Update parameters in \( q(z) \), using \( q(z_i) \sim GIG(\frac{1}{2}, \tilde{a}_q, \tilde{b}_q) \).

Step 7. Update parameters in \( q(\beta_p) \), using \( q(\beta_j) \sim N(\mu_{q_j}, \omega_{q_j}) \).

Step 8. Update the lower bound \( l \), if the difference between two consecutive \( l \) is bigger than the tolerance level specified, repeat Steps 3 \( \sim 8 \).
3. Simulation studies

We compare the variational inference with the Gibbs sampling method in terms of accuracy and speed using simulated data. CPU time is used to measure the speed of different algorithms and predictive mean squared error (MSE) is used to measure the accuracy. Assuming independent and identically (i.i.d) distributed errors, we conduct the simulation using the following models.

1. Sparse case with Gaussian noise: \( \beta_1 = (3, 1.5, 0, 0, 2, 0, 0, 0) \), \( \epsilon_i \sim N(0, 0.6^2) \).

2. Dense case with Gaussian noise: \( \beta_2 = (0.85, 0.85, 0.85, 0.85, 0.85, 0.85, 0.85, 0.85) \), \( \epsilon_i \sim N(0, 0.6^2) \).

3. Very sparse case with Gaussian noise: \( \beta_3 = (2, 4, 0, \ldots, 0) \), \( \epsilon_i \sim N(0, 0.6^2) \).

4. High-dimensional: \( \beta_4 = (2, \ldots, 2, 0, \ldots, 0, 3, \ldots, 3) \), \( \epsilon_i \sim N(0, 0.6^2) \)

For first three models, we set the sample size \( n \) equal to 1000. And the sample size for the last model is 50. In model 1~3 we run the regression using variational inference without the lasso penalty (Algorithm 2). And variational inference with the lasso penalty is applied in the high-dimensional case. Gibbs sampling are applied in all four cases for comparison. Fig. 3.1 and Fig. 3.2 show the CPU time and predictive MSE using variational inference and Gibbs sampling under different quantiles, respectively.

The Gibbs sampling on quantile regression is conducted using the \texttt{bayesQR} function in R.
Figure 3.1. CPU time at different quantiles
Figure 3.2. Predictive MSE at different quantiles
package bayesQR (Benoit and den Poel, 2017). In the sparse and dense case, variational inference has a comparable speed compared with Gibbs sampling, but variational inference maintains a lower MSE. Variational inference tends to need more time for extreme quantiles. In the very sparse case and the case when predictor is more than sample size, variational inference spends less time than quantile regression but has a slightly larger MSE. Variational inference could be used as a faster alternative to Gibbs sampling when the dimension of the predictor is high, while provides a comparable accuracy in terms of MSE. We also compare the number of iterations needed to converge using quantile regression with the lasso penalty and Gibbs sampling under quantile $p = \{0.25, 0.5, 0.75\}$. The results are shown in Fig. 3.3 and Fig. 3.4. It shows that the two methods take almost the same number of iterations to converge. However, turning points of variational inference usually occur before that in Gibbs sampling, which indicates that the declining of MSE in variational inference is usually faster in the first few iterations.
Figure 3.3. Iteration trajectories of variational inference and Gibbs sampling
Figure 3.4. Iteration trajectories of variational inference and Gibbs sampling
4. Conclusions

This thesis derive the variational inference algorithm for quantile regression with and without the lasso regularization. Simulated studies show that, in comparison with Gibbs sampling, variational inference has a faster MSE declining within few iterations. Usually variational inference could maintain a comparable accuracy with Gibbs sampling. In very sparse data sets and the case when predictor is more than sample size, variational inference could usually perform better without sacrificing significant accuracy.


C. Reed and K. Yu. A partially collapsed Gibbs sampler for Bayesian quantile regression. 01 2009.


