

การทดสอบการแจกแจงปกติโดยแผนภาพของเศษตกค้างในการทดสอบอย่างเส้น

Graphical Normality Tests on Residuals in Linear Regression

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บทคัดย่อ

ลักษณะที่ไม่ปกติของการแจกแจงประชากร เช่น ความเบี้ยว ความโค้ง ทางขวาหรือทางซ้าย สามารถระบุได้จากแผนภาพความน่าจะเป็นปกติซึ่งการทดสอบสมมติฐานการแจกแจงปกติแบบไม่ใช้แผนภาพจะไม่สามารถใช้วินิจฉัยลักษณะเหล่านี้ได้ สำหรับการทดสอบทวนวรรณกรรมทางสถิติ ช่วงความน่าจะเป็นทางชั้นขนาด $1-\alpha$ บนแผนภาพความน่าจะเป็นปกติสำหรับตัวอย่างสุ่มอย่างมีใช้กันอยู่แล้ว เมื่อ α คือ ระดับนัยสำคัญ วัตถุประสงค์หลักของงานวิจัยชิ้นนี้ คือ การสร้างช่วงความน่าจะเป็นทางชั้นบนแผนภาพความน่าจะเป็นปกติสำหรับเศษตกค้างจากการทดสอบอย่างเส้นเพื่อ ก่อให้เกิดการตัดสินใจที่เชื่อถือได้ว่าเศษตกค้างนั้นเรียงกันเป็นเส้นตรงหรือไม่ สำหรับการทดสอบสำหรับวิธีการทดสอบโดยใช้ภาพจะลูกபெரியமெயினกับการทดสอบแบบไม่ใช้แผนภาพเพื่อประเมินว่าแบบใดจะมีอำนาจการทดสอบที่ดีกว่ากัน ท้ายที่สุดตัวอย่างจะถูกแสดงเพื่อสะท้อนถึงประสิทธิภาพของการทดสอบ

คำสำคัญ: การทดสอบโดยใช้ภาพ แผนภาพความน่าจะเป็นปกติ เศษตกค้าง ช่วงความน่าจะเป็นทางชั้น

Abstract

Non-normal features of the population distribution such as skewness, kurtosis, long or short tails can be easily identified from the normal probability plot. The non-graphical hypotheses tests of normality do not have this diagnostic feature. For the statistical literature, $1-\alpha$ simultaneous probability intervals for augmenting a normal probability plot for a simple random sample are available where α is a significance level. The main objective of this research is on construction of simultaneous probability intervals on normal probability plots for residuals from linear regression providing objective judgements whether on residuals fall close to a straight line. We then compare the powers of these graphical tests and some non-graphical tests for residuals in order to assess the power performances of the graphical tests and to identify the ones that have better power. Finally, the example is provided to illustrate the effectiveness of the tests.

Keywords: Graphical Test, Normal Probability Plot, Residuals, Simultaneous Probability Interval

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Introduction

First of all, the theoretical background of a linear regression model is introduced so that it enables to extend the tests of normality for a simple random sample to the vector of residuals from a linear regression model. It is more convenient to deal with multiple regression models if they are expressed in matrix notation. The model is given by $\mathbf{y} = \mathbf{X}\beta + \varepsilon$ or in terms of matrix form as

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1p} \\ 1 & x_{21} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

$$\text{where } \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}_{n \times 1}, \mathbf{X} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1p} \\ 1 & x_{21} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{bmatrix}_{n \times (p+1)}, \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}_{(p+1) \times 1}, \text{ and } \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}_{n \times 1}.$$

In general, \mathbf{y} is an $n \times 1$ vector of the observations, \mathbf{X} is an $n \times (p+1)$ matrix of the levels of the regressor variables or the design matrix, β is a $(p+1) \times 1$ vector of the regression coefficients, and ε is an $n \times 1$ vector of random errors.

The least squares estimator of β results from minimizing the sum of squared residuals is given by $\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$ provided that the inverse matrix $(\mathbf{X}^T \mathbf{X})^{-1}$ exists. Therefore, the vector of fitted values ($\hat{\mathbf{y}}$) corresponding to the vector of observed values (\mathbf{y}) is

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = \mathbf{Hy}$$

where $\mathbf{H} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$ is called the hat matrix. The vector of residuals can be written in matrix form as

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} = \mathbf{y} - \mathbf{Hy} = (\mathbf{I} - \mathbf{H})\mathbf{y} = (\mathbf{I} - \mathbf{H})\varepsilon$$

then the residuals $\mathbf{e} = (e_1, e_2, \dots, e_n)^T$ have the multivariate normal distribution since

$$\text{Var}(\mathbf{e}) = \text{Var}[(\mathbf{I} - \mathbf{H})\varepsilon] = (\mathbf{I} - \mathbf{H})\text{Var}(\varepsilon)(\mathbf{I} - \mathbf{H})^T = \sigma^2(\mathbf{I} - \mathbf{H})$$

where $\text{Var}(\varepsilon) = \sigma^2 \mathbf{I}$ and $\mathbf{I} - \mathbf{H}$ is symmetric and idempotent.

This leads to residuals which follow the normal distribution $N(\mathbf{0}, \sigma^2(\mathbf{I} - \mathbf{H}))$. Therefore, the regression residuals are neither independent nor homoscedastic because the covariance matrix $\sigma^2(\mathbf{I} - \mathbf{H})$ is not a diagonal matrix. The variance of the k^{th} residual is $\text{Var}(e_k) = \sigma^2(1 - h_{kk})$ where h_{kk} is the k^{th} diagonal element of the hat matrix for $k = 1, \dots, n$. The unknown error variance σ^2 is assumed to be estimated by the mean residual sum of

$$\text{square } S_e = \sqrt{\frac{\mathbf{e}^T \mathbf{e}}{n-p-1}}. \text{ Note that the studentized residuals can be defined as } r_k = \frac{e_k}{S_e \sqrt{1-h_{kk}}} \text{ for } k=1, \dots, n$$

which replaces the standardized residuals $\frac{e_k}{S_e}$.

As known in general statistical textbooks, one of the major assumptions of the linear regression model which we have concerned is the normality of random errors (ε). Our objective is to test normality of the error vector with the hypothesis

$$H_0: \varepsilon \sim N(\mathbf{0}, \sigma^2 \mathbf{I}).$$

However, ε is unobservable data, the residuals \mathbf{e} will be the estimator of ε to construct the tests on normality.

Basically, there are two types of procedures for assessing whether a population has a normal distribution based on a random sample. One of them is the graphical tests (e.g., normal probability plots) and the other is non-graphical tests (e.g., the Anderson-Darling and Shapiro-Wilk tests). The normal probability plot is a graphical technique for assessing whether or not a data set is approximately normally distributed. The data are plotted against a theoretical normal distribution in such a way that the points should form an approximate straight line. Specifically, the normal probability plot of the residuals is a simple graphical method to detect the normality assumption in linear regression if and only if the n points of residuals fall close to a straight line, the random errors are claimed to be normally distributed. As concerned, the graphical tests are more intuitive and more easily interpretable than non-graphical ones. However, the drawback is that different people can make different interpretations of the plots. Thus, graphical tests are usually regarded as informal techniques because the conclusions arrived at may be influenced by the subjectivity of users.

In methodology section, the construction of graphical tests on normal probability plot are developed to provide the $1-\alpha$ simultaneous probability intervals for the residuals as objective judgement. Then, we compare the powers of graphical tests on normal probability plot and non-graphical tests to identify the tests shown in results and discussion section. Finally, the conclusion of this research is presented in the subsequent section.

Methodology

Let $\mathbf{e} = (e_1, e_2, \dots, e_n)^T$ be the vector of residuals from a normal error in linear regression with $\mathbf{e} \sim N(\mathbf{0}, \sigma^2 (\mathbf{I} - \mathbf{H}))$ and $e_{[1]} \leq \dots \leq e_{[n]}$ be the residual arranged in ascending order. In addition, the unknown error variance σ^2 is estimated by $S_e = \sqrt{\frac{\mathbf{e}^T \mathbf{e}}{n-p-1}}$ as before.

Normal probability plot for residuals consists of the n points $(z_k, e_{[k]}), k=1, \dots, n$. There are several ways to choose the reference values z_k . Denote that $\Phi(\cdot)$ is the cumulative distribution function of the standard normal distribution and $\Phi^{-1}(\cdot)$ is the inverse function of $\Phi(\cdot)$. One can be used a set of plotting positions $0 < p_1 < \dots < p_n < 1$, that is, $\Phi(z_k) = p_k$ for $k=1, \dots, n$. According to [1], plotting position proposed by Blom (1958) is most suitable in the normal distribution. Thus, through this research we will use $p_k = \frac{k - 0.375}{n + 0.25}$ for $k=1, \dots, n$ as plotting positions [2].

We introduced two graphical tests considered in this article as follows:

1. The first test on normal probability plot based on Kolmogorov-Smirnov (1933) statistic [3] is

$$D = \max_{1 \leq k \leq n} \left| \Phi\left(\frac{e_{[k]}}{S_e \sqrt{1 - h_{kk}}}\right) - \frac{k - 0.375}{n + 0.25} \right|.$$

Let c_D be a critical constant so that $P\{D < c_D\} = 1 - \alpha$ under H_0 . The probability statement $P\{D < c_D\} = 1 - \alpha$ can be rewritten as

$$\begin{aligned} 1 - \alpha &= P\{D < c_D\} \\ &= P\left\{ \max_{1 \leq k \leq n} \left| \Phi\left(\frac{e_{[k]}}{S_e \sqrt{1 - h_{kk}}}\right) - \left(\frac{(k - 0.375)}{(n + 0.25)}\right) \right| < c_D \right\} \\ &= P\left\{ e_{[k]} \in S_e \sqrt{1 - h_{kk}} \Phi^{-1}\left(\left(\frac{(k - 0.375)}{(n + 0.25)}\right) \pm c_D\right) \text{ for } k = 1, \dots, n \right\}. \end{aligned}$$

Therefore, the simultaneous intervals of $e_{[k]}$ for $k = 1, \dots, n$ is given by

$$S_e \sqrt{1 - h_{kk}} \Phi^{-1}\left(\left(\frac{(k - 0.375)}{(n + 0.25)}\right) \pm c_D\right).$$

2. The second test on normal probability plot constructed based on Michael [4] is

$$D_{sp} = \max_{1 \leq k \leq n} \left| \frac{2}{\pi} \arcsin \sqrt{\Phi\left(\frac{e_{[k]}}{S_e \sqrt{1 - h_{kk}}}\right)} - \frac{2}{\pi} \arcsin \sqrt{\frac{k - 0.375}{n + 0.25}} \right|.$$

Let c_{sp} be a critical constant so that $P\{D_{sp} < c_{sp}\} = 1 - \alpha$ under H_0 . The $1 - \alpha$ simultaneous probability intervals associated with the probability statement $P\{D_{sp} < c_{sp}\} = 1 - \alpha$ can be rewritten as

$$\begin{aligned} 1 - \alpha &= P\{D_{sp} < c_{sp}\} \\ &= P\left\{ \max_{1 \leq k \leq n} \left| \frac{2}{\pi} \arcsin \sqrt{\Phi\left(\frac{e_{[k]}}{S_e \sqrt{1 - h_{kk}}}\right)} - \frac{2}{\pi} \arcsin \sqrt{\frac{k - 0.375}{n + 0.25}} \right| < c_{sp} \right\}. \end{aligned}$$

Therefore, the simultaneous intervals of $e_{[k]}$ for $k = 1, \dots, n$ is given by

$$S_e \sqrt{1 - h_{kk}} \Phi^{-1}\left(\sin^2\left(\arcsin \sqrt{\left(\frac{(k - 0.375)}{(n + 0.25)}\right) \pm \frac{\pi}{2} c_{sp}}\right)\right).$$

In power comparison, we include the Anderson-Darling [5] and Shapiro-Wilk [5] tests as the non-graphical based tests. That is, the Anderson-Darling statistic is

$$AD = -\frac{1}{n} \left[\sum_{k=1}^n (2k-1) \left\{ \ln Z_k + \ln(1-Z_{n-k+1}) \right\} \right] - n$$

where $Z_k = \Phi \left(\frac{e_{[k]}}{S_e \sqrt{1-h_{kk}}} \right)$. The critical constant c_{AD} which corresponding to $P\{AD < c_{AD}\} = 1 - \alpha$ can be

determined by simulation as the critical constant c_D .

The Shapiro-Wilk statistic is

$$SW = \left\{ \sum_{k=1}^n a_k \frac{e_{[k]}}{S_e \sqrt{1-h_{kk}}} \right\}^2 \left/ \sum_{k=1}^n \left(\frac{e_{[k]}}{S_e \sqrt{1-h_{kk}}} \right)^2 \right.$$

where a_k are coefficients tabulated by Shapiro and Wilk. The critical constant c_{SW} which corresponding to $P\{SW < c_{SW}\} = 1 - \alpha$ can be determined by simulation as the critical constant c_D .

To compute power results among graphical and non-graphical tests when standardized and studentized residuals are applied for linear regression with one explanatory variable, 10,000 simulations are used. Similarly, the $\varepsilon_1^*, \dots, \varepsilon_n^*$ are drawn from the given distribution. Note that μ is the mean of the given distribution as shown in the next section. Then the error vector is $\varepsilon = (\varepsilon_1^* - \mu, \dots, \varepsilon_n^* - \mu)$. The residual vector can be computed by $e = (I - H)\varepsilon$ applying to test e . The proportion of times that H_0 is rejected taking as the power of the test when compare with critical values in [6].

In our simulation study, we use $\alpha = 0.05$ and the two different forms of design matrix X which are presented by [6]. For the symmetrical design matrix (say Design 1), we generate the first $\frac{n}{2}$ observations of column vector for explanatory variable in X are set to be -1 and the remaining $\frac{n}{2}$ observations are set equal to 1. Conversely, for the asymmetrical design matrix (say Design 2) the first observation is set equal to -1 and the remaining observations are set equal to 1.

Group I of the given distributions is asymmetric on the support $(0, \infty)$ including χ_1^2 , exponential(0,1) and χ_4^2 . Group II of three distributions is on interval (0,1) and includes uniform(0,1), beta(1,2) and beta(2,2). In addition, Group III of distributions are symmetric on the support $(-\infty, \infty)$ consisting of t(1), t(3) and t(6).

In practice, the $1 - \alpha$ simultaneous probability intervals can then be used to test H_0 based on corresponding graphical tests in the following procedure:

1. Choose a significance level α and the graphical test.
2. Calculate the critical constant which depends on α , sample size n and the number of simulation.
3. Sort e_k 's in ascending order $e_{[1]} \le \dots \le e_{[n]}$ and plot $(\Phi^{-1}(p_k), e_{[k]})$, $k = 1, \dots, n$. This step produces normal probability plot.
4. For each k , plot the vertical intervals corresponding to $e_{[k]}$ based on the graphical test considered for $k = 1, \dots, n$.
5. Join the upper bounds and the lower bounds of all n vertical intervals from step 4 which becomes the bands.
6. Reject the null hypothesis H_0 at level α if at least one point $(\Phi^{-1}(p_k), e_{[k]})$, $k = 1, \dots, n$ falls outside the bands.

Results and Discussion

From the power comparison among all alternative distributions in Group I, II and III given in Table 1 and 2, the following observations can be made as follows:

For overall results of power comparison in Table 1, D test performs quite badly in comparison with the other tests but the performance of D test seems better on other situations (especially Group III). The reason is because the characteristics of \mathbf{X} is choose as in Methodology section. In General, SW test gives highest power among all tests for Group I, but it performs as good as AD test based on distributions in Group II and III. Although the D_{sp} test is not the best test for all cases, it still gives higher powers than the D test in almost all cases.

Table 1 Power comparison among D, D_{sp} , AD and SW tests where \mathbf{X} comes from Design 1

Distributions	n	D	D_{sp}	AD	SW
χ^2_1	8	22.94	23.28	31.52	35.04
	12	47.53	49.13	56.68	60.11
	24	86.14	93.41	94.08	95.79
	48	99.68	99.98	99.95	99.97
	60	99.97	100	100	100
exponential(0,1)	8	13.75	13.71	17.13	20.15
	12	27.50	27.52	35.36	38.74
	24	59.99	73.31	76.12	81.10
	48	92.43	99.09	98.57	99.41
	60	97.29	99.92	99.70	99.94
χ^2_4	8	8.71	8.53	10.42	11.86
	12	15.35	15.29	19.92	22.38
	24	33.86	41.40	46.90	54.09
	48	64.23	86.67	83.98	90.71
	36	75.97	95.12	92.40	96.51
uniform(0,1)	8	6.60	7.16	7.24	7.40
	12	8.27	8.82	8.90	7.84
	24	12.50	14.31	19.70	18.84
	48	26.88	39.39	51.56	59.26
	60	34.45	56.37	65.34	75.45
beta(1,2)	8	7.22	7.27	8.13	8.40
	12	10.34	10.24	11.89	11.79
	24	20.22	24.17	27.78	29.06
	48	43.27	73.21	63.93	71.06
	60	54.84	88.83	78.82	86.05
beta(2,2)	8	4.99	5.11	5.21	5.21
	12	5.63	5.45	5.69	4.71
	24	6.31	5.96	7.21	5.66
	48	9.10	9.06	13.46	12.34
	60	10.55	12.38	16.59	17.11
t(1)	8	24.98	26.68	32.35	35.91
	12	48.41	51.85	55.10	57.52
	24	83.41	86.53	88.78	88.86

Distributions	n	D	D _{sp}	AD	SW
	48	98.69	98.93	99.50	99.41
	60	99.56	99.63	99.87	99.86
t(3)	8	6.72	7.04	7.85	8.11
	12	12.48	13.78	15.76	12.77
	24	23.52	28.67	31.78	26.11
	48	43.34	50.00	56.42	44.52
	60	49.85	55.73	63.52	51.62
t(6)	8	5.48	5.43	5.66	6.14
	12	6.61	6.90	8.24	9.17
	24	9.32	12.08	13.17	16.59
	48	13.36	18.03	20.18	26.73
	60	15.70	20.45	23.49	31.06

Table 2 power comparison among D, D_{sp}, AD and SW tests where X comes from Design 2

Distributions	n	D	D _{sp}	AD	SW
χ^2_1	8	25.54	13.83	17.80	15.25
	12	45.78	37.14	42.04	32.76
	24	85.51	86.23	90.73	77.61
	48	99.64	99.99	99.97	99.40
	60	100	100	100	99.91
exponential(0,1)	8	14.69	6.82	8.32	6.31
	12	26.64	19.57	20.62	14.57
	24	58.96	55.69	60.36	40.20
	48	91.51	95.15	96.79	82.21
	60	97.08	99.37	99.37	93.50
χ^2_4	8	9.65	4.76	5.24	3.76
	12	16.17	10.55	10.10	6.27
	24	32.73	28.47	28.18	14.58
	48	64.72	61.04	70.70	37.80
	36	75.93	76.22	84.63	52.22
uniform(0,1)	8	6.26	3.50	4.98	4.07
	12	6.74	4.24	5.43	2.79
	24	10.58	10.97	9.77	0.95
	48	23.22	33.98	33.80	1.12
	60	31.89	50.75	49.98	2.20
beta(1,2)	8	7.59	3.26	3.97	3.5
	12	9.11	5.58	4.59	4.82
	24	18.30	14.49	10.93	14.38
	48	40.48	31.82	41.14	40.13
	60	51.86	45.65	58.19	56.80
beta(2,2)	8	5.25	3.94	4.47	4.20
	12	4.40	3.33	3.30	3.60
	24	5.80	4.95	3.70	4.03
	48	7.44	6.93	6.44	6.10
	60	9.95	9.45	9.91	9.87

Distributions	n	D	D_{sp}	AD	SW
t(1)	8	29.01	32.09	34.01	32.50
	12	54.44	59.44	60.32	56.61
	24	86.59	88.50	90.87	87.40
	48	99.10	99.03	99.69	99.14
	60	99.76	99.80	99.93	99.84
t(3)	8	8.75	11.83	10.88	8.76
	12	13.86	18.93	18.39	13.64
	24	26.13	31.26	34.62	26.16
	48	45.44	52.65	59.98	43.10
	60	54.14	62.24	69.47	50.63
t(6)	8	6.55	7.71	6.76	6.88
	12	7.59	10.00	9.32	10.14
	24	9.98	12.75	14.61	16.98
	48	14.20	20.20	23.28	26.24
	60	17.34	24.64	28.01	31.66

For the conclusion made by Table 2, It is very interestingly that there is a slight difference among D_{sp} , AD and SW tests in several cases. Obviously, the D test performs well in χ^2_1 , exponential(0,1), χ^2_4 and beta(2,2). The D_{sp} test shows impressive powers for the rest even though it is a graphical test.

Montgomery [7] studied on the rocket propellant and the authors suspected whether the shear strength is related to the age in weeks of the batch of sustainer propellant or not. The twenty observations on shear strength and the age of the corresponding batch of propellant have been collected when shear strength is a dependent variable and age of propellant (weeks) is an explanatory variable in simple linear regression. To estimate the model parameter, least squares method is applicable to obtain the least squares equation as $\hat{y} = 2627.82 - 37.15x$.

Now, we will apply the procedure of $1 - \alpha$ simultaneous probability intervals in the methodology section to produce the vertical intervals for each residual. The objective judgement on normal probability plot is that if at least one point $(\Phi^{-1}(p_k), e_{[k]})$, $k = 1, \dots, n$ in the normal probability plot is not included in the corresponding vertical interval, ones can claim that H_0 is not supported by the observed data.

To draw the conclusion that the random errors follow normal assumption by Figure 1, all residuals must lie within the corresponding intervals. The top panel of Figure 1 shows that each residual $e_{[k]}$ $k = 1, \dots, n$ falls inside the corresponding vertical interval based on the D test. Hence, the inference is that the random errors are normally distributed under the D test. However, from the bottom panel of Figure 1, $e_{[2]} = -213.6$ does not lie inside the corresponding interval $(-204.9496, -72.5683)$. Thus, we can draw the conclusion that the errors do not follow a normal distribution based on the D_{sp} test. Additionally, by the statistical software, we also make a conclusion that the null hypothesis H_0 is rejected at $\alpha = 0.05$ under AD and SW tests.

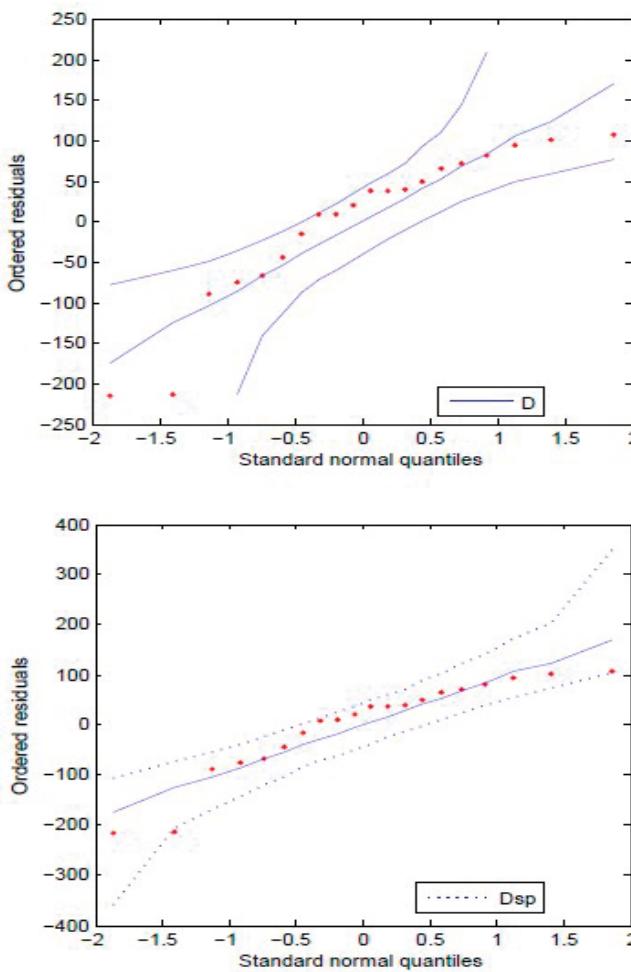


Figure 1 Simultaneous intervals for testing normality of residuals based on rocket

propellant data for graphical based D and D_{sp} tests at $\alpha = 0.05$

Conclusion

Based on the investigations set out in the previous sections, the SW and AD tests are non-graphical tests, they may not be more powerful than the graphical tests. In general, the D_{sp} test, which is effectively graphical test for normality based on residuals in linear regression, is good enough to detect normality on residuals as shown in above figure similar to the SW and AD tests. Therefore, the graphical test on normal probability plot becomes a useful tool for practitioners who look for the objective judgement on the normal probability plot.

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