

GOODNESS-OF-FIT FOR THE EXTREME VALUE DISTRIBUTION

BY

MICHAEL A. STEPHENS

TECHNICAL REPORT NO. 7

JULY 18, 1977

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1. Introduction

In this paper we discuss the test of fit that a random sample comes from the extreme value distribution

$$(1) \quad F(x) = \exp[-\exp\{-(x-\xi)/\theta\}] , \quad -\infty < x < \infty .$$

This is the most important of the three distributions which arise as the asymptotic distribution of the largest value, suitably normalized, of a sample taken from any of a wide class of distributions (see e.g. Johnson and Kotz (1970), p. 272). It arises also in applied research; the present work was motivated by a question arising in biology. Suppose the sample is in ascending order $x_1 \leq x_2 \leq x_3 \leq \dots \leq x_n$, and the null hypothesis is formally stated as H_0 : the sample comes from distribution (1), with possibly one or both of the location and scale parameters ξ , θ unknown. Following Stephens (1974, 1976) we distinguish four situations:

Case 0: Both ξ and θ are known, so that $F(x)$ is completely specified.

Case 1: θ known, ξ to be estimated.

Case 2: ξ known, θ to be estimated.

Case 3: ξ , θ both unknown, and to be estimated.

We suppose the parameters will be estimated by maximum likelihood from the given example; the estimates, for Case 3, are given by the equations (Johnson and Kotz (1970), p. 283):

$$(2) \quad \hat{\theta} = \Sigma_j x_j / n - [\Sigma_j x_j \exp(-x_j / \hat{\theta})] / [\Sigma_j \exp(-x_j / \hat{\theta})]$$

and

$$(3) \quad \hat{\xi} = -\hat{\theta} \ln[\sum_j \exp(-x_j/\hat{\theta})/n] .$$

Equation (2) is solved iteratively, and then (3) can be solved. In Case 1, θ is known; then $\hat{\xi}$ is given by (3) with θ replacing $\hat{\theta}$. In Case 2, ξ is known; suppose then that $y = x_i - \xi$; $\hat{\theta}$ is given by solving

$$(4) \quad \hat{\theta} = \{\sum_j y_j - \sum_j y_j \exp(-y_j/\hat{\theta})\}/n .$$

2. The Goodness-of-Fit Tests

The tests discussed below are based on EDF statistics, measuring the discrepancy between the empirical distribution function and the theoretical distribution (1); in Cases 1, 2, and 3, the m.l. estimates are inserted for unknown parameters in (1). The statistics discussed are those usually called W^2 , U^2 and A^2 . Asymptotic theory for the statistics will be given in Section 3; this is based on work of Anderson and Darling (1952), for Case 0, and on papers by Darling (1955), Sukhatme (1972), Durbin (1973) and Stephens (1976) for situations where parameters must be estimated. The reader is referred to these papers for the theory behind the methods which follow; in particular, we follow closely the general lines of Stephens (1976). In that paper, for example, will be found the definitions of W^2 , U^2 and A^2 ; here we shall give only the practical steps in making a test of H_0 . These are:

(a) Calculate $z_i = F(x_i)$ where $F(x)$ is as given in (1) with the appropriate m.l. estimates inserted for unknown parameters in Cases 1, 2, or 3. Recall that the x_i are supposed in ascending order, giving z_i also in ascending order. Let $\bar{z}$ be the mean of the z_i .

(b) Calculate the test statistic desired:

$$W^2 = \sum_{i=1}^n (z_i - \frac{2i-1}{2n})^2 + \frac{1}{12n}$$

$$U^2 = W^2 - n(\bar{z} - \frac{1}{2})^2$$

$$A^2 = -[\sum_i (2i-1)\{\ln z_i + \ln(1-z_{n+1-i})\}]/n - n.$$

(c) Refer to Table 1, first calculating the modified statistic and then comparing these with the (upper tail) points given in the table, for the appropriate case. For example, if a sample of size 10, Case 3, gave $W^2 = 0.119$, the modified W^2 is, say, $W^* = 0.119(1-0.2/J_{10}) = 0.1265$; this is just significant at the 5% level.

3. Asymptotic Theory of the Tests

The following is a summary, taken from the papers referenced above, of the steps needed to calculate the asymptotic distributions of W^2 , U^2 or A^2 in the various cases.

For Case 0, when $F(x)$ is completely specified, it is well-known that $z = F(x)$ gives a random variable z which is uniformly distributed between 0 and 1; further, if $z_i = F(x_i)$, $i = 1, 2, \dots, n$, and if $F_n(z)$ is the EDF of the z_i sample, then $y_n(z) = \sqrt{n}\{F_n(z) - z\}$ tends asymptotically to a Gaussian process $y(z)$, $0 < z < 1$, with $E(y(z)) = 0$ for all z , and

$$(5) \quad E(y(s)y(t)) = \rho_0(s,t) = s - st, \quad 0 \leq s \leq t \leq 1,$$

where E is the expectation operator.

Unknown parameters. Suppose now that the (continuous) distribution under test is $F(x)$ (not necessarily (1)), with density $f(x)$, containing k parameters $\theta_1, \theta_2, \dots, \theta_k$; these are unknown and will be estimated by maximum likelihood. Suppose Z is the matrix with entries Z_{ij} given by

$$(6) \quad Z_{ij} = -E \left(\frac{\partial^2 \ln f(x)}{\partial \theta_i \partial \theta_j} \right), \quad i, j = 1, 2, \dots, k,$$

and let Σ be its inverse. Further, define $s = F(x)$, and

$$(7) \quad g_i(s) = \frac{\partial s}{\partial \theta_i}.$$

Let $u(s)$ be a k -vector whose i -th component is $g_i(s)$. Then, under appropriate regularity conditions (see e.g. Durbin (1973)), $y_n(z)$ now tends to a Gaussian process $y(z)$ with mean zero as before, and with covariance

$$(8) \quad \rho(s, t) = \rho_0(s, t) - u'(s) \Sigma u(t).$$

The statistic W^2 is $\int_0^1 y_n^2(z) dz$ and, again under regularity conditions, its asymptotic distribution will be that of $\int_0^1 y^2(z) dz$.

Anderson and Darling (1952) and Darling (1955) have shown how another Gaussian process may be constructed, with mean 0 and given covariance function $\rho(s, t)$ and the distribution (the word asymptotic will be dropped) of W^2 is calculated from the new process. We must first solve

$$(9) \quad f(x) = \lambda \int_0^1 \rho(x, y) f(y) dy$$

for eigenfunctions $f_i(y)$ and corresponding eigenvalues λ_i . If $D(\lambda)$ is the Fredholm determinant associated with (9), the characteristic function of the distribution of W^2 will be $\{D(2it)\}^{-1/2}$. The distribution of W^2 will then be the same as that of

$$(10) \quad S = \sum_{i=1}^{\infty} w_i / \lambda_i$$

where the w_i are independent χ_1^2 variables. The cumulants of the distribution are

$$(11) \quad K_j = 2^{j-1} (j-1)! \int_0^1 \rho_j(s, s) ds$$

where $\rho_1(s, t) = \rho(s, t)$, and, for $j \geq 2$, $\rho_j(s, t)$ is defined by

$$\rho_j(s, t) = \int_0^1 \rho_{j-1}(s, u) \rho(u, t) du.$$

The cumulants can also be found from the representation (10):

$$(12) \quad K_j = 2^{j-1} (j-1)! \sum_{i=1}^{\infty} (1/\lambda_i)^j.$$

Statistics U^2 and A^2 . These statistics are respectively functionals of $y_n(z) - \bar{y}_n(z)$ and of $y_n(z) w(z)$ where $w(z) = \{z(1-z)\}^{-1/2}$; $Y_n(Z) - \bar{Y}_n(Z)$ these processes tend asymptotically to Gaussian processes with covariances $\rho(s, t)$, which, for a given case, can be found from the corresponding covariance for W^2 ; then Equation (9) must again be solved, and the sum S in (10), with the new λ_i , will give the distribution of U^2 or A^2 . The characteristic function comes from the Fredholm determinant of (9) as before.

Thus the practical problem is to find $\rho(s,t)$ for different cases, then to solve (9) for λ_i , and then to use (12) to approximate the distribution (assuming, as is nearly always so except for Case 0, that the characteristic function cannot be inverted).

4. Asymptotic Results for the Extreme Value Distribution

The above results apply to any suitably regular distribution. For the distribution (1) considered here, we find, after some algebra,

$$(13) \quad Z = -\frac{1}{\theta^2} \begin{pmatrix} 1 & \gamma-1 \\ \gamma-1 & c^2 \end{pmatrix}$$

where $\gamma = .57712$ is Euler's constant and c^2 is

$$\Gamma''(3) + \Gamma''(1) - 2\Gamma''(2) - 1 = \pi^2/6 + (\gamma-1)^2 = 1.82368 ,$$

giving $c = 1.350437$; $\Gamma''(x)$ is the second derivative of the Gamma function $\Gamma(x)$. The asymptotic variances of $\hat{\xi}$ (Case 1) and $\hat{\theta}$ (Case 2), when $\theta = 1$, are then n^{-1} and $(c^2 n)^{-1}$, respectively. The functions $g(s)$, with subscript to indicate the case, are

$$g_1(s) = \frac{s \ln s}{\theta} ,$$

$$g_2(s) = \frac{s \ln s [-\ln(-\ln s)]}{\theta} ,$$

and these give covariance functions $\rho_j(s,t)$ for Case j , $j = 1, 2$:

$$(14) \quad \rho_j(s,t) = \rho_0(s,t) - \phi_j(s) \phi_j(t)$$

with

$$\phi_1(s) = s \ln s$$

and

$$\phi_2(s) = s \ln s [-\ln(-\ln s)]/1.350437 .$$

For Case 3 we first define σ_1^2 , σ_2^2 , and ρ by writing $Z^{-1} = \Sigma$ as

$$(15) \quad \Sigma = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix} .$$

The large-sample variances of $\hat{\xi}$ and $\hat{\theta}$, in Case 3, are then σ_1^2/n and σ_2^2/n respectively, and the correlation between them is ρ . Inversion of Z gives (for $\theta = 1$), $\sigma_1^2 = 1.10867$, $\sigma_2^2 = 0.60793$ and $\rho = 0.313$.

Note that the variances are different from those in Cases 1 and 2 because of the presence of correlation.

Since Σ is positive definite, it can be written $\Sigma = BB'$ where B is upper triangular; an example given by Sukhatme (1972) is

$$(16) \quad B = \begin{pmatrix} \sigma_1(1-\rho^2)^{1/2} & \rho\sigma_1 \\ 0 & \sigma_2 \end{pmatrix} .$$

If we define $v(s) = B'u(s)$, with two components $\psi_1(s)$, $\psi_2(s)$, the covariance for Case 3 becomes, from (8),

$$(17) \quad \rho_3(s,t) = \rho_0(s,t) - \psi_1(s) \psi_1(t) - \psi_2(s) \psi_2(t) .$$

Another possible matrix decomposition is $\Sigma = CC'$ where

$$C = \begin{pmatrix} \sigma_1 & 0 \\ \rho\sigma_2 & (1-\rho^2)^{1/2} \sigma_2 \end{pmatrix} .$$

If there were no asymptotic correlation between $\hat{\xi}$ and $\hat{\theta}$ in Case 3, $\rho_3(s,t)$ would take the form of (17), but with $\phi_i(\cdot)$ replacing $\psi_i(\cdot)$.

5. Calculation of Weights

With covariance $\rho_j(s,t)$ known for Case j, the next problem is to solve (9) for the weights λ_i . This is done as follows.

Let $0 < \lambda_1 < \lambda_2 < \lambda_3 \dots$ be the weights and $f_i(x)$ the associated normalized eigenfunctions, for Case 0. (For W^2 , these are

$\lambda_i = 1/\pi^2 i^2$ and $f_i(x) = \sqrt{2} \sin \pi i x$.) Set $D_0(\lambda) = \prod_i (\lambda - \lambda_i)$. Expand

$\phi_1(x) = \sum_i a_i f_i(x)$, so that $a_i = \int_{-\infty}^{\infty} \phi_1(x) f_i(x) dx$; similarly let

$b_i = \int_{-\infty}^{\infty} \phi_2(x) f_i(x) dx$. Let

$$S_a(\lambda) = 1 + \lambda \sum \frac{a_i^2}{\lambda - \lambda_i} ;$$

$$S_b(\lambda) = 1 + \lambda \sum \frac{b_i^2}{\lambda - \lambda_i} ;$$

$$S_{ab}(\lambda) = \lambda \sum \frac{a_i b_i}{\lambda - \lambda_i} .$$

In general, the λ_i of Cases 1 and 2 are then given by setting the Fredholm determinant to zero; this implies, for Case 1, solving $D_0(\lambda) S_a(\lambda) = 0$, and for Case 2, $D_0(\lambda) S_b(\lambda) = 0$. For Case 3, suppose $\psi_1(x)$, $\psi_2(x)$ replace $\phi_1(x)$, $\phi_2(x)$ in the definitions of a_i and b_i above, and define

$$T(\lambda) = S_a(\lambda) S_b(\lambda) - \{S_{ab}(\lambda)\}^2;$$

solutions for Case 3 are then given by $D_0(\lambda) T(\lambda) = 0$.

Weights for W^2 . For W^2 , the λ_i of Case 0, which we call the standard weights, each occur only once. In, say, Case 1, if a value i exists so that $a_i = 0$, then $\lambda = \lambda_i$ would be a solution of $D_0(\lambda) S_a(\lambda) = 0$; otherwise $(\lambda - \lambda_i)$ in $D_0(\lambda)$ cancels $(\lambda - \lambda_i)$ in the term in $S_a(\lambda)$ and $\lambda = \lambda_i$ is not a solution. For distribution (1) the a_i are never zero for W^2 , so the λ_i are then given only by $S_a(\lambda) = 0$. Similarly, for Case 2 we solve $S_b(\lambda) = 0$, and for Case 3, $T(\lambda) = 0$ (see Stephens (1976) for examples where $a_i = 0$).

Weights for A^2 and U^2 . For A^2 a similar situation exists; the functions $f_i(x)$ for Case 0 are $P_1^1(2x-1)$, where $P_1^1(t)$ are Ferrer associated Legendre functions, and the standard $\lambda_i = i(i+1)$. No coefficient a_i or b_i is zero, and solutions for λ_i for Cases 1, 2, and 3 are given by $S_a(\lambda) = 0$, $S_b(\lambda) = 0$, and $T(\lambda) = 0$, respectively.

For U^2 the discussion is more complicated. The roots λ_i of $D_0(\lambda) = 0$ are double roots, given by $\lambda_i = 4\pi^2 i^2$, and the corresponding eigenfunctions are $f_i(x) = \sqrt{2} \sin 2\pi i x$ and $f_i^*(x) = \sqrt{2} \cos 2\pi i x$. Suppose a

and a_i^* , b_i and b_i^* are the coefficients obtained using $f_i(x)$ and $f_i^*(x)$ respectively. Then $S_a(\lambda)$ becomes

$$S_a(\lambda) = 1 + \lambda \left(\sum_i \frac{a_i^2}{1-\lambda/\lambda_i} + \sum_i \frac{a_i^{*2}}{1-\lambda/\lambda_i} \right),$$

and

$$S_{ab}(\lambda) = \lambda \left(\sum_i \frac{a_i b_i}{1-\lambda/\lambda_i} + \sum_i \frac{a_i^* b_i^*}{1-\lambda/\lambda_i} \right).$$

$S_b(\lambda)$ is defined similarly to $S_a(\lambda)$. In Case 1, although no coefficient a_i , a_i^* , b_i or b_i^* is zero, one factor $\lambda - \lambda_i$ in $D_0(\lambda)$ cancels denominators in $S_a(\lambda)$, but the other factor remains, so $\lambda = \lambda_i$ is a solution of $D_0(\lambda) S_a(\lambda) = 0$; other solutions are given directly by $S_a(\lambda) = 0$. Similarly, for Cases 2 and 3, the standard weights occur once in addition to those given respectively by $S_b(\lambda) = 0$ and $T(\lambda) = 0$.

As a check on calculations, the weights for Case 3, for all three statistics, were found using the $\phi_1(s)$ and $\phi_2(s)$ given by both transformations B and C of Section 2; these, of course, give different coefficients a_i, a_i^*, b_i, b_i^* but the same final distribution for S in (10).

6. Direct Calculation of Means and Variances

The means and variances of the various distributions can be found directly from (11). For example, for the mean μ_j for Case j , (11) gives

$$(18) \quad \mu_j = \int_0^1 \rho_1(s,s)ds = \int_0^1 \rho_0(s,s)ds - \int_0^1 \phi_1^2(s)ds = \mu_0 - \int_0^1 \phi_1^2(s)ds.$$

The mean drops from its Case 0 value ($\mu_0 = 1/6$) by the last integral

in (18), which we will call Δ_j ; this can sometimes be directly calculated. For example, for W^2 Case 1, using integration by parts,

$$\Delta_1 = \int_0^1 \phi_1^2(s) ds = \int_0^1 s^2 \ln^2 s ds = .07407 .$$

Similarly, for Case 2, let b be $(1.350437)^{-2}$; then

$$\Delta_2 = \int_0^1 \phi_2^2(s) ds = b \int_0^1 s^2 \ln^2 s \{\ln(-\ln s)\}^2 ds .$$

Let $s = e^{-z}$; then

$$\Delta_2 = b \int_0^\infty e^{-3z} z^2 \ln^2 z dz .$$

Integrals of this type can easily be evaluated by use of appropriate substitutions and the identities

$$\Gamma(m) = \int_0^\infty e^{-y} y^{m-1} dy ,$$

$$\Gamma'(m) = \int_0^\infty e^{-y} y^{m-1} \ln y dy ,$$

$$\Gamma''(m) = \int_0^\infty e^{-y} y^{m-1} \ln^2 y dy .$$

For Δ_2 above, substitute $u = 3z$;

$$\begin{aligned} \Delta_2 &= \frac{b}{27} \int_0^\infty e^{-u} u^2 (\ln u - \ln 3)^2 du \\ &= b\{\Gamma''(3) - 2 \ln 3 \Gamma'(3) + \ln^2 3 \Gamma(3)\}/27 \\ &= 0.01750 . \end{aligned}$$

For W^2 Case 3, using the notation of Section 4, after Equation (16), we have

$$\begin{aligned}\Delta_3 &= \int_0^1 \psi_1^2(s) ds + \int_0^1 \psi_2^2(s) ds \\ &= \int_0^1 v'(s) v(s) ds \\ &= \int_0^1 u'(s) \Sigma u(s) ds \\ &= \sigma_1^2 \Delta_1 + 2\rho\sigma_1\sigma_2 \Delta_{12} + \sigma_2^2 \Delta_2\end{aligned}$$

where we define

$$\Delta_{12} = \int_0^1 \phi_1(s) \phi_2(s) ds .$$

Let c be $1/1.350437$; then

$$\Delta_{12} = \int_0^1 s^2 \ln^2 s \{-\ln(-\ln s)\} ds = c \int_0^\infty e^{-3z} z^2 \ln z dz = 0.0096445 .$$

Thus finally $\Delta_3 = 0.1083$. The three means for Cases 1, 2, 3 are then $\mu_1 = 0.0926$, $\mu_2 = 0.1492$, $\mu_3 = 0.0584$. For U^2 the calculations are on similar lines but are somewhat more complicated; the results are $\mu_0 = 1/12$, $\mu_1 = 0.0718$, $\mu_2 = 0.0683$, $\mu_3 = 0.0559$. For A^2 the integrals are intractable and have been calculated numerically to give $\mu_0 = 1$, $\mu_1 = 0.5959$, $\mu_2 = 0.8619$, $\mu_3 = 0.3869$.

In principle, variances could be calculated from (11), as was done in Stephens (1976) for the case of the normal distribution, but here the integrals were too complicated. It is important, however, to have the exact means, as (12) usually converges too slowly to give them correctly.

7. Calculation of Percentage Points

When the λ_i are found, and the exact means, the percentage points of S in (10) can be found by a modification of Imhof's method, given by Durbin and Knott (1972). Alternatively, the first four cumulants can be found from (12) and Pearson curves fitted to the data. Imhof's method can be made very accurate for a finite sum in (10), though it is expensive in computer time; in adapting it for an infinite sum an element of approximation is introduced. Thus both techniques give approximate percentage points. The Imhof method gives more accurate points in the lower tail (see Solomon and Stephens (1975) for a fuller discussion), but this is not, of course, the tail which would generally be used in goodness of fit work. Both techniques will depend on the accuracy of the λ_i , in turn dependent on the accuracy of the numerical integrations in a_i and b_i .

Both methods were used here to find the percentage points given in Table 1; they were in agreement to the accuracy given. Points for Case 0 are included to show how much the points drop in the other cases (and to show, therefore, how important it is to use the correct points).

8. Monte Carlo Results for Finite n

Monte Carlo studies were made to determine the percentage points of the various statistics, for sample sizes $n = 10, 20$, and 50 ; 5,000 samples were used for each case. Previous experience had suggested (Stephens (1974)) that convergence to the asymptotic points would be rapid, and a plot of percentage points against $1/n$ proved this to be so.

The Monte Carlo points were used to calculate the modified forms given in Table 1; for further details on how these are found, see Stephens (1970, 1976).

Comment. It is interesting that the asymptotic process in Case 1 above has exactly the same covariance ($\rho_1(s,t)$ in (14)) as in a test for the exponential distribution $F(x) = 1 - \exp(-x/\theta)$, with θ unknown; see Case 4 of Stephens (1976). The asymptotic distributions of all the EDF statistics are therefore the same in Case 1 above as in the exponential test.

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Table 1

Percentage Points for Modified Statistics W^2 , U^2 , A^2

For the appropriate case, the statistic should be modified as shown,
and compared with the given percentage points.

Statistic	Modification	Upper Tail Percentage Points					
		α :	0.75	0.90	0.95	0.975	0.99
W^2							
Case 0	$(W^2 - 0.4/n + 0.6/n^2)(1.0 + 1.0/n)$			.347	.461	.581	.743
1	$W^2(1 + 0.16/n)$		.116	.175	.222	.271	.338
2	None		.186	.320	.431	.547	.705
3	$W^2(1 + 0.2/\sqrt{n})$		.073	.102	.124	.146	.175
U^2							
Case 0	$(U^2 - 0.1/n + 0.1/n^2)(1.0 + 0.8/n)$			.152	.187	.221	.267
1	$U^2(1 + 0.16/n)$		.090	.129	.159	.189	.230
2	$U^2(1 + 0.15/n)$		.086	.123	.152	.181	.220
3	$U^2(1 + 0.2/\sqrt{n})$		.070	.097	.117	.138	.165
A^2							
Case 0	None			1.933	2.492	3.070	3.857
1	$A^2(1 + 0.3/n)$		.736	1.062	1.321	1.591	1.959
2	None		1.060	1.725	2.277	2.854	3.640
3	$A^2(1 + 0.2/\sqrt{n})$		.474	.637	.757	.877	1.038

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) In this paper we present goodness-of-fit tests for the extreme value distribution, based on the EDF statistics W^2 , U^2 and A^2 . Asymptotic percentage points are given for each of the three statistics, for the three cases where one or both of the parameters of the distribution must be estimated from the data. Slight modifications of the calculated statistics are given to enable the points to be used with finite samples.		

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