Quantile regression for compositional covariates

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Abstract

Quantile regression is a very important tool to explore the relationship between the response variable and its covariates. Motivated by mean regression with LASSO for compositional covariates proposed by Lin et al. (2014), we consider quantile regression with no-penalty and penalty function. We develop the computational algorithms based on linear programming. Numerical studies indicate that our methods provides the better alternative than mean regression under many settings, particularly for heavy-tailed or skewed distribution of the error term. Finally, we study the fat data using the proposed method.

Key words: compositional data; quantile regression; linear programming; mean regression; adaptive LASSO.

MSC2010 subject classifications: Primary 62J05; secondary 62J07.

1 Introduction

Compositional data are defined traditionally as constrained data, like proportions or percentages, with a fixed constant sum constraint (such as unit-sum constraint), which can find applications in a wide range of geology, sociology, economics, biology and so on (Shanmugam (2018)). Sometimes, we are especially interested in relative information, not the absolute values, such as geochemical compositions of rocks. Since the seminal work of Aitchison (1982), statistical methodologies have been proposed for compositional data analysis. However, owing to the special nature of compositional data, the usual linear regression model is inappropriate for our purposes. The linear log-contrast model of Aitchison and Bacon-Shone (1984) is a very common method for regression to deal with compositional data. To the best of authors' knowledge, statistical methods discussed mean regression. As we known, mean regression is not robust against outliers. For the testing problem, we address quantile regression in the paper.

Quantile regression is robust to outliers and heavy-tailed conditional error distributions. Moveover, it can provide a more complete picture than mean regression when the conditional distribution of the response variable is asymmetric. Hence, quantile regression has been applied in survival analysis, financial economics, investment analysis and so on (Koenker and Basseet (1978), Koenker and Geling (2001) and Yu et al. (2003)). Variable selection is an important issue in statistical modeling. In recent years, many different types of penalties have been introduced. Tibshirani (1996) proposed LASSO, which imposed the same penalty on every regression coefficient leading to excessive compression of larger coefficients. To tackle the problem, Fan and Li (2001) developed SCAD, which has three properties: unbiasedness, sparsity, continuity. Zou (2006) introduced the adaptive LASSO by using adaptive penalizing weights for different coefficients in the LASSO penalty, which

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meets above three properties. Besides, there are fused LASSO (Tibshirani et al. (2005)), elastic net (Zou and Hastie (2005)) and MCP (Zhang (2010)). We also refer to Wu and Liu (2009).

For compositional data, Lin et al. (2014) studied variable selection in mean regression by LASSO. However, this method is sensitive to outliers. When the error follows the heavy-tailed distribution or asymmetric distribution, it works not well. In this paper, we develop a novel method to overcome these difficulties via combining quantile regression with the adaptive LASSO penalty, showing the new algorithms based on linear programme.

The paper is organized as follows. In Section 2, we introduce the proposed methods of quantile regression and its variable selection, and give a method for selecting the tuning parameter. In Section 3, we present the computational algorithms. Simulation studies and an empirical example are presented in Section 4. The article concludes in Section 5.

2 Quantile regression for compositional data

Let (Y_i, X_i) be an observation collected from the subject (i = 1, ..., n), where $Y_i \in R$ is the response of interest, $X_i = (X_{i1}, ..., X_{ip})^{\top} \in R^p$ is the p-dimensional covariates lying in the (p-1)-dimensional positive simplex $S^{p-1} = \{(X_{i1}, ..., X_{ip}) | X_{ij} > 0, \sum_{j=1}^p X_{ij} = 1\}$. $Y = (Y_1, ..., Y_n)^{\top}$. We apply the log-ratio transformation of Aitchison (1982), and lead to the linear log-contrast model

$$Y = Z^p \beta_{\backslash p} + \varepsilon, \tag{1}$$

where $Z^p = \{\log(X_{ij}/X_{ip})\}$ is an $n \times (p-1)$ log-ratio matrix with the pth component as the reference component, $\beta_{\backslash p} = (\beta_1, \dots, \beta_{p-1})^{\top}$, ε is an n-vector of independent error term.

In the model (1), the reference component selection is not easy. As Lin et al. (2014), let $\beta_p = -\sum_{j=1}^{p-1} \beta_j$, the expression can be rewritten as

$$Y = Z\beta + \varepsilon, \quad \sum_{j=1}^{p} \beta_j = 0, \tag{2}$$

where $Z = \{\log x_{ij}\}_{n \times p} = (Z_1, \dots, Z_n)^{\top}, \ \beta = (\beta_1, \dots, \beta_p)^{\top}$. Note that the intercept is not included in the model, since it can be eliminated by centring the response and predictor variables. So, the estimator quantile regression is to minimize the following objective function

$$\arg\min_{\beta} \sum_{i=1}^{n} \rho_{\tau} (Y_i - Z_i^{\top} \beta),$$

$$s.t. \sum_{j=1}^{p} \beta_j = 0,$$
(3)

where $\rho_{\tau}(u) = u(\tau - I(u < 0))$ is called the check function. $\tau \in (0, 1)$ is the quantile, and $I(\cdot)$ is an indicative function. $\beta = (\beta_1, \dots, \beta_p)^{\top}$ is the unknown parameter vector.

Now, we consider quantile regression with the adaptive LASSO, which is motivated by the LASSO penalty mean regression proposed by Lin et al. (2014). As we known, the adaptive LASSO penalty function is a generalization of the LASSO penalty via adaptive weights. Hence, we consider the constrained optimization problem

$$\arg\min_{\beta} \left(\sum_{i=1}^{n} \rho_{\tau} (Y_i - Z_i^{\top} \beta) + \lambda \sum_{j=1}^{p} w_j |\beta_j| \right),$$

$$s.t. \sum_{j=1}^{p} \beta_j = 0,$$

$$(4)$$

where $w_j = \frac{1}{|\tilde{\beta}_j|^{\kappa}}$, and $\kappa > 0$. $\tilde{\beta}$ is the solution of model (3). Here, λ is the tuning parameter. As the suggestion of Zou (2006), we set $\kappa = 1$ in our paper.

In the problem (4), the tuning parameter is very important because the penalty method depends on the choice of it. We can use the BIC criterion to select the parameter λ (Wang et al. (2007)), which is defined as

$$BIC(\lambda_n) = \log\left(\sum_{i=1}^{n} \rho_{\tau}(Y_i - Z_i^{\top}\beta)\right) + \frac{\log n}{n} \times df$$

where df is the number of nonzero coefficients. The optimal regularization parameter $\lambda_{opt} = \arg\min_{\lambda_n} \mathrm{BIC}(\lambda_n)$.

3 Algorithms

From (3) and (4), they are the constrained optimization problems. First of all, we deal with quantile regression with the adaptive LASSO. Here, we give the computational algorithm, which introduces some slack variables replacing the objective function with an equality constraint so that (4) can be transformed into a linear programming problem.

Let $u_i = \max(0, Y_i - Z_i^{\top}\beta)$, $v_i = \max(0, -(Y_i - Z_i^{\top}\beta))$, $\beta_j^+ = \max(0, \beta_j)$, $\beta_j^- = \max(0, -\beta_j)$. $\beta_j = \beta_j^+ - \beta_j^-$ and $|\beta_j| = \beta_j^+ + \beta_j^-$. $w = (w_1, \dots, w_p)^{\top}$. By the expressions of slack variables, (4) can be re-expressed as

$$\begin{split} &\sum_{i=1}^{n} \rho_{\tau}(Y_{i} - Z_{i}^{\top}\beta) + \lambda \sum_{j=1}^{p} w_{j} |\beta_{j}| \\ &= \sum_{i=1}^{n} \left(\tau u_{i} + (1-\tau)v_{i}\right) + \lambda \sum_{j=1}^{p} w_{j} (\beta_{j}^{+} + \beta_{j}^{-}) \\ &= \tau I_{n}^{\top} u + (1-\tau) I_{n}^{\top} v + \lambda w^{\top} \beta^{+} + \lambda w^{\top} \beta^{-} \\ &= (\lambda w^{\top}, \lambda w^{\top}, \tau I_{n}^{\top}, (1-\tau) I_{n}^{\top}) ((\beta^{+})^{\top}, (\beta^{-})^{\top}, u^{\top}, v^{\top})^{\top} \\ &= A\gamma \end{split}$$

Here $u = (u_1, \dots, u_n)^{\top}$ and $v = (v_1, \dots, v_n)^{\top}$. $\beta^+ = (\beta_1^+, \dots, \beta_p^+)^{\top}$ and $\beta^- = (\beta_1^-, \dots, \beta_p^-)^{\top}$. I_n denotes the n-vector of ones. $A = (\lambda w^{\top}, \lambda w^{\top}, \tau I_n^{\top}, (1-\tau)I_n^{\top})$ and $\gamma = ((\beta^+)^{\top}, (\beta^-)^{\top}, u^{\top}, v^{\top})^{\top}$. The constrained condition is

$$Y - Z\beta = u - v$$

Elementary calculations show that

$$\begin{bmatrix} Z & -Z & E_n & -E_n \end{bmatrix} \begin{bmatrix} \beta^+ \\ \beta^- \\ u \\ v \end{bmatrix} = Y$$

where E_n denotes the $n \times n$ identity matrix.

Let

$$B = \begin{bmatrix} I_p^\top & -I_p^\top & 0_n^\top & -0_n^\top \\ Z & -Z & E_n & -E_n \end{bmatrix}$$

and

$$H = (0, Y^{\top})^{\top}.$$

where 0_n denotes the *n*-vector of zeros. Combined with $\sum_{j=1}^p \beta_j = 0$, the constrained optimization problem (4) can be transformed into a linear programming problem

$$\min A\gamma$$

$$s.t.B\gamma = H$$

Similarly, quantile regression without penalty model (3) can also transform into a linear programming problem

$$\min A_1 \gamma_1$$

$$s.t. B_1 \gamma_1 = H_1$$

where $A_1 = (0_n^{\top}, 0_n^{\top}, \tau I_n^{\top}, (1 - \tau) I_n^{\top}), B_1 = B, \gamma_1 = \gamma, \text{ and } H_1 = H.$

4 Numerical studies

4.1 Simulations

As Lin et al. (2014), we generate the covariate data in the following way. We first generate an $n \times p$ data matrix $O = (o_{ij})$ from a multivariate normal distribution $N_p(\mu, \Sigma)$, and then obtain the covariate matrix $X = (x_{ij})$, where $x_{ij} = \exp(o_{ij}) / \sum_{k=1}^{p} \exp(o_{ik})$. Here $\mu = (\mu_1, \dots, \mu_p)^{\top}$. We repeat 500 times for each setting. The error term ε is generated from five distributions.

Case 1. $\varepsilon \sim N(0,1)$.

Case 2. $\varepsilon \sim t(3)$, which is symmetric and heavy-tail distribution.

Case 3. $\varepsilon \sim pareto(2,1)$, which is the heavy-tail distribution.

Case 4. $\varepsilon \sim gpd(0.2, 0, 1.2)$, which is the skewed distribution.

Case 5. $\varepsilon \sim gev(0.2, 3, 1.5)$, which is the extreme value distribution, and the skewed distribution.

In Example 1, we examine the performance of mean regression (MR) and quantile regression (QR, $\tau=0.5$). In Example 2, we conduct the Monte Carlo comparisons for variable selection.

Example 1. Let

$$\mu_j = \begin{cases} \log(0.5 * p), & j = 1, 2, 3 \\ 0, & \text{others} \end{cases}$$

and $\Sigma = \rho^{|i-j|}$ with $\rho = 0.2$. We set $n = \{50, 100, 200, 500\}$, and generate the responses according to model (2) with $\beta = (1, -0.8, 0.6, -1.5, -0.5, 1.2)^{\top}$. We evaluate the performance through the following two criteria:

(1)
$$b_j = \frac{1}{500} \sum_{m=1}^{500} |\hat{\beta}_j^{(m)} - \beta_j|$$

(2)
$$L_1 = \frac{1}{500} \sum_{m=1}^{500} \sum_{j=1}^{p} |\hat{\beta}_j^{(m)} - \beta_j|$$

Here $\hat{\beta}_{j}^{(m)}$ is the estimator of β_{j} based on the m-th sample. We compare the performance of quantile regression (QR) with mean regression (MR).

Table 1 summarizes the simulation results. We can draw the following conclusions:

- (1) When the error distribution follows the normal distribution, MR is slightly better than QR. As the sample size increases, the differences between them are decreasing.
- (2) When the error distribution is the heavy-tailed or skewed, QR performs better than MR since these distributions have outliers.

Table 1: Simulation results for Example 1

Distribution	n	Method	b_1	b_2	b_3	b_4	b_5	b_6	L_1
N(0,1)	50	MR	0.114	0.118	0.118	0.118	0.119	0.114	0.701
		QR	0.143	0.149	0.142	0.148	0.145	0.143	0.870
	100	MR	0.074	0.079	0.083	0.082	0.082	0.077	0.477
		QR	0.095	0.101	0.105	0.105	0.099	0.098	0.603
	200	MR	0.054	0.057	0.058	0.057	0.056	0.054	0.336
		QR	0.070	0.071	0.074	0.072	0.069	0.068	0.424
	500	MR	0.033	0.035	0.034	0.036	0.037	0.034	0.209
		QR	0.040	0.044	0.043	0.044	0.045	0.042	0.259
t(3)	50	MR	0.186	0.191	0.196	0.200	0.202	0.184	1.159
		QR	0.157	0.167	0.172	0.173	0.166	0.160	0.995
	100	MR	0.128	0.133	0.133	0.139	0.143	0.128	0.803
		QR	0.110	0.114	0.112	0.113	0.115	0.110	0.674
	200	MR	0.090	0.090	0.092	0.095	0.097	0.088	0.553
		QR	0.075	0.076	0.077	0.077	0.078	0.074	0.457
	500	MR	0.056	0.058	0.060	0.058	0.062	0.060	0.355
		QR	0.047	0.048	0.049	0.047	0.049	0.047	0.287
pareto(2,1)	50	MR	0.198	0.212	0.217	0.221	0.219	0.193	1.261
		QR	0.077	0.083	0.084	0.080	0.084	0.078	0.486
	100	MR	0.162	0.169	0.173	0.166	0.168	0.160	0.999
		QR	0.050	0.053	0.053	0.054	0.053	0.053	0.317
	200	MR	0.128	0.130	0.129	0.130	0.134	0.128	0.779
		QR	0.037	0.039	0.040	0.039	0.039	0.036	0.231
	500	MR	0.079	0.091	0.084	0.081	0.086	0.083	0.506
		QR	0.024	0.025	0.025	0.025	0.025	0.024	0.147
gpd(0.2, 0, 1.2)	50	MR	0.209	0.217	0.224	0.217	0.210	0.206	1.284
		QR	0.147	0.154	0.155	0.162	0.156	0.149	0.924
	100	MR	0.141	0.150	0.146	0.148	0.143	0.140	0.868
		QR	0.099	0.109	0.107	0.109	0.104	0.104	0.632
	200	MR	0.104	0.105	0.111	0.107	0.113	0.102	0.641
		QR	0.071	0.075	0.076	0.075	0.078	0.073	0.448
	500	MR	0.064	0.070	0.068	0.067	0.068	0.068	0.404
		QR	0.045	0.049	0.048	0.048	0.049	0.045	0.285
gev(0.2, 3, 1.5)	50	MR	0.291	0.316	0.323	0.318	0.314	0.312	1.874
		QR	0.255	0.272	0.279	0.286	0.271	0.264	1.627
	100	MR	0.200	0.213	0.216	0.210	0.217	0.213	1.270
		QR	0.166	0.188	0.191	0.191	0.186	0.186	1.109
	200	MR	0.146	0.150	0.152	0.157	0.158	0.137	0.900
		QR	0.128	0.133	0.134	0.128	0.134	0.125	0.781
	500	MR	0.093	0.097	0.096	0.097	0.097	0.093	0.573
		QR	0.082	0.085	0.081	0.085	0.084	0.079	0.495

Example 2. Let

$$\mu_j = \begin{cases} \log(0.5 * p), & j = 1, \dots, 5 \\ 0, & \text{others} \end{cases}$$

and $\beta = (1, -0.8, 0.6, 0, 0, -1.5, -0.5, 1.2, 0, \dots, 0)^{\top}$. We set $(n, p) = \{(50, 10), (100, 10), (100, 20), (200, 20)\}$. To summarize the variable selection results and evaluate estimation accuracy, we consider the following criteria:

(1) TP: the average number of true positives, which denotes the average number of the true zero correctly set to zero.

- (2) TN: the average number of true negatives, which denotes the average number of the true nonzero correctly set to nonzero.
- (3) FP: the average number of false positives, which denotes the average number of the true zero incorrectly set to nonzero.
- (4) FN: the average number of false negetives, which denotes the average number of the true nonzero incorrectly set to zero.

We compare three method: quantile regression with adaptive LASSO (QR-ALA, $\tau = 0.5$), mean regression with LASSO (MR-LA) and adaptive LASSO (MR-ALA). The other settings are the same as Example 1.

From Tables 2 and 3, we can get the following comments:

- (1) From L_1 , QR-ALA is better than MR-LA and MR-ALA, especially for the heavy-tail or skewed distribution. Even if N(0,1), QR-ALA is still slightly better, which implies that QR-ALA is more accurate. The performances of three methods increase gradually with n.
- (2) For variable selection, QR-ALA and MR-ALA outperform than MR-LA, which is more inclined to set zero coefficients to nonzero since FP is very large. When the error term follows the normal distribution, MR-ALA is better than QR-ALA. However, when the error term follows other distributions, QR-ALA is superior to MR-ALA, which clearly indicates that the proposed method is more efficient.

Table 2: Simulation results for Example 2 (Cases 1–2)

Distribution	(n, p)	Method	L_1	TP	TN	FP	FN
N(0, 1)	(50, 10)	MR-LA	1.197	5.952	2.318	1.682	0.048
, , ,	,	MR-ALA	1.245	5.770	3.856	0.144	0.230
		QR-ALA	1.160	5.740	3.598	0.402	0.260
	(100, 10)	MR-LA	0.915	5.996	2.596	1.404	0.004
		MR-ALA	1.047	5.952	3.988	0.012	0.048
		QR-ALA	0.728	5.968	3.752	0.248	0.032
	(100, 20)	MR-LA	1.251	5.998	11.154	2.846	0.002
		MR-ALA	1.048	5.936	13.930	0.070	0.064
		QR-ALA	0.832	5.950	13.488	0.512	0.050
	(200, 20)	MR-LA	0.850	6.000	11.478	2.522	0.000
		MR-ALA	0.943	5.990	13.998	0.002	0.010
		QR-ALA	0.511	6.000	13.724	0.276	0.000
t(3)	(50, 10)	MR-LA	2.139	5.242	2.558	1.442	0.758
		MR-ALA	1.934	4.920	3.626	0.374	1.080
		QR-ALA	1.648	5.110	3.702	0.298	0.890
	(100, 10)	MR-LA	1.502	5.750	2.746	1.254	0.250
		MR-ALA	1.426	5.472	3.838	0.162	0.528
		QR-ALA	0.840	5.878	3.832	0.168	0.122
	(100, 20)	MR-LA	2.125	5.418	11.964	2.036	0.582
		MR-ALA	1.525	5.330	13.566	0.434	0.670
		QR-ALA	1.029	5.812	13.518	0.482	0.188
	(200, 20)	MR-LA	1.492	5.910	12.034	1.966	0.090
		MR-ALA	1.098	5.848	13.816	0.184	0.152
		QR-ALA	0.586	5.988	13.818	0.182	0.012

Table 3: Simulation results for Example 2 (Cases 3–5)

Distribution	(n, p)	Method	L_1	TP	TN	FP	FN
pareto(2,1)	(50, 10)	MR-LA	2.162	5.132	2.394	1.606	0.868
1 () /	, ,	MR-ALA	2.193	4.992	3.538	0.462	1.008
		QR-ALA	0.640	5.898	3.824	0.176	0.102
	(100, 10)	MR-LA	1.643	5.472	2.514	1.486	0.528
		MR-ALA	1.750	5.344	3.702	0.298	0.656
		QR-ALA	0.345	6.000	3.956	0.044	0.000
	(100, 20)	MR-LA	2.335	5.046	11.156	2.844	0.954
		MR-ALA	1.959	5.048	13.278	0.722	0.952
		QR-ALA	0.415	5.998	13.844	0.156	0.002
	(200, 20)	MR-LA	1.921	5.382	10.794	3.206	0.618
		MR-ALA	1.582	5.438	13.548	0.452	0.562
		QR-ALA	0.270	6.000	13.940	0.060	0.000
gpd(0.2, 0, 1.2)	(50, 10)	MR-LA	2.235	5.210	2.382	1.618	0.790
		MR-ALA	2.241	4.772	3.560	0.440	1.228
		QR-ALA	1.470	5.356	3.732	0.268	0.644
	(100, 10)	MR-LA	1.621	5.702	2.312	1.688	0.298
		MR-ALA	1.665	5.242	3.778	0.222	0.758
		QR-ALA	0.806	5.896	3.844	0.156	0.104
	(100, 20)	MR-LA	2.500	4.972	10.716	3.284	1.028
		MR-ALA	1.894	5.074	13.314	0.686	0.926
		QR-ALA	0.967	5.860	13.554	0.446	0.140
	(200, 20)	MR-LA	1.851	5.608	9.502	4.498	0.392
		MR-ALA	1.347	5.654	13.680	0.320	0.346
		QR-ALA	0.577	6.000	13.748	0.252	0.000
gev(0.2, 3, 1.5)	(50, 10)	MR-LA	3.186	4.350	2.532	1.468	1.650
		MR-ALA	3.355	3.956	3.162	0.838	2.044
		QR-ALA	2.779	3.940	3.696	0.304	2.060
	(100, 10)	MR-LA	2.409	5.008	2.510	1.490	0.992
		MR-ALA	2.560	4.234	3.620	0.380	1.766
		QR-ALA	1.759	4.996	3.826	0.174	1.004
	(100, 20)	MR-LA	3.500	4.732	9.034	4.966	1.268
		MR-ALA	2.919	3.996	12.762	1.238	2.004
		QR-ALA	2.056	4.946	13.358	0.642	1.054
	(200, 20)	MR-LA	2.477	5.566	8.206	5.794	0.434
		MR-ALA	2.031	4.666	13.682	0.318	1.334
		QR-ALA	1.239	5.732	13.468	0.532	0.268

4.2 Application

In this section, to illustrate the usefulness of the proposed procedure, we apply the proposed method in the dataset fat, which contains many physical measurements of 252 males can be found in R package "UsingR". Body.fat is the response variable. The following X-variables are used as covariates: neck (circumference), chest (circumference), abdomen (circumference), hip (circumference), thigh (circumference), knee (circumference), ankle (circumference), bicep (circumference), forearm (circumference) and wrist (circumference). We transform covariates into compositional data. As the suggestion of

Shanmugam (2018), $Y = \log (\text{body.fat}/(100 - \text{body.fat}))$. There are 251 observations after removing suspicious observations. Here, the ten-fold cross-validation method is used to select the tuning parameter. To evaluate the performance of MR-ALA and QR-ALA, we divide the data set into a test set and a training set, 9 copies as the training set, and 1 copy as the test set at random. We repeat 100 simulations and use NMSE to compare two methods. NMSE is defined by

$$NMSE = \frac{\sum (Y_i - \hat{Y}_i)^2}{\sum (Y_j - \overline{Y})^2}.$$

where \overline{Y} is the mean of the response variable, \hat{Y}_i is the predictive value of the test data set using the model obtained from the training set.

As Table 4, NMSE of QR-ALA is less than MR-ALA whether it is the raw data or transformed compositional data, which QR-ALA is better than that MR-ALA since there are outliers in the dataset fat. It is surprised that the performances of the two methods with compositional data are better than the corresponding models with original data, which implies this transform may be necessary and meaningful in application.

Table 4: NMSE for dataset fat

	MR-ALA	QR-ALA
Original data	0.426	0.376
Compositional data	0.424	0.353

5 Discussion

In this paper, we study quantile regression with compositional data, and propose penalized quantile regression with the adaptive-LASSO penalty function. Due to linear programming, the proposed of the algorithm works not well when dimension p is much larger than sample size n. This problem may be achieved by ADMM Yu and Lin (2017) proposed. We will study it in our future research.

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