Biometrika (1988), **75**, 3, *pp.* 569–75
Printed in Great Britain

Testing for normal errors in designs with many blocks

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SUMMARY

Goodness-of-fit tests are provided for the assumption of homoscedastic normal errors in experimental designs where the number of fitted parameters is large. Asymptotic critical points are given for the Cramér–von Mises statistic, Watson's statistic and the Anderson–Darling statistic. An expansion of the covariance function of the empirical process of standardized residuals is given. The corresponding weak convergence result is established for one-way layouts when the number of parameters grows linearly with the sample size. A Monte Carlo study is given to aid in the use of the tables.

Some key words: Anderson–Darling statistic; Cramér–von Mises statistic; Goodness-of-fit; Watson's statistic.

1. INTRODUCTION

When fitting regression models $y_i = x_i\beta + \varepsilon_i$ for $i = 1, \ldots, N$ it is common to assume that the errors are independent $N(0, \sigma^2)$ variates. In this paper we study tests of this null hypothesis based on the standardized residuals $e_i = w_i(y_i - x_i\hat{\beta})/\hat{\sigma}$, where $\hat{\beta}$ is the usual least-squares estimate, $\hat{\sigma}^2 = \nu^{-1}\Sigma(y_i - x_i\hat{\beta})^2$, $\nu = N - p$, p is the dimension of β and $\text{var}\,(y_i - x_i\hat{\beta}) = \sigma^2/w_i^2$. If X is the design matrix with ith row x_i then w_i^{-2} is the ith diagonal entry in the matrix $I - X(X'X)^{-1}X'$.

If ν is large then e_i will be close to $\tilde{e}_i = w_i(y_i - x_i\hat{\beta})/\sigma$. The $\tilde{e}_i$ have standard normal marginal distributions. Thus the variates $\Phi(e_i)$, where Φ is the standard normal distribution function, are approximately uniformly distributed on [0, 1]. Suppose $u_1 < \ldots < u_N$ are the values of $\Phi(e_i)$ arranged in increasing order. We study tests of the null hypothesis of homoscedastic normal errors based on three statistics: the Cramér–von Mises statistic

$$W^2 = \sum_{i=1}^{N} \{u_i - (2i-1)/(2N)\}^2 + 1/(12N), \tag{1}$$

Watson's statistic

$$U^2 = W^2 - N(\bar{u} - \tfrac{1}{2})^2, \tag{2}$$

where $\bar{u} = \Sigma\, u_i/N$, and the Anderson–Darling statistic

$$A^2 = -N^{-1} \sum_{i=1}^{N} (2i-1)\{\log u_i + \log\,(1 - u_{N+1-i})\} - N. \tag{3}$$

The large-sample theory of such statistics may be deduced from the asymptotic behaviour of the empirical process

$$Z_N(t) = N^{-\frac{1}{2}} \sum_{i=1}^{N} [1\{\Phi(e_i) \leq t\} - t].$$

When the number, p, of parameters is fixed as N increases Mukantseva (1977), Pierce & Kopecky (1979) and Loynes (1980) have shown that Z_N converges weakly to a mean zero Gaussian process with covariance function

$$\rho(s, t) = \min(s, t) - st - J_1(s)J_1(t) - \tfrac{1}{2}J_2(s)J_2(t). \tag{4}$$

Here $J_1(s) = \phi\{\Phi^{-1}(s)\}$, ϕ is the standard normal density and $J_2(s) = \Phi^{-1}(s)J_1(s)$. This is exactly the result obtained by Stephens (1976) when $p = 1$ and each $x_i = 1$; Stephens calls this Case 3. When p^2/N is bounded as N tends to infinity the work of Portnoy (1986) suggests that this result remains true under suitable conditions on the x_i. His work does not deal with the case where σ is unknown but allows for estimators other than the least-squares estimates.

In many common experimental situations the data are arranged in blocks. In order to collect more data, more blocks and more block effects are introduced. Thus the number of parameters, p, increases linearly with N. We concentrate on this situation.

We consider four designs which we describe in some detail to fix notation.

Design 1: The one-way layout. We have data y_{jk} for $k = 1, \ldots, K$ and $j = 1, \ldots, n$. Our model is $y_{jk} = \mu_j + \varepsilon_{jk}$. The weights used in computing the e_{jk} are $w_{jk} = \{K/(K-1)\}^{\frac{1}{2}}$.

Design 2: The two-way layout. We have data y_{ijl} for $l = 1, \ldots, L$, $i = 1, \ldots, I$ and $j = 1, \ldots, n$. Thus I treatments are replicated L times each in each of n blocks. Our model is $y_{ijl} = \mu_j + t_i + \varepsilon_{ijl}$, where $\Sigma_i t_i = 0$. The weights are

$$w_{ijl} = \{1 - (nL)^{-1} - (IL)^{-1} + (nIL)^{-1}\}^{-\frac{1}{2}}.$$

The quantity $K = IL$ will be needed in the sequel.

Design 3: Balanced incomplete blocks. We have data y_{jl}, the response to treatment l in block j; not all pairs j, l have observations. We have L treatments of which K occur in each block. There are n blocks. Each pair of treatments occurs $\lambda = nK(K-1)/\{L(L-1)\}$ times together in a block. The weights are $w_{jl} = [(K-1)\{K^{-1} - (\lambda L)^{-1}\}]^{-\frac{1}{2}}$. Our model is $y_{jl} = \mu_j + t_l + \varepsilon_{jl}$, where $\Sigma_l t_l = 0$.

Design 4: Latin squares. We have data y_{ijl} arranged in an n by n Latin square. Our model is $y_{ijl} = \mu_j + r_i + t_l + \varepsilon_{ijl}$, where $\Sigma_i r_i = \Sigma_l t_l = 0$. The weights are $w_{ijl} = n/(n^2 - 3n + 2)^{\frac{1}{2}}$.

In § 2 we tabulate the limiting distributions of W^2, U^2 and A^2 in the above designs when n tends to ∞ with I, K and L remaining fixed. A practical problem arises. The limiting distribution as $K \to \infty$ with n fixed is different from the limit as $n \to \infty$ with K fixed. Consider a one-way layout with $K = 8$ replicates and $n = 8$ cells. Which limit should be used? In § 2 we indicate, on the basis of a Monte Carlo study, how best to enter the tables for particular values of the parameters. Section 2 concludes with a brief example.

In § 3 we present, for general designs, an expansion of the covariance function of Z_N with a remainder of order ν^{-1}. We give a similar expansion for a process uniformly close to Z_N. The corresponding weak convergence result is proved for one-way layouts.

In § 4 we make some remarks concerning consistency of the tests and discuss related problems.

2. The tests

To test the null hypothesis of homoscedastic normal errors in any of Designs 1–4 proceed as follows.

(i) Fit the model by least-squares.
(ii) Compute the standardized residuals using the weights appropriate to the design and arrange them in increasing order to obtain $e_{(1)} < \ldots < e_{(N)}$.
(iii) Compute $u_i = \Phi(e_{(i)})$.
(iv) Compute W^2, U^2 or A^2 using (1), (2) or (3).
(v) Refer the computed statistic to the table of critical points, Table 1, using the value of K given above in the discussion of the designs to find the appropriate line in the table. For Latin squares use $K = \infty$. For the two-way layout the value K should be taken as the smaller of the number of rows and the number of columns times the number of observations per cell. In other words the factor called 'blocks' should be the factor with the larger number of levels.

Table 1. *Critical points for W^2, U^2 and A^2*

		Upper tail significance level (%)							
	K	25	15	10	5	2·5	1	0·5	0·1
W^2	2	0·0658	0·0859	0·103	0·133	0·164	0·207	0·241	0·320
	3	0·0728	0·0886	0·101	0·122	0·143	0·172	0·193	0·242
	4	0·0729	0·0889	0·102	0·123	0·145	0·173	0·195	0·246
	5	0·0732	0·0894	0·102	0·124	0·146	0·175	0·198	0·250
	10	0·0737	0·0902	0·103	0·126	0·148	0·178	0·201	0·254
	20	0·0739	0·0904	0·103	0·126	0·149	0·179	0·202	0·255
	∞	0·0739	0·0904	0·104	0·126	0·149	0·179	0·202	0·255
U^2	2	0·0658	0·0859	0·103	0·133	0·164	0·207	0·241	0·320
	3	0·0696	0·0847	0·0966	0·117	0·137	0·164	0·185	0·232
	4	0·0688	0·0837	0·0954	0·115	0·135	0·162	0·182	0·228
	5	0·0688	0·0838	0·0955	0·116	0·136	0·162	0·182	0·229
	10	0·0691	0·0841	0·0960	0·116	0·137	0·163	0·184	0·231
	20	0·0691	0·0842	0·0961	0·116	0·137	0·164	0·184	0·231
	∞	0·0692	0·0843	0·0962	0·117	0·137	0·164	0·184	0·232
A^2	2	0·426	0·536	0·627	0·789	0·957	1·187	1·365	1·789
	3	0·465	0·551	0·618	0·731	0·843	0·992	1·104	1·366
	4	0·464	0·551	0·619	0·734	0·849	1·002	1·117	1·386
	5	0·466	0·554	0·623	0·740	0·858	1·014	1·132	1·410
	10	0·468	0·558	0·629	0·749	0·870	1·031	1·153	1·440
	20	0·469	0·560	0·631	0·751	0·873	1·034	1·158	1·447
	∞	0·469	0·560	0·631	0·752	0·873	1·035	1·159	1·448

The points in the tables are critical points from the limiting distributions of the test statistics achieved as $n \to \infty$ with the numbers of all other parameters fixed. In § 4 we establish that under these conditions the covariance function of Z_N converges to

$$\rho(s, t; K) = \min(s, t) - st + (K-1)[\Phi_2\{\Phi^{-1}(s), \Phi^{-1}(t); -(K-1)^{-1}\} - st] - KJ_2(s)J_2(t)/\{2(K-1)\}, \tag{5}$$

where $\Phi_2(x, y; \rho)$ is the bivariate cumulative distribution function for a normal distribution with mean vector equal to 0, unit variances, and correlation coefficient ρ. For the one-way layout, Z_N converges to a mean zero Gaussian process with covariance $\rho(s, t; K)$. As $K \to \infty$ this covariance converges to $\rho(s, t; \infty)$ given by (4).

It follows that W^2 and U^2 have limiting distributions of the form $\Sigma\, \lambda_i \omega_i$, where $\omega_1, \omega_2, \ldots$ have independent chi-squared distributions on 1 degree of freedom. The weights λ_i are the eigenvalues of the Fredholm equation

$$\lambda f(s) = \int f(t)\chi(s, t)\, dt. \tag{6}$$

For W^2 the kernel χ is just ρ of (5). For U^2 we have

$$\chi(s, t; K) = \rho(s, t; K) - \int_0^1 \rho(u, t; K)\, du - \int_0^1 \rho(s, u; K)\, du + \int_0^1 \int_0^1 \rho(u, v; K)\, du\, dv.$$

For A^2 the limiting distribution should be of the same form with

$$\chi(s, t; K) = \rho(s, t; K)/\{s(1-s)t(1-t)\}^{\frac{1}{2}}.$$

This does not quite follow from the weak convergence result. See Durbin (1973) for a discussion of this problem in related settings.

The points in the table were computed as follows. The integral equation (6) was replaced by the discretized version

$$\lambda v_i = \sum_{j=1}^{M} v_j \chi\{(i-\tfrac{1}{2})/M, \quad (j-\tfrac{1}{2})/M\}/M \quad (i = 1, \ldots, M),$$

where M is a large integer. In practice $M = 100$ was found to be adequate. The M eigenvalues, $\{\tilde{\lambda}_1, \ldots, \tilde{\lambda}_M\}$, of the discretized equations were computed numerically. Critical points were then found for the distribution of $\tilde{\lambda}_1 \omega_1 + \ldots + \tilde{\lambda}_M \omega_M$ using the numerical Fourier inversion technique of Imhof (1961).

A Monte Carlo study checked the adequacy of the asymptotic points. For one- and two-way layouts with n and K equal to 2, 5, 10 and 20 we generated 10 000 Monte Carlo samples. Using the procedure set down above we compared each of the calculated statistics with the asymptotic upper tail 5% point. The tests using the asymptotic points were found to be conservative when the total sample size is less than about 25 and close to their nominal levels in larger designs.

Box & Cox (1964) present data from a completely randomized 3×4 factorial design with 4 observations per cell. The observations are survival times for animals treated with one of four treatments after receiving one of three poisons. We fit a model with interactions so that for the purposes of testing for normality the experiment may be regarded as a one-way layout with $K = 4$ and $n = 12$. The statistics are $W^2 = 0{\cdot}279$, $U^2 = 0{\cdot}276$ and $A^2 = 1{\cdot}561$, all of which are significant at the 0·1% point. The Box-Cox transformation analysis based on the transformation $z = y^\lambda$ leads to a fitted value of λ of approximately $-0{\cdot}81$. For the transformed values we obtain $W^2 = 0{\cdot}0938$, $U^2 = 0{\cdot}0838$ and $A^2 = 0{\cdot}535$, which all yield P-values around 15%. Thus the analysis based on the assumption of normality for the transformed data appears to be justified. Box & Cox use a model with no interactions to obtain a fitted value for λ of $-0{\cdot}75$ for which the conclusions are not perceptibly different.

The overall significance level of a test of the hypothesis that the Box-Cox transformation is appropriate for some value of λ will be lower than the asymptotic points suggest because another parameter, not one of location, has been estimated. It may not be possible to derive useful asymptotic theory for tests of the hypothesis that z is exactly normal for some value of lambda since z is necessarily positive.

3. General designs

An approximate covariance for Z_N may be obtained as follows. The joint distribution of the e_i has been studied by Ellenberg (1973). In particular the e_i have identical marginal distribution functions

$$G_\nu(x) = T_\nu[x\{(\nu-1)/(\nu-x^2)\}^{\frac{1}{2}}] \quad (x^2 \leq \nu),$$

where T_ν is the t-distribution on ν degrees of freedom. The distribution G_ν is called an inverted t-distribution on ν degrees of freedom. The corresponding density is

$$g_\nu(x) = \Gamma(\tfrac{1}{2}\nu)(\pi\nu)^{-\frac{1}{2}}(1-x^2/\nu)^{(\nu-3)/2}/\Gamma(\tfrac{1}{2}\nu-\tfrac{1}{2}) \quad (x^2<\nu).$$

Let $\tilde{e}_i = w_i(y_i - x_i\hat{\beta})/\sigma$. The $\tilde{e}_i$ have a mean zero multivariate normal distribution with unit variances and

$$\operatorname{cov}(\tilde{e}_i, \tilde{e}_j) = \rho_{ij} = H_{ij}/(H_{ii}H_{jj})^{\frac{1}{2}},$$

where $H = I - X(X'X)^{-1}X'$. Then e_i, e_j have joint density

$$g_\nu(t_1, t_2, \rho_{ij}) = (\nu-2)(1-\rho_{ij}^2)^{-\frac{1}{2}}(2\pi\nu)^{-1}(1-r^2/\nu)^{\frac{1}{2}(\nu-4)} \quad (r^2<\nu),$$

where $r^2 = (t_1^2 + t_2^2 - 2\rho_{ij}t_1t_2)/(1-\rho_{ij}^2)$. Let $G_\nu(t_1, t_2, \rho_{ij})$ be the corresponding joint cumulative distribution function. The process $N^{-\frac{1}{2}}\Sigma[1\{G_\nu(e_i)\leq t\}-t]$ has covariance function

$$\rho_N(s,t) = \min(s,t) - st + N^{-1}\textstyle\sum_{i\neq j}[G_\nu\{G_\nu^{-1}(s), G_\nu^{-1}(t), \rho_{ij}\} - st]. \tag{7}$$

The covariance function of Z_N is thus $\rho_N[\Phi\{G_\nu^{-1}(s)\}, \Phi\{G_\nu^{-1}(t)\}]$ which has the same limit, if any, as $\rho_N(s,t)$.

In an unpublished Simon Fraser University thesis, S. G. Meester used bivariate Edgeworth and Cornish-Fisher expansions to obtain

$$G_\nu\{G_\nu^{-1}(s_1), G_\nu^{-1}(s_2); \rho\} = \Phi_2\{\Phi^{-1}(s_1), \Phi^{-1}(s_2); \rho\} - (4\nu)^{-1}\phi_2\{\Phi^{-1}(s_1), \Phi^{-1}(s_2); \rho\}$$
$$\times\{2\Phi^{-1}(s_1)\Phi^{-1}(s_2) - \rho\Phi^{-1}(s_1) - \rho\Phi^{-1}(s_2)\} + O(\nu^{-2}).$$

This gives an expansion for ρ_N with a remainder of order N/ν^2. This is negligible for the designs considered here for which ν is proportional to N.

For Designs 1 to 4 of § 2 the expansion

$$\Phi_2\{\Phi^{-1}(s_1), \Phi^{-1}(s_2); \rho\} = s_1s_2 + \rho J_1(s_1)J_1(s_2) + O(\rho^2)$$

can now be used to show that ρ_N converges to $\rho(s, t, K)$ given by (5).

For designs with sufficient structure it is possible to prove that Z_N converges in distribution to a mean zero Gaussian process with covariance given by the limit of ρ_N. We give a proof for the one-way layout. More general results are available in unpublished work of J. R. Leslie and R. A. Lockhart. Portnoy (1986) gives results for designs with p^2/N bounded as $N\to\infty$. Of the designs considered here only the Latin square meets this criterion. This design does not seem to satisfy the conditions imposed by Portnoy.

Suppose now the data are collected in n cells with K observations per cell. We fit a model $y_{jk} = \mu_j + \varepsilon_{jk}$. We assume K is fixed and study the empirical process as n tends to infinity. In this case Z_N converges to a mean zero Gaussian process with covariance function $\rho(s, t; K)$.

We sketch a proof of the result. Without loss of generality take $\sigma = 1$ and $\beta = 0$. Let $w^2 = K/(K-1)$ and $\tilde{e}_{jk} = w(y_{jk} - \bar{y}_j)$, so that $\tilde{e}_{jk}$ is the standardized residual after fitting the model with σ known. As j ranges over $1, \ldots, n$ with k fixed the variates $\tilde{e}_{jk}$ are independent with standard normal distributions. Let $\tilde{Z}_k$ be the empirical process of these normal variates, namely,

$$\tilde{Z}_k(t) = n^{-\frac{1}{2}} \sum_j [1\{\Phi(\tilde{e}_{jk}) \leq t\} - t].$$

Let $H_N(t) = \Phi\{\hat{\sigma} G_\nu^{-1}(t)\}$. Then

$$Z_N(t) = (n/N)^{\frac{1}{2}} \sum_k \tilde{Z}_k\{H_k(t)\} + N^{\frac{1}{2}}\{H_N(t) - t\}.$$

A Taylor expansion can be used to establish that

$$N^{\frac{1}{2}}\{H_N(t) - t\} = N^{\frac{1}{2}}\{(\hat{\sigma}^2 - 1)J_2(t)/2\} + o_p(1).$$

Here and throughout the remainder term is small uniformly in $t \in [0, 1]$. Moreover $\nu\hat{\sigma}^2 = n \sum_k s_k^2 / w^2$, where $s_k^2 = \sum_j \tilde{e}_{jk}^2 / n$. Thus

$$Z_N(t) = (n/N)^{\frac{1}{2}} \sum_k [\tilde{Z}_k\{H_k(t)\} + n^{\frac{1}{2}}(s_k^2 - 1)J_2(t)/(2w^2)] + o_p(1).$$

The vectors $(e_{j1}, \ldots, e_{jK})$ are independent as j runs from 1 to n. The multivariate central limit theorem can be used together with the fact that each Z_k converges to a Brownian bridge to show that the vector $\{\tilde{Z}_k, n^{\frac{1}{2}}(s_k^2 - 1); k = 1, \ldots, K\}$ converges in distribution.

Now follow the discussion of Billingsley (1968, p. 144ff) of random changes of time to finish the proof.

The argument given above leads in general designs to an approximate covariance for Z_N. As above let

$$\tilde{Z}_N(t) = N^{-\frac{1}{2}} \sum [1\{\Phi(\tilde{e}_i) \leq t\} - t], \quad H_N(t) = \Phi\{\hat{\sigma} G_\nu^{-1}(t)\}.$$

Then $Z_N(t) = \tilde{Z}_N\{H_N(t)\} + N^{\frac{1}{2}}\{H_N(t) - t\}$. If $\tilde{Z}_N$ converges to a continuous process then Z_N is uniformly close to $\hat{Z}_N(t) = \tilde{Z}_N(t) + \frac{1}{2}N^{\frac{1}{2}}(\hat{\sigma}^2 - 1)J_2(t)$. The process $\hat{Z}_N$ has mean 0 and covariance

$$\hat{\rho}_N(s, t) = \min(s, t) - st + N^{-1} \sum_{i \neq j} [\Phi_2\{\Phi^{-1}(s), \Phi^{-1}(t); \rho_{ij}\} - st] - \tfrac{1}{2} N J_2(s) J_2(t)/\nu.$$

Again for Designs 1 to 4 above this converges to the covariance given by (5).

4. COMMENTS

The critical points for all three statistics depend very little on K for $K \geq 3$. For $K \geq 4$ the critical points for a fixed α increase with K. Use of the $K = \infty$ points in designs with the number, p, of fitted parameters large but not more than roughly $\frac{1}{4}N$ may be expected to give conservative tests. In small samples the Monte Carlo levels are smaller still so that the tests using the $K = \infty$ points would be even more conservative. The Monte Carlo studies suggest the extent of this effect is quite small, not reducing the level of a 5% test below 4% except in the smallest designs.

In designs where p is of the order of $\frac{1}{2}N$ the asymptotic critical points are rather larger. Tests using these asymptotic points are conservative in the Monte Carlo studies but not unduly so for designs with at least 20 degrees of freedom for error. Even in a design with only 4 degrees of freedom for error the observed level of a nominal 5% test is $2\frac{3}{4}$%.

In designs more complicated than those considered here it is not clear that tables of asymptotic critical points would be practical. It seems to us that direct calculation of a sum of weighted chi-squared approximation using the exact covariance (7) of the process $N^{-\frac{1}{2}} \sum [1\{G_\nu(e_i) \leq t\} - t]$ would be preferable. We hope to put together a software package which would find eigenvalues numerically and calculate P-values by Imhof's method.

In the designs considered here the block effects are not estimated consistently as $n \to \infty$. As a result the tests do not actually compare a consistent estimate of the distribution function of the ε_i with the normal distribution. For example, in the one-way layout with $K=2$ the two fitted residuals in the ith block are $\pm(\varepsilon_{i1}-\varepsilon_{i2})$. In this design we can hope to estimate and test hypotheses about the law of the ε_i only if that law is characterized by the law of $\varepsilon_{i1}-\varepsilon_{i2}$. For the normal distribution this is indeed the case. For any asymmetric error distribution, such as the important extreme value distribution, the law of $\varepsilon_{i1}-\varepsilon_{i2}$ is unchanged by replacing the law of ε_i with its mirror image, namely, the law of $-\varepsilon_i$. For a discussion of such characterization problems, see Small (1983).

In summary, the tests given are consistent tests of the hypothesis of normality. The corresponding tests of other distributions would not be consistent for $K=2$. Of course for such other distributions there remains the difficult problem of computing the distribution of the fitted residuals.

As part of the Monte Carlo study we examined the effect of using the exact probability integral transformation $u_i = G_\nu(e_{(i)})$ in place of $\Phi(e_{(i)})$. In virtually every case the normal transformation gave critical points closer to the asymptotic values. This was particularly true for small samples where the tests using asymptotic points have actual levels significantly lower than the nominal levels.

Acknowledgements

This paper is based on the M.Sc. project of the first author undertaken while both authors were at Simon Fraser University. Part of the work was done while the second author was on sabbatical at the University of Waterloo whose support is gratefully acknowledged. The research was supported by grants from the Natural Sciences and Engineering Research Council of Canada. Both authors have benefited from many conversations with Dr M. A. Stephens. The comments of a referee improved the presentation.

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[*Received October* 1987. *Revised February* 1988]