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Quasi-Likelihood Ratio Tests for Homoscedasticity in Linear Regression

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Two quasi-likelihood ratio tests are proposed for the homoscedasticity assumption in the linear regression models. They require few assumptions than the existing tests. The properties of the tests are investigated through simulation studies. An example is provided to illustrate the usefulness of the new proposed tests.

Keywords: Bootstrap, homoscedasticity test, quasi-likelihood, regression model, variance function

Introduction

Homoscedasticity or constant variance is a standard assumption in regression models. The violation of this assumption can lead to inefficient estimation or incorrect inference (Ruppert et al., 2003). Former research studied homoscedasticity tests in different parametric and nonparametric regression models. For the linear regression model, Cook and Weisberg (1983) proposed a score test statistic for parametric variance functions; Breusch and Pagan (1979) proposed a Lagrange multiplier test for a fairly wide class of alternative hypotheses; Diblasi and Bowman (1997) constructed a nonparametric test of constant variance. All of them require the assumption that the errors have the normal distribution. Koenker (1981) proposed a variant of the Breusch-Pagan test by relaxing the normality assumption, but the alternative hypotheses still cannot include all of the possible heteroscedastic models.

For nonparametric regression models, Eubank and Thomas (1993), Müller and Zhao (1995), respectively, presented tests for nonparametric and semi-parametric variance functions under the assumption of normal distributed errors; Dette and Munk (1998), Dette (2002), Liero (2003), and Wang and Zhou (2005) developed tests by comparing variance estimators under two hypotheses under the Lipschitz continuous assumption; Francisco-Fernández and Vilar-Fernández (2008) proposed two new tests based on nonparametric smoothing; Dette et al. (2007) and Dette and Hetzler (2008) considered tests of a parametric form of conditional variance. For partially linear regression models, You and Chen (2005), Lin and Qu (2012), respectively, presented heteroscedasticity tests based on the research of Dette and Munk (1998) and Dette (2002); Dette and Marchlewski (2008) considered testing a parametric form of the conditional variance.

Linear regression models are the most popular models. The homoscedasticity tests for linear models in the literature referenced above require assumptions, such as normality and parametric variance functions. These assumptions greatly restrict their applications to real data analysis.

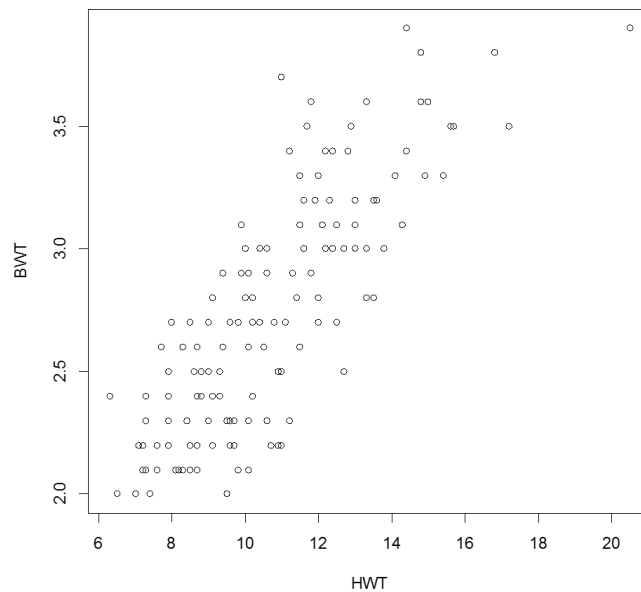


Figure 1. Scatter plot of BWT versus HWT

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As an example, consider the Cats data in MASS package in R. 144 adult [over 2kg (kilograms) in weight] cats used for experiments with the drug digitalis had their heart in g (grams) and body weight in kg recorded. The interest is if the heart weight (HWT) is associated with the body weight (BWT) for cats. A scatter plot of BWT versus HWT is given in Figure 1, which indicates a linear relationship. A linear regression line can be fit to investigate their association. However, the variances of the observations may be different. In order to choose appropriate inference methods to obtain efficient estimation or correct inference, check the homoscedasticity assumption for the linear regression model. Shown in Figure 1. the variances are larger for the middle response values than small and large response values. This suggests the researchers to consider the variance as a function of the mean. However, it is hard to specify the form of the variance function, which is required by the existing homoscedasticity tests for the linear regression model. As will be shown, if the true variance function is not in the specified alternative, the test is not reliable, i.e., cannot maintain the probability of the type-I error and has low power. Therefore, in order to obtain the reliable test results, homoscedasticity tests are proposed in which the alternative hypothesis includes all possible heteroscedastic models, for the linear regression model.

Two powerful quasi-likelihood ratio tests are proposed for linear regression models with minimum assumptions, that is, they do not require a known distribution and specific variance function forms of the data. This is achieved due to the good properties of quasi-likelihood. As shown in Wedderburn (1974), the quasi-likelihood has similar properties as the log-likelihood function. It only requires assumptions on the first two moments which is much easier to postulate than the entire distribution of the data. Due to these properties, quasi-likelihood ratio tests have the potential to achieve high power but require fewer assumptions. In addition, these tests can be easily extended to more complex models, such as partially linear models and nonparametric models, with minimum assumptions.

Two Quasi-Likelihood Ratio Tests for Homoscedasticity

Consider the linear model

$$y_i = \mu_i + \varepsilon_i, \quad i = 1, \dots, n \quad (1)$$

where ε_i are identically and independently distributed with mean zero and unknown variances $\sigma^2(\mu_i)$; y_i has mean $\mu_i = \mathbf{X}_i^T \boldsymbol{\beta}$ where \mathbf{X}_i is a p -dimensional vector of known

constants and $\boldsymbol{\beta}$ is a vector of parameters. The homoscedasticity test for model (1) is to test if the variance $\sigma^2(\mu_i)$ is constant.

$$\begin{aligned} H_0 : \sigma^2(\mu_i) &= \sigma^2 \text{ for } i = 1, \dots, n \\ H_1 : \sigma^2(\mu_i) &\neq \sigma^2 \text{ for at least one } i = 1, \dots, n \end{aligned}$$

for some unknown positive constant σ^2 .

First Test: Quasi-Likelihood Ratio Test

Quasi-likelihood proposed by Wedderburn (1974) is defined as follows:

$$Q = \frac{1}{n} \sum_{i=1}^n \int_{y_i}^{\mu_i} \frac{y_i - a}{\sigma^2(a)} da. \quad (2)$$

In (2), it is assumed the variance is a function of the mean, but the form of the variance function is not specified. Therefore, few assumptions are required for the proposed tests based on the quasi-likelihood. The score function of the quasi-likelihood (2) is derived as its first derivative as

$$\mathbf{U}_{\boldsymbol{\beta}} = \frac{1}{n} \sum_{i=1}^n \mathbf{X}_i^T (y_i - \mathbf{X}_i^T \boldsymbol{\beta}) / \sigma^2(\mu_i).$$

Wedderburn (1974) showed that quasi-likelihood (2) has similar properties to the log-likelihood. Then the test statistic is constructed as

$$QLR_1 = -2(Q_0 - Q_1),$$

where Q_0 is the quasi-likelihood function under H_0 and Q_1 is the quasi-likelihood function under H_1 . Next, we will explain how to calculate these quasi-likelihood functions.

To calculate Q_0 under H_0 (i.e., the data are homoscedasticity), we estimate $\boldsymbol{\beta}$ by the least squares estimator $\tilde{\boldsymbol{\beta}}$ for model (1). Then we calculate $\tilde{\mu}_i = \mathbf{X}_i^T \tilde{\boldsymbol{\beta}}$ and $\tilde{\sigma}^2 = 1/n \sum_{i=1}^n (y_i - \tilde{\mu}_i)^2$. Therefore, the quasi-likelihood under H_0 can be calculated as

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$$Q_0 = \frac{1}{n} \sum_{i=1}^n \int_{y_i}^{\hat{\mu}_i} \frac{y_i - a}{\hat{\sigma}^2} da.$$

To calculate Q_1 under H_1 (i.e., the data are heteroscedasticity), we first estimate $\boldsymbol{\beta}$ by maximizing the quasi-likelihood (2), which is same as solving the score function $\mathbf{U}_{\boldsymbol{\beta}} = 0$. In $\mathbf{U}_{\boldsymbol{\beta}}$, we approximate the variance function $\sigma^2(\mu_i)$ as a spline function. Specifically, the variance function is approximated by a basis expansion

$$\sigma^2(\mu_i) = \sum_{j=1}^J \mathbf{B}_j(\mu_i) \gamma_j,$$

where J is the number of B -spline basis functions, $\mathbf{B}_j, j = 1, \dots, J$, are the B -spline basis functions (De Boor, 2001) and $\gamma_j, j = 1, \dots, J$, are unknown spline coefficients to be estimated. The number J is determined by the degree of the splines and the number of knots, the choices of which will be introduced in the following algorithm. Then the score function is approximated by

$$\tilde{\mathbf{U}}_{\boldsymbol{\beta}} = \frac{1}{n} \frac{\sum_{i=1}^n \mathbf{X}_i^T (y_i - \mu_i)}{\sum_{j=1}^J \mathbf{B}_j(\mu_i) \gamma_j},$$

which is a function of μ_i . Therefore, the estimator $\hat{\boldsymbol{\beta}}$ is the solution of $\tilde{\mathbf{U}}_{\boldsymbol{\beta}} = 0$. We use the following algorithm to obtain $\hat{\boldsymbol{\beta}}$ and calculate the quasi-likelihood under H_1 :

- (1) Initialize the variances with $\hat{\sigma}^{2(0)}(\mu_i) = 1$.
- (2) At the $(k + 1)^{\text{th}}$ step,
 - (a) For the given variance $\hat{\sigma}^{2(k)}(\mu_i)$, the parameter estimates $\hat{\boldsymbol{\beta}}^{(k+1)}$ are obtained by maximizing the quasi-likelihood (2) using the Newton-Raphson with scoring method.
 - (b) For given $\hat{\boldsymbol{\beta}}^{(k+1)}$, calculate $\hat{\mu}_i = \mathbf{X}_i^T \hat{\boldsymbol{\beta}}^{(k+1)}$ and the basis expansions $\mathbf{B}_j(\hat{\mu}_i)$. Then the estimators $\hat{\gamma}_j$ of γ_j are obtained by the least squares method for the following model:

$$\hat{\varepsilon}_i^2 = \sum_{j=1}^J \mathbf{B}_j(\hat{\mu}_i) \gamma_j + \phi_i,$$

where $\hat{\varepsilon}_i^2 = (y_i - \hat{\mu}_i)^2$ are the 'observed' values of the variances $\sigma^{2(k+1)}(\mu_i)$ and $\phi_i, i = 1, \dots, n$, are error terms with mean zero and constant variance. Now $\sigma^{2(k+1)}(a)$ is calculated by $\hat{\sigma}^{2(k+1)}(a) = \sum_{j=1}^J \mathbf{B}_j(a) \hat{\gamma}_j$, where $J = n_{\text{knots}} + d - 1$ and n_{knots} and d are the number of knots and the degree of the spline, respectively. In the algorithm, we use a cubic B -spline, so $d = 3$, and the `bs` function in R software is used to choose the quantiles as knots for a given number of knots. The number of knots is varied in the range from 1 to 15, out of which we select the one that minimizes the Akaike-like (AIC-like) criterion (Yu & Peace, 2012)

$$\text{AIC-like} = \sum_{i=1}^n \frac{y_i - \hat{\mu}_i}{\hat{\sigma}^{2(k+1)}(\hat{\mu}_i)} + 2(n_{\text{knots}} + d - 1).$$

- (c) Repeat Steps (a)-(b) until $|\hat{\boldsymbol{\beta}}^{(k+1)} - \hat{\boldsymbol{\beta}}^{(k)}| < l |\hat{\boldsymbol{\beta}}^{(k+1)}|$, where l is the prespecified convergence criterion. The converged estimators are $\hat{\boldsymbol{\beta}}$ and the corresponding variance estimators are $\hat{\sigma}^2(\cdot)$. Chiou and Müller (1999) proved that under regularity conditions, both $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}^2(\cdot)$ are consistent estimators.
- (3) The quasi-likelihood under H_1 is calculated as

$$Q_1 = \frac{1}{n} \sum_{i=1}^n \int_{y_i}^{\hat{\mu}_i} \frac{y_i - a}{\hat{\sigma}^2(a)} da.$$

Now we are ready to calculate the quasi-likelihood ratio test statistic as

$$QLR_1 = -2 \times \frac{1}{n} \left(\sum_{i=1}^n \int_{y_i}^{\hat{\mu}_i} \frac{y_i - a}{\tilde{\sigma}^2} da - \sum_{i=1}^n \int_{y_i}^{\hat{\mu}_i} \frac{y_i - a}{\hat{\sigma}^2(a)} da \right).$$

Second Test: Modified Quasi-Likelihood Ratio Test

A modified quasi-likelihood is proposed:

$$Q^* = \frac{1}{n} \sum_{i=1}^n \int_{y_i}^{\mu_i} \frac{y_i - a}{\sigma^2(\mu_i)} da. \quad (3)$$

It is easy to see that (3) has the same first derivative as (2). In other words, (3) and (2) have the same score functions. Then (3) has similar properties to the log likelihoods as well based on the Theorem 1 in Wedderburn (1974, p. 440). Therefore, it can be used to construct likelihood ratio test as well. Moreover, the estimators of β are same by maximizing (3) or (2) because they have the same score functions.

The motivation of the modified quasi-likelihood is that it has the same value under H_0 as (2). In addition, the calculation for (3) is much less time consuming than the calculation for (2). First, we only need to calculate the variances at $\hat{\mu}_i$ values for (3) but need to calculate all values in the integral for (2). Second, the integration of (3) has a closed form. However, (2) does not have a closed form and we need approximations in the calculation.

The test statistic based on (3) is constructed as

$$QLR^* = -2(Q_0^* - Q_1^*),$$

where Q_0^* is the modified quasi-likelihood function under H_0 and Q_1^* is the modified quasi-likelihood function under H_1 . Because the estimators of β based on (3) are same as those based on (2) under both H_0 and H_1 , use the same procedures to estimate the β and $\sigma^2(\mu_i)$. Then

$$Q_0^* = Q_0 = \frac{1}{n} \sum_{i=1}^n \int_{y_i}^{\tilde{\mu}_i} \frac{y_i - a}{\tilde{\sigma}^2} da$$

and

$$Q_1^* = \frac{1}{n} \sum_{i=1}^n \int_{y_i}^{\tilde{\mu}_i} \frac{y_i - a}{\hat{\sigma}^2(\hat{\mu}_i)} da.$$

The quasi-likelihood ratio test statistic is

$$\begin{aligned} QLR_2 &= -2 * \frac{1}{n} \left(\sum_{i=1}^n \int_{y_i}^{\tilde{\mu}_i} \frac{y_i - a}{\tilde{\sigma}^2} da - \sum_{i=1}^n \int_{y_i}^{\hat{\mu}_i} \frac{y_i - a}{\hat{\sigma}^2(\hat{\mu}_i)} da \right) \\ &= \frac{1}{n} \left(\frac{1}{\tilde{\sigma}^2} \sum_{i=1}^n (y_i - \tilde{\mu}_i)^2 - \sum_{i=1}^n \frac{1}{\hat{\sigma}^2(\hat{\mu}_i)} (y_i - \hat{\mu}_i)^2 \right) \end{aligned}$$

Remark. Comparing QLR_1 and QLR_2 , we see that the only difference between them is the denominator $\hat{\sigma}^2(\cdot)$ of quasi-likelihood under H_1 . For different patterns of the variance functions, either one of the proposed tests can be more powerful than the other one.

Bootstrap Procedure for the Critical Values of the Test

Because the quasi-likelihood has the properties of log likelihood, the proposed quasi-likelihood ratio tests follow the Chi-square distribution based on the theory of the likelihood ratio tests. However, it is well known that for nonparametric smoothing tests, the asymptotic theory does not provide accurate approximations to the distribution of the test statistic when the sample size is small or moderate (Hardle & Mammen, 1993). Alternatively, bootstrap method is often used to approximate the distribution of the test statistic. Therefore, a similar bootstrap procedure as in Wang and Zhou (2005) is proposed to approximate the critical values of the tests in practical applications. The bootstrap procedure is proposed as follows. Denote B as the sufficient large number of bootstrapping. Therefore, for $b = 1, \dots, B$,

- (1) For $i = 1, \dots, n$, let $y_{i,b}^* = \mathbf{X}_i^T \tilde{\boldsymbol{\beta}} + \varepsilon_i^*$, where ε_i^* is a bootstrap sample from centered $\tilde{\varepsilon}_i = (y_i - \tilde{\mu}_i)$.
- (2) With the bootstrap sample $\left\{ (\mathbf{X}_i, y_{i,b}^*), i = 1, \dots, n \right\}$, calculate QLR_{1b} and QLR_{2b} for each bootstrapping sample using the new proposed methods.
- (3) Let $QLR_{1\eta}$ be the η^{th} order statistic of $QLR_{11}, \dots, QLR_{1B}$; then $QLR_{1|(1-\alpha)B|}$ approximates the $(1 - \alpha)$ -quantile of the distribution of QLR_1 under the null hypothesis. Similarly, calculate $QLR_{2|(1-\alpha)B|}$ to approximate the $(1 - \alpha)$ -quantile of the distribution of QLR_2 under the null hypothesis.

Simulations

The performance of the proposed tests is investigated for finite samples. Compare the two quasi-likelihood ratio tests with the parametric score test proposed by Cook and Weisberg (CW test) (Cook & Weisberg, 1983), the Breusch-Pagan test (BP test) (Breusch & Pagan, 1979), and its variant proposed by Koenker (VBP test) (Koenker, 1981). These tests require assumptions, such as normal error and some specific functional forms of the variance.

Evaluate Size (Type-I Error) of the Test

Homoscedastic data is generated under H_0 from $y_i = 1 + x_i + \varepsilon_i$, where the x_i are generated from the standard normal distribution. Consider two different distributions for ε_i : the standard normal distribution $[N(0, 1)]$, and the t distribution with 4 degree of freedom $[t(4)]$. Sample sizes are 70 and 100. The test is calculated with 1000 simulation runs for each scenario and nominal level 0.05. We use $B = 500$ bootstrap samples per run to obtain the critical values. The results are summarized in Table 1 and it can be seen that the proposed tests maintain the specified nominal level satisfactory. For CW and BP tests, when the error term follows t distribution, the probability of type-I errors is much higher or lower than the nominal level 0.05. Clearly, CW and BP tests are not robust. However, VBP test is robust for the non-normal distributed data.

Empirical Power of the Test

In order to investigate the power of the tests, consider two alternatives:

$$\text{Alternative I: } y_i = 1 + x_i + 0.5\exp(2x_i)\varepsilon_i$$

$$\text{Alternative II: } y_i = 1 + x_i + 0.5[1 + \sin(3x_i)]\varepsilon_i$$

where both x_i and ε_i are generated from the standard normal distribution. Table 2 summarizes the results. Alternative I satisfies all of the assumptions required by the CW, BP, and VBP tests, and they are more powerful than the quasi-likelihood ratio tests. However, in alternative II, the true form of the variance function does not fit the general formulation of the alternative hypotheses in the CW, BP, and VBP tests, and their powers are much lower than the new proposed quasi-likelihood ratio tests. The power of the quasi-likelihood ratio tests is satisfactory. The first quasi-likelihood ratio test is more powerful than the second test for alternative I, but less powerful for alternative II. Although the classical tests are powerful against the

Table 1. Empirical size of the tests

N		N(0, 1)	t(4)
70	Test I	0.045	0.040
	Test II	0.054	0.067
	CW	0.051	0.170
	BP	0.051	0.170
	VBP	0.044	0.052
100	Test I	0.038	0.049
	Test II	0.063	0.047
	CW	0.044	0.193
	BP	0.044	0.193
	VBP	0.044	0.050

Table 2. Empirical power of the tests

N		Alternative I	Alternative II
70	Test I	0.548	0.570
	Test II	0.355	0.964
	CW	1.000	0.179
	BP	1.000	0.179
	VBP	1.000	0.041
100	Test I	0.588	0.848
	Test II	0.464	0.981
	CW	1.000	0.178
	BP	1.000	0.178
	VBP	1.000	0.043

specified alternative, they may have very low power if the true variance forms are not in the specified direction. However, the new proposed quasi-likelihood tests have satisfactory powers for different true variance forms because they include all possible variance forms in the alternative hypothesis.

Cats Data Analysis

The usefulness of the new quasi-likelihood ratio tests is illustrated on the Cats data, which is introduced in the Introduction section. The intent is to investigate if the heart weight (HWT) is associated with the body weight (BWT) for cats. Scatter plot (Figure 1) shows the linear relationship between BWT and HWT. Therefore, the following linear regression model is fitted to the data:

$$BWT_i = \beta_0 + \beta_1 HWT_i + \varepsilon_i, \tag{4}$$

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where ε_i is the error term with mean zero and variance $\sigma^2(\mu_i)$ and $\mu_i = \beta_0 + \beta_1 HWT_i$. First, we check the normality assumption of the data. Q-Q plot (Figure 2) shows that the data satisfies the normality assumption. In order to see the variance form, Figure 3 shows the plot of $\hat{\varepsilon}_i^2$ versus $\hat{\mu}_i$, where $\hat{\varepsilon}_i = BWT_i - \hat{\beta}_0 - \hat{\beta}_1 HWT_i$, $\hat{\beta}_0, \hat{\beta}_1$ are the least squares estimators of β_0, β_1 in model (4), and $\hat{\mu}_i = \hat{\beta}_0 + \hat{\beta}_1 HWT_i$. It indicates the homoscedasticity assumption is not satisfied. Because the normality assumption is satisfied, the CW and the BP tests may be used to check the homoscedasticity assumption. Both the CW and the BP tests got a p -value 0.11 by assuming the variance of BWT $\sigma^2(\mu_i)$ is a function of the mean μ_i . It concludes the data is not heteroscedastic.

However, as shown in Figure 3, the variance form is not exponential, which is assumed by the CW test, so the CW test has low power. For the BP test, although the variance form is sufficiently general to include a fairly wide class of heteroscedastic models, it does not include some heteroscedastic models, such as $\sigma_i^2 \propto \mu_i^2$. From Figure 3, the square of the mean may contribute to the shape of the variance function. This may be the reason that the BP test has low power and hence is not significant. Then, apply the two quasi-likelihood tests to this linear regression model. The first test gives a p -value 0.03, and the second test gives a p -value 0.2. The first test is significant and the second one is not. This suggests the heteroscedastic variance structure of this dataset is easier to be identified by the

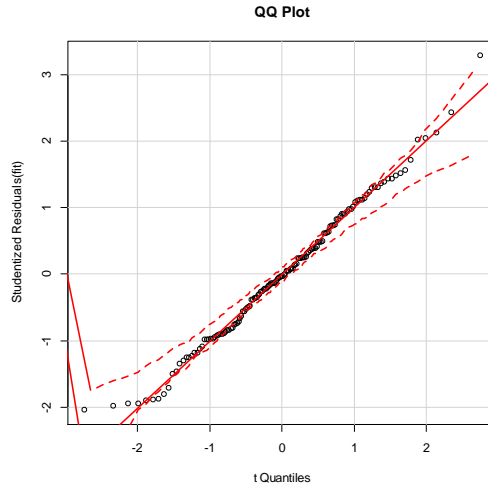


Figure 2. Q-Q plot to check the normality assumption

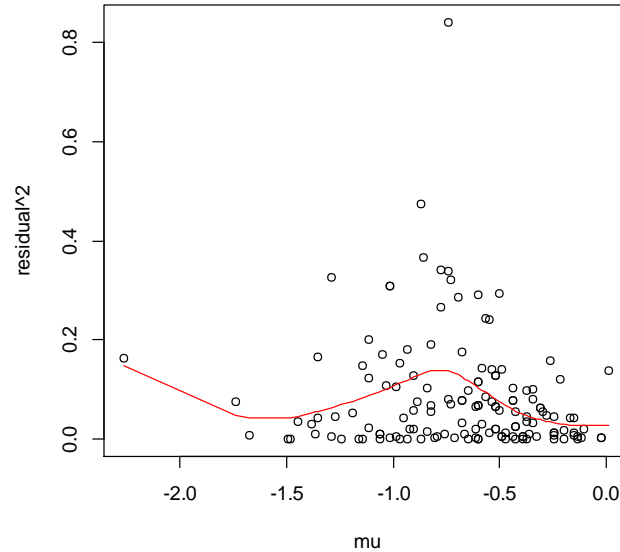


Figure 3. Plot of checking the variance function

first test than the second one, so the first test is more powerful than the second one. Because the quasi-likelihood ratio tests can test for all possible heteroscedastic models, their test results are reliable, and we conclude that the data is heteroscedastic.

Discussions and Conclusions

The classical homoscedasticity tests for linear regression models, such as the CW and the BP tests, cannot test for all possible heteroscedastic models. If the true variance form is not in the specified alternative hypotheses, the tests are not reliable. However, for real data, the true variance form is usually unknown and is hard to specify, so we do not know if the test results are valid or not. In this paper, we proposed two quasi-likelihood ratio tests, which can test for all possible heteroscedastic models. Hence, they are valid for all real data and have wider applications than the classical homoscedasticity tests for linear regression models. Moreover, the quasi-likelihood ratio tests have the potential to achieve greater power due to its log-likelihood properties. Furthermore, the quasi-likelihood ratio tests are easy to be implemented. The simulation shows the new proposed quasi-

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likelihood ratio tests maintain the probability of type-I error well and have satisfactory powers. The real data analysis shows the new proposed tests are useful.

A new form of quasi-likelihood is proposed for the second test. It has a simpler form that results in easy and less time-consuming computations. Simulations show the quasi-likelihood ratio test based on this new form is more powerful for some scenarios. The proposed tests can be easily extended to other models by using the estimators in the quasi-likelihood for the corresponding models. Future research can be conducted to extend these two tests to other models, such as nonparametric models or partial linear models.

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