Scientia Africana, Vol. 21 (No. 1), April, 2022. Pp 233-244 https://dx.doi.org/10.4314/sa.v21i1.20

ISSN 1118 – 1931

QUANTILE CROSSING AS IT PERTAINS TO SAMPLE SIZE AND GOODNESS OF FIT: A SIMULATION STUDY

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Received: 05-02-2022
Accepted: 30-03-2022

ABSTRACT

Estimation of quantile regression curves individually causes quantile crossing, which eventually leads to an invalid estimation of the predictor effect. This work implemented quantile regression coefficient modeling (QRCM) where the regression coefficients are modeled as parametric functions of the order of the quantile in other to eliminate crossing. Four different samples of sizes 30, 50, 100 and 500 were simulated in other to investigate the effect of sample size on crossing and also to investigate the effect of crossing on model fit. The results show that as the sample sizes were increased crossing was reduced, but with a very large sample size crossing was not observed at all. The results also revealed that the presence of crossing caused the models not to be well specified but with the elimination of crossing the models were seen to be well specified.

Keywrods: Quantile Crossing, Quantile Regression, Goodness of Fit, Cross Index and Quantile Function.

INTRODUCTION

Quantiles are said to be points in a distribution that pertains to the rank order of values in that distribution. Quantiles seem inseparably linked to the operations of ordering and sorting the sample observations that are usually used to define them. So it comes as a mild surprise to observe that we can define the quantiles through a simple alternative expedient as an optimization problem. Just as we can define the sample mean as the solution to the problem of minimizing a sum of squared residuals, we can define the median as the solution to the problem of minimizing a sum of absolute residuals, (Koenkerand Hallock,2001). Given a set of covariates, the linear-regression model (LRM) specifies the conditional mean function whereas the Quantile Regression model (QRM) specifies the conditional-quantile function. The LRM is a standard statistical method that focuses on modeling the conditional mean of a response variable without accounting for the full conditional distributional properties of the response variable. In contrast, the QRM facilitates analysis of the full conditional distributional properties of the response variable. The QRM and LRM are similar in certain respects, as both models deal with a continuous response variable that is linear in unknown parameters, but the QRM and LRM model deal with different quantities and rely on different assumptions about error terms. The issue of crossing arises during multiple percentiles estimation, the quantile curves can cross, leading to an invalid distribution for the response, such as wrong coefficient effects Nwakuya and

Onyegbuchulam (2021) investigated the effects of crossing on regression coefficients and they found out that crossing has a significant effect on regression coefficients. It's paramount that crossing should be eliminated in quantile regression analysis. Some authors like Lui and Wu(2011), proposed a new kernel-based multiple QR estimate technique called simultaneous non-crossing quantile regression, the method applies constraints on the kernel coefficients to avoid crossing. Chernozhukov et al. (2010) proposed estimating noncrossing quantile curves via a monotonic rearrangement of the original nonmonotonic function. Most recently Santos and Kneib (2020) considered a flexible Bayesian quantile regression model with Gaussian process adjustment to achieve a noncrossing property. Jiang and Yu(2022) considered single-index models and developed methods for QR that guarantees non-crossing quantile curves which they extended to composite quantile regression. Patto and Matteo (2016) described an approach for modeling the regression coefficients as parametric functions of the order of the quantile. The method proved to be advantageous in terms of parsimony, efficiency and removal of crossing. Patto et al. (2021) applied this approach to longitudinal data were they described how the QRCM paradigm can be applied to longitudinal data. This work aims at investigating crossing as it relates to sample size and goodness of fit while modeling the regression coefficients as parametric functions of the order of the quantile, following the work of Patto and Matteo (2016).

The quantile regression model is given by;

$$Q_\tau(y_i) = \beta_0(\tau) + \beta_1(\tau)x_{i1} + \cdots + \beta_p(\tau)x_{ip} + e_i \quad (1)$$

Where p is the number of predictor variables, $\beta(\tau)$is the τth effect on the response variable while e and x are the error term and predictor variable respectively. The best median Quantile regression line is found by minimizing median absolute deviation.

$$MAD = \frac{1}{n}\sum_{i=1}^{n} \rho_\tau\left(y_i - \left(\beta_0(\tau) + \beta_1(\tau)x_{i1} + \cdots + \beta_p(\tau)x_{ip}\right)\right) \quad (2)$$

Here the function ρ is the check function which gives asymmetric weights to the error depending on the quantile and the overall sign of the error.

$$\rho_\tau(e) = e(\tau - 1(e < 0)) = \begin{cases} \tau|e|, & e \geq 0 \\ (1-\tau)|e|, & e \leq 0 \end{cases}$$

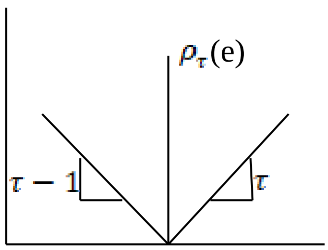

Figure 1.1 Loss Function

Scientia Africana, Vol. 21 (No. 1), April, 2022. Pp 233-244 https://dx.doi.org/10.4314/sa.v21i1.20
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In figure 1.1, $\rho_\tau(0) = 0$ increases linearly with slope τ as e moves away from zero to the right and it increases linearly with slope $1 - \tau$ as e moves away from zero on the left. Nwakuya (2020) opined that the traditional frequentist quantile regression makes minimum assumptions that tolerate errors that are not normal given that the response variable (y) is continuous even in Bayesian framework. John & Nduka (2009) concluded that quantile regression offers a comprehensive strategy for completing the regression picture as it goes beyond this primary goal of determining only the conditional mean, and enables one to pose the question of relationship between the response variable and explanatory variables at any quantile of the conditional distribution function. Studying For better understanding of the intuition of quantile regression, let's begin with the intuition of ordinary least squares. Given the model

$$y_i = \beta' X_i + \varepsilon_i \tag{3}$$

the least squares estimate minimizes the sum of the squared error terms

$$\sum_i^N \sum (y_i - \hat{y}_i)^2 \tag{4}$$

Comparatively, quantile regression minimizes a weighted sum of the positive and negative error terms:

$$\tau \sum_{y_i > \hat{\beta}_\tau' X_i} |y_i - \hat{\beta}_\tau' X_i| + (1-\tau) \sum_{y_i < \hat{\beta}_\tau' X_i} |y_i - \hat{\beta}_\tau' X_i| \tag{5}$$

where τ is the quantile level.

The τ^{th} conditional quantile $\tau \in 0,1$ of a real valued random variable Y given a vector of *k* predictors is given by;

$$Q_\tau(Y|X) = \inf\left(\Pr\left(Y \le y|X\right)\right) \ge \tau. \tag{6}$$

The earliest research by Koenker and Bassset (1978) recognized that the solutions were determined by fitting certain observations exactly. When the quantile regression were introduced, it was found out that fitting certain observations exactly forced the regression quantile fits to cross, thus causing the conditional quantile function to be non-monotonic in its statement, τ at some values of the predictor variables, Koenker (2005). Crossing in quantile regression happens when regression predictions for different quantile probabilities do not increase as probability increases.

QUANTILE CROSSING

In view of the fact that quantile regression curves are estimated individually, these curves may cross, leading to an invalid distribution for the response. Reviewing the conditional distribution of the response given the predictor, one of the processes is to estimate multiple conditional quantile functions. Theoretically, the various conditional quantile functions ought not to cross each other as claimed by the basic principle of conditional distribution functions. However, this naive individual estimation can lead to estimated conditional quantile functions that may cross each other. Authors that worked on non-crossing include, He (1997) that suggested a technique to estimate the quantile curves while ensuring that it does not cross. Nevertheless, the approach presumes a heteroscedastic regression model for the response, which permits the predictors to have effect on the distribution of the response via a location and scale change of an underlying base distribution. Wu and Liu (2009) suggested a technique to ensure non-crossing, by fitting the quantiles sequentially and constraining the current curve to not cross the previous curve. Dette and Volgushev (2008) and Chernozhukov et al. (2009), all secured non-crossing by the approach of modifying the estimation of the conditional distribution function. The indirect technique is considered if focus is purely in estimation of the conditional quantile. However, when our focus is on quantifying the effects of the predictors, the quantile curves are typically modeled via a parametric form, such as linear predictor effects, and a direct estimation approach is required.

METHODOLOGY

Let y denote the outcome of interest conditional on a p dimensional vector x, where y is a continuous random variable with cumulative distribution function $F_{y_i}(.)$ and let $Q_{y_i}(\tau|x)$ be the quantile function· The Quantile regression model with the τth quantile for response (y|x) is of the form; $Q_\tau(y|x) = \inf(\Pr(Y \leq (y|x) \geq \tau$, it is assumed that for $\tau \in 0{,}1$ and that there is a p dimensional vector $\beta(\tau)$ such that;

$$Q(\tau/x) = X^T\beta(\tau) \tag{7}$$

$\beta(\tau)$, describes the effect of predictors on the τ^{th} quantile of the response variable and we assume that the quantile regression coefficient function $\beta(.)$ can be modeled parametrically as $\beta(\tau) = \beta(\tau/\theta)$, where θ is an unknown parameter. We can define $\beta(\tau)$ as a function of τ that depends on a finite-dimensional parameter θ, so that;

$$\beta(\tau/\theta) = \theta b(\tau) \tag{8}$$

Where $b(\tau)$ =$[b_1(\tau), \ldots, b_k(\tau)]^T$ is a set of k known functions of τ. θ is a matrix with entries θ_{ij}. Hence the conditional quantile function is;

$$Q(\tau/x,\theta) = x^T\theta b(\tau)\ , \tag{9}$$

this can be written as; $y = x^T\theta b(\tau)$ (10)

Considering a simple model given as $y_i = \beta_o(\tau/\theta) + \beta_1(\tau/\theta)x$ (11)

If we denote the quantile function of distribution of a standard normal distribution as $z(\tau)$then;

$\beta_o(\tau/\theta) = \theta_{00} + \theta_{01}\xi(\tau)and\beta_1(\tau/\theta) = \theta_{10}$, where $\beta_1$is linear in τ and β_0 depends on $\xi(\tau)$.

In this model θ_{00} is the intercept of $\beta_o(\tau/\theta)$, θ_{10} is the slope associated with $\xi(\tau)$ and the regression coefficient $\beta_1(\tau/\theta)$ is assumed to be constant across quantiles enforcing homoscedasticity. In other to estimate the τ^{th}quantile regression coefficients under equation (7) we minimize the objective function;

$$L(\beta(\tau)) = \sum_i^n(\tau - w_{\tau,i})(y_i - X^T\beta(\tau_t)) \tag{12}$$

Subject to $X_i^T\beta_{\tau t} \geq X_i^T\beta_{\tau t-1}$, t=2,…,q

Scientia Africana, Vol. 21 (No. 1), April, 2022. Pp 233-244 https://dx.doi.org/10.4314/sa.v21i1.20
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Given that; $w_{\tau,i} = I\left(y_i \leq X_i^T\beta(\tau)\right)$ where I(.) is an indicator function. $\theta$is estimated by minimizing the integrated objective function given in equation (13)below with respect to the order of the quantile.

$$L(\theta) = \int_0^1 L(\,\beta(\tau/\theta))d\tau \qquad (13)$$

This approach allows the estimation of the entire quantile process without allowing crossing. This work applied simulated datasets with sample sizes 30, 50, 100 and 500 in other to investigate effect of sample size on crossing and to check the fitness of the model without crossing and with crossing.The simulated dataset with crossing was generated for binomial and uniform distribution, while the response was generated as a function of both the predictors from both distributions, for sample size n = 30, 50, 100 and 500. The work was analyzed using Quantreg package and qrcm package in R.

Goodness of fit test:

Let $F_n(X)$ denote the empirical distribution function of the data defined by $F_n(X) = \frac{1}{n}\sum_{i-1}^{n} I(x_i \leq x), -\infty < x < \infty$, where the indicator function $I(a,b)$ is defined as 1 for a ≤ b and as 0 otherwise. Since $F_n(X)$ is the proportion of observations less than or equal to $x\ if\ F(X)$ is the true distribution of X, we expect $F_n(X)$ to be close$F(X)$. The closeness of $F_n(X)$ to $F(X)$ is assessed by the Cramer-von Mises statistics defined by Richard A. L. (2019) as;

$$w_n^2 = n\int_{-\infty}^{\infty}[F_n(X) - F(X)]^2 dF(X)$$

The hypothesis is given as;

$H_0: \tau_1, \dots, \tau_q \sim u(0,1)$ (model is correctly specified)

$H_1: \tau_1, \dots, \tau_q \nsim u(0,1)$ (model is not correctly specified)

Cross index: Cross index is the average length, across observations, of the sub-intervals of τ. Cross index lies from 0 to 1, with 0 indicating no crossing and 1 indicating that observations cross at all quantiles. Cross index close to 0 indicates minimal crossing while cross index close to 1 indicates high crossing.

RESULTS

Sample size = 30. The dataset had crossing with a cross index of 0.3105, which is minimal crossing.

Table 4.1: Quantile regression coefficient results at different quantiles with crossing:

Quantiles	Coefficients	Estimate	std.err	z value	p(>|z|))
25%	Intercept	0.6659	5.2904	0.126	0.900
	β_1	2.3316	2.6715	0.873	0.383
	β_2	5.3758	4.9869	1.078	0.281
50%	Intercept	0.5452	5.7178	0.095	0.924
	β_1	2.9888	5.0242	0.595	0.552
	β_2	6.3411	7.0616	0.898	0.369
75%	Intercept	5.708	17.947	0.318	0.750
	β_1	2.239	6.435	0.348	0.728
	β_2	1.607	16.995	0.095	0.925
95%	Intercept	33.74	18.92	1.784	0.0745
	β_1	-7.32	11.11	-0.659	0.5099
	β_2	-17.76	15.51	-1.145	0.2522

*Significant at 0.05 level of significance

Table 4.1 presents the quantile regression coefficients with crossing and it shows that all the predictors are insignificant.

AFTER REMOVING CROSSING: Number of observations that crossed is 0 (0%), with cross index of 0.0005462.

Table 4.2 Quantile regression coefficient results at different quantiles after removal of crossing:

Quantiles	Coefficients	Estimate	std.err	z value	p(>|z|))
25%	Intercept	-0.9878	6.8540	-0.144	0.885410
	β_1	2.8530	0.8106	3.519	0.000433*
	β_2	7.0496	7.0053	1.006	0.3143
50%	Intercept	0.8662	0.5311	1.631	0.103
	β_1	2.5729	0.2969	8.667	<2e-16*
	β_2	6.0500	0.6023	10.044	<2e-16*
75%	Intercept	3.131	6.440	0.486	0.627
	β_1	2.805	1.444	1.943	0.050*
	β_2	4.076	6.336	0.643	0.520
95%	Intercept	23.5386	17.3947	1.353	0.176
	β_1	0.2412	10.3794	0.023	0.981
	β_2	-10.3701	14.8580	-0.698	0.485

*Significant at 5% level of significance.

The table 4.2 above shows that the removal of crossing affected the effects of the predictors. We can see that β_1 is now significant at the 25th, 50th and 75th quantiles but it showed no effect at the 95th quantile.

Scientia Africana, Vol. 21 (No. 1), April, 2022. Pp 233-244 https://dx.doi.org/10.4314/sa.v21i1.20
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Table 4.3: Goodness of fit test result

Test Statistics	statistic	p-value
Cramer-Von Mises (With Crossing)	0.036759	0.03061224
Cramer-Von Mises (Without Crossing)	0.065670	0.68141414

With crossing the model was seen not to be well specified but it can be seen that the removal of the crossing resulted to a well specified model. Table 4.3 shows that the model without crossing is well specified.

SAMPLE SIZE = 50

Number of observations that crossed were 28, the analysis shows that 56% of the observations has crossing somewhere in the domain with a cross index of 0.167.

Table 4.4: Quantile regression coefficient results at different quantiles with crossing:

Quantiles	Coefficients	Estimate	std.err	z value	p(>|z|))
25%	Intercept	-0.3813	29.6825	-0.013	0.990
	β_1	2.4084	0.4750	5.070	3.97e-07*
	β_2	6.8926	29.6886	0.232	0.816
50%	Intercept	-0.1664	18.7418	-0.009	0.992916
	β_1	2.8370	0.8352	3.397	0.000682*
	β_2	7.0754	18.7010	0.378	0.7052
75%	Intercept	0.7110	1.1470	0.620	0.535
	β_1	3.0647	0.7577	4.045	5.23e-05*
	β_2	6.7818	0.8928	7.596	3.05e-14*
95%	Intercept	3.314	5.162	0.642	0.5210
	β_1	3.183	4.682	0.680	0.4967
	β_2	6.168	2.902	2.125	0.0335*

*Significant at 5% level of significance

Table 4.4 above shows that at all quantiles at least one predictor is significant. The effects in this result are similar to the effects in 25th quantile without crossing. We can say that even with crossing a little increase in the sample reveals some effects that were not visible with a smaller sample size.

After Removing Crossing

Number of observations that crossed: 0 (0%) with cross index of 0.00.

Table 4.5: Quantile regression coefficient results at different quantiles after removing crossing:

Quantiles	Coefficients	Estimate	std.err	z value	p(>|z|))
25%	Intercept	-0.006231	0.956783	-0.007	0.995
	β_1	2.490053	0.223359	11.148	< 2e-16*
	β_2	6.4684	0.9532	6.786	1.15e-11*
50%	Intercept	0.2236	1.5700	0.142	0.886766
	β_1	2.7864	0.8063	3.456	0.000549*

	β_2	6.6696	1.2180	5.476	4.36e-08*
75%	Intercept	1.100	2.016	0.546	0.58525
	β_1	3.202	0.464	6.900	5.19e-12*
	β_2	6.217	2.100	2.960	0.0031*
95%	Intercept	3.390	10.245	0.331	0.741
	β_1	3.621	4.319	0.838	0.402
	β_2	5.477	8.133	0.673	0.501

*Significant at 5% level of significance

The Table 4.5 above reveals that after the removal of crossing all the predictors were seen to have a significant effect except for the 95th quantile. This also reveals an improvement in the significance of the predictors when crossing was removed.

Table 4.6: Goodness of fit test result

Test Statistics	statistic	p-value
Cramer-Von Mises (With Crossing)	0.0269145	0.04061224
Cramer-Von Mises (Without Crossing)	0.0556175	0.9895233

We can see that the removal of the crossing resulted in a well specified model. But with crossing the model is seen not to be well specified.

SAMPLE SIZE = 100

Number of observations that crossed: 4 (4%), the analysis shows that 4% of the observations has crossing somewhere in the domain with a cross index of 0.2018, which is minimal crossing.

Table 4.7: Quantile regression coefficient results at different quantiles with crossing:

Quantiles	Coefficients	Estimate	std.err	z value	p(>|z|))
25%	Intercept	0.8173	2.1689	0.377	0.706
	β_1	2.2319	2.3523	0.949	0.343
	β_2	5.5892	4.8617	1.150	0.250
50%	Intercept	0.7969	0.4585	1.738	0.0822
	β_1	3.1353	0.3558	8.813	<2e-16*
	β_2	5.4893	0.4666	11.765	<2e-16*
75%	Intercept	1.105	2.830	0.390	0.696
	β_1	3.570	3.004	1.188	0.235
	β_2	5.824	1.435	4.059	4.93e-05*
95%	Intercept	1.763	13.935	0.127	0.899
	β_1	4.108	7.459	0.551	0.582
	β_2	6.047	5.236	1.1556	0.248

*Significant at 5% level of significance

Scientia Africanna, Vol. 21 (No. 1), April, 2022. Pp 233-244 https://dx.doi.org/10.4314/sa.v21i1.20
 ISSN 1118 – 1931

The Table 4.7 above shows that only at 50th and 75th quantile were the predictors significant.

After Removing Crossing

Number of observations that crossed: 0 (0%) with cross index: 0.0005462.

Table 4.8: Quantile regression coefficient results at different quantiles after removing crossing:

Quantiles	Coefficients	Estimate	std.err	z value	p(>|z|))
25%	Intercept	0.4839	0.1712	2.827	0.00469*
	β_1	2.7247	0.2083	13.080	< 2e-16*
	β_2	5.7347	0.2707	21.182	< 2e-16*
50%	Intercept	0.7592	0.5305	1.431	0.152
	β_1	3.0785	0.3651	8.432	<2e-16*
	β_2	5.6786	0.3911	14.520	<2e-16*
75%	Intercept	1.2280	0.5583	2.199	0.0279*
	β_1	3.3802	0.6632	5.097	3.46e-07*
	β_2	5.8394	0.3644	16.024	<2e-16*
95%	Intercept	2.0509	0.8777	2.337	0.01946*
	β_1	4.1482	1.3904	2.984	0.00285*
	β_2	5.3353	0.8545	6.244	4.27e-10*

*Significant at 5% level of significance

The Table 4.8 above shows that after removing crossing all the predictors at all the quantiles were seen to be significant. Showing that the increase in the sample size has a role to play in reducing crossing.

Table 4.9: Goodness of fit test result

Test Statistics	statistic	p-value
Cramer-Von Mises (With Crossing)	0.0465311	0.00
Cramer-Von Mises (Without Crossing)	0.098252	0.72433

We can see that the removal of the crossing resulted to a well specified model.

SAMPLE SIZE = 500

Number of observations that crossed: 0 (0%), the analysis shows that 0% of the observations has crossing somewhere in the domain with a cross index of 0.000713. This shows us that when the sample size is very large crossing is eliminated.

Table 4.10: Quantile regression coefficient results at different quantiles after removing crossing:

Quantiles	Coefficients	Estimate	std.err	z value	p(>|z|))
25%	Intercept	0.22442	0.06062	3.702	0.000214*
	β_1	2.51083	0.08875	28.291	< 2e-16*
	β_2	6.89674	0.15379	44.844	<2e-16*
50%	Intercept	0.6673	0.1685	3.96	7.5e-05*
	β_1	3.0750	0.1279	24.05	< 2e-16*
	β_2	6.6703	0.1870	35.67	< 2e-16*

75%	Intercept	1.3039	0.2549	5.116	3.12e-07*
	β_1	3.5608	0.1693	21.035	< 2e-16*
	β_2	6.7486	0.2995	22.534	< 2e-16*
95%	Intercept	2.5857	0.5098	5.072	3.94e-07*
	β_1	4.1522	0.2778	14.944	< 2e-16*
	β_2	7.4926	0.4412	16.984	<2e-16*

*Significant at 5% level of significance

From table 4.10, we can see that all of the covariates were significant at the P-value 0.05.

We also noticed that as the sample size increase the number of observations that crossed reduces significantly. With a sample size of 500, no crossing was observed at any point.

CONCLUSION

This paper investigated the effect of sample on crossing and also looked at how crossing affects model fitness. The analysis modeled the regression coefficients as parametric functions of the order of the quantile. This process removes crossing as was shown by Patto and Matteo (2016). In the analysis four different datasets were simulated with sample sizes 30, 50, 100 and 500. Using sample size of 30 with crossing all the predictors was seen to be insignificant and after crossing removal some of the predictors showed significant effects. There was an improvement when the sample size was increased to 50, even with crossing some predictors were seen to be significant and after removing crossing all the predictors were seen to be significant except the 95th quantile. For sample size 100, after the removal of crossing all the predictors were seen to significant and also at sample size of 500, there was no crossing at all. We also looked at the goodness of fit of the models and we discovered that without crossing the models were well specified while the presence of crossing produced models that were not well specified Based on the findings we can conclude that this work has been able to show that increase in sample size reduces crossing but with very large samples sizes crossing is totally eliminated. Also the work has been able to show that crossing affects the fit of a model by producing unspecified models while removal of crossing produces well specified model.

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