

Saddlepoint approximation in exponential models with boundary points

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A saddlepoint approximation is developed for the likelihood ratio test statistic in non-regular exponential models. For the one-parameter case, it is proved that the saddlepoint correction has a relative error of order $O(n^{-1})$, assuming that the canonical statistic has four finite moments. The results are applied in reliability theory and survival analysis, testing for exponentiality. Note that we are using the saddlepoint method for statistics without moment generating function.

Keywords: higher-order asymptotics; likelihood ratio test; reliability theory; survival analysis models

1. Introduction

The asymptotic distribution of the likelihood ratio test statistic, when the null model is embedded in the boundary of the parameter space, is not usually a χ_n^2 distribution. Often, when certain regularity conditions are fulfilled, the asymptotic distribution is a mixture of χ_n^2 distributions. We refer to Self and Liang (1987) and Geyer (1994) for further information on regularity conditions in non-standard cases.

In non-regular exponential models the standard regularity conditions do not always work, because the null model does not have a natural extension to an open neighbourhood. This fact is closely related to the steepness of the cumulant generating function and to the moments of the limit distribution. Examples of interest are conjugate families of non-negative random variables without a moment generating function, the singly truncated normal distribution which includes the exponential distribution in the boundary (del Castillo and Puig 1999a) and several situations in reliability theory and survival analysis, see del Castillo and Puig (1999b).

This paper shows that saddlepoint approximation provides a modified likelihood ratio test with finite-sample distribution closer to its asymptotic distribution, for non-regular exponential models, assuming that the canonical statistic has four finite moments. We have merged the results of the likelihood ratio test under non-standard conditions (see Self and Liang 1987) and the saddlepoint approximation for the likelihood ratio test of Jensen (1992). The paper shows when and why saddlepoint approximation works in non-regular exponential models. Surprisingly, it works well even for statistics without moment

generating function. For more information, see also Goutis and Casella (1999), Jensen (1995), Barndorff-Nielsen and Cox (1994) or Reid (1996).

Section 2 clarifies the regularity conditions for exponential models with boundary points in order to obtain first-order asymptotic results with the simplest assumptions. At this point the concepts of steep and non-steep exponential models are especially important. Section 3 develops the high-order asymptotic methods for the likelihood ratio test statistic for non-regular exponential models, following Jensen (1992). Section 4 shows how to use the previous results for practical cases. Testing for exponentiality in reliability theory and survival analysis models is also considered. The numerical accuracy of the saddlepoint approximation is illustrated by means of an example on real data.

2. Exponential family models with boundary points

Let X be a continuous random variable with probability density function $f(x)$ and cumulant generating function $\kappa(\theta)$. Let Θ be the set of points in \mathbb{R} where $\kappa(\theta)$ is finite. Let \mathcal{F} be the *conjugate family* of $f(x)$ given by

$$f(x; \theta) = e^{\theta x - \kappa(\theta)} f(x), \quad \theta \in \Theta, \quad (2.1)$$

which is a *full exponential model* (see Barndorff-Nielsen and Cox, 1994, Chapter 1). The parameter set Θ is a convex set containing the origin, and $\kappa(\theta)$ is infinitely differentiable and strictly convex on the interior of Θ . For $\theta = 0$, $f(x; 0)$ is the initial distribution $f(x)$.

If Θ is an open set then \mathcal{F} is called a *regular exponential model*. Otherwise, if Θ includes some of its topological boundary points, \mathcal{F} is called a non-regular exponential model. A non-regular exponential model such that $|\kappa'(\theta)|$ tends to infinity as θ tends to the boundary points of Θ is called *steep*. A necessary and sufficient condition for the maximum likelihood estimator (MLE) to be the unique solution of the likelihood equation is the steepness property. However, in this steep case with boundary points, the asymptotic distribution of the MLE or the asymptotic distribution of the likelihood ratio test is unknown when θ belongs to the boundary.

Examples of exponential models with boundary parameter are obtained from continuous positive random variables, with cumulant generating function not defined in a neighbourhood of 0, as a consequence of the following:

Example 1. Let $X > 0$ be a continuous positive random variable with probability density function $f(x)$. In this case the cumulant generating function, $\kappa(\theta)$, is finite for all $\theta \leq 0$. Hence, if $E[X^k] = \infty$, for some $k \geq 1$, the conjugate family given by (2.1) has 0 as a boundary point of Θ .

In this section we find the asymptotic distribution of the likelihood ratio test for $\theta = 0$, from independent and identically distributed samples, in some relevant examples of the situation (2.1) where 0 is a boundary point. Since the cumulant generating function is not defined in a neighbourhood of 0, not all the moments of X need exist. Without loss of generality we can assume that Θ is the interval $c < \theta \leq 0$, where c is some constant.

Proposition 1. Let \mathcal{F} be the statistical model given by (2.1), with $\Theta = \{c < \theta \leq 0\}$. If $\mu_0 = E[X]$ is finite then $\kappa'(\theta) \uparrow \mu_0$ as $\theta \uparrow 0$. Hence, \mathcal{F} is a non-steep model.

Proof. $\kappa(\theta)$ is a strictly convex function, so $E_\theta[X] = \kappa'(\theta)$ is strictly increasing. The result follows from the dominated convergence theorem. \square

Corollary 1. Under the same assumptions on \mathcal{F} as in Proposition 1, given a sample of independent and identically distributed components, the solution of the likelihood equation

$$\kappa'(\theta) = \bar{x}$$

is $\hat{\theta} < 0$, for $\bar{x} < \mu_0$, and otherwise $\hat{\theta} = 0$, for $\bar{x} \geq \mu_0$. Moreover, since $\kappa'(\theta)$ is strictly increasing, the MLE, $\hat{\theta}(\bar{x})$ is a continuous function at 0. Therefore, because of the law of large numbers, the MLE is consistent, $\hat{\theta} = o_p(1)$.

Given a normal variable with mean μ and variance σ^2 we denote by $N_+(\mu, \sigma^2)$ the positive truncated normal distribution with probability density function

$$f_+(x; \mu, \sigma) = \frac{\phi((x - \mu)\sigma^{-1})}{\sigma\Phi(\mu\sigma^{-1})}, \quad x > 0, \tag{2.2}$$

where $\phi(x)$ and $\Phi(x)$ are the density function and the distribution function of the standard normal. On the other hand, we say that X is a random variable from a negative truncated normal distribution, denoted $N_-(\mu, \sigma^2)$, if $-X$ is distributed according to $N_+(\mu, \sigma^2)$.

We now derive the same asymptotic distribution given by Self and Liang (1987) for the MLE as well as for the likelihood ratio test, weakening their assumptions to the existence of the second moment of X .

Proposition 2. Let \mathcal{F} be the model given by (2.1), with $\Theta = \{c < \theta \leq 0\}$, where the variance of X , σ_0^2 , is finite. The asymptotic distribution of $\sqrt{n}\hat{\theta}$ is a fifty-fifty mixture of the constant 0 and the negative truncated normal $N_-(0, 1/\sigma_0^2)$,

$$\sqrt{n}\hat{\theta} \xrightarrow{d} \frac{1}{2}N_-(0, 1/\sigma_0^2) + \frac{1}{2}\delta_0.$$

Proof. For $\bar{x} < \mu_0$ consider $\hat{\theta}(\bar{x})$ as in Corollary 1. We can extend it to a continuously differentiable function, $\tilde{\theta}(\bar{x})$, in the neighbourhood of μ_0 , by $\tilde{\theta}(\bar{x}) = (\bar{x} - \mu_0)/\sigma_0^2$, for $\bar{x} \geq \mu_0$. From the central limit theorem $\sqrt{n}(\bar{x} - \mu_0) \xrightarrow{d} N(0, \sigma_0^2)$, and with the δ -method

$$\sqrt{n}\tilde{\theta}(\bar{x}) \xrightarrow{d} N(0, 1/\sigma_0^2).$$

By definition of $\hat{\theta}$ we have the correspondence $\hat{\theta} = \tilde{\theta}$ for $\tilde{\theta} < 0$ and $\hat{\theta} = 0$ for $\tilde{\theta} \geq 0$. Then the asymptotic distribution of the MLE follows. \square

For an exponential model \mathcal{F} given by (2.1), with $\Theta = \{c < \theta \leq 0\}$, the likelihood ratio statistic for testing $\theta = 0$, denoted by w , becomes

$$w = 2n\{\hat{\theta}\bar{x} - \kappa(\hat{\theta})\}. \tag{2.3}$$

It is well known from Self and Liang (1987) that if the null model has a natural extension to an open neighbourhood, the asymptotic distribution of w is a fifty–fifty mixture of a χ^2_1 distribution and the unit mass at the origin δ_0 . We denote this mixture by $\tilde{\chi}^2_1$. Here we give a proof of the result with the simplest assumptions.

Corollary 2. *Let \mathcal{F} be a model given by (2.1), with $\Theta = \{c < \theta \leq 0\}$, where the variance of X , σ_0^2 , is finite. The asymptotic distribution of the likelihood ratio test w for $\theta = 0$ is a $\tilde{\chi}^2_1$ distribution.*

Proof. From Proposition 2 the asymptotic distribution of $n\sigma_0^2\hat{\theta}^2$ is a $\tilde{\chi}^2_1$ distribution. Hence, it is sufficient to prove that $w - n\sigma_0^2\hat{\theta}^2 = o_p(1)$. If we extend w , for $\hat{\theta} > 0$, to $\tilde{w}(\hat{\theta}) = n\sigma_0^2\hat{\theta}^2$ then \tilde{w} is a continuously differentiable function in the neighbourhood of 0. Therefore, applying Taylor’s expansion to \tilde{w} , the result follows. □

In an exponential model where the variance of X is not finite, in particular in a steep model, the asymptotic distribution of the likelihood ratio statistic does not generally have to be a $\tilde{\chi}^2_1$ or even a χ^2_1 . However, this does not contradict Self and Liang (1987) because their sufficient conditions are not fulfilled.

The result that links the existence of moments and the derivatives of the characteristic function at zero (Billingsley 1995, Chapter 5) can be extended to one-sided Taylor expansion for the cumulant generating function in our case.

Lemma 1. *Let \mathcal{F} be a model given by (2.1), with $\Theta = \{c < \theta \leq 0\}$, where the absolute moment $E|X|^k$ is finite. Then the derivatives of the cumulant generating function $\kappa^{(r)}(\theta)$, $r \leq k$, defined for $\theta < 0$, extend continuously up to $\theta = 0$. Hence, we have*

$$\kappa(\theta) = \kappa_1\theta + \frac{1}{2}\kappa_2\theta^2 + \frac{1}{3!}\kappa_3\theta^3 + \dots + \frac{1}{k!}\kappa_k\theta^k + o(|\theta|^k), \tag{2.4}$$

where κ_r are the cumulants at $\theta = 0$.

Proof. The result is equivalent to proving that the derivatives of the moment generating function, $M(\theta) = e^{\kappa(\theta)}$, extend continuously.

In the interior points, $c < \theta < 0$, the derivatives exist and are expressed as

$$M^{(r)}(\theta) = \int_{-\infty}^{\infty} x^r e^{\theta x} f(x) dx.$$

To prove continuity we only need to show that the dominated convergence theorem can be applied. We consider two situations.

If $x \geq 0$, then $e^{\theta x} \leq 1$ and

$$\int_0^{\infty} x^r e^{\theta x} f(x) dx \leq \int_0^{\infty} |x|^r f(x) dx < \infty$$

If $x < 0$, we have

$$\frac{|x|^r}{r!} \leq e^{|x|} = e^{-x}.$$

For $\varepsilon > 0$, replacing x by εx we have

$$|x|^r e^{\theta x} \leq r! \varepsilon^{-r} e^{(\theta-\varepsilon)x}$$

we can choose ε small enough to have $c < \theta - \varepsilon < 0$. Therefore,

$$\left| \int_{-\infty}^0 x^r e^{\theta x} f(x) dx \right| \leq r! \varepsilon^{-r} \int_{-\infty}^0 e^{(\theta-\varepsilon)x} f(x) dx < \infty.$$

□

3. Saddlepoint approximation at the boundary

In this section we assume that \mathcal{F} is an exponential model given by (2.1), with $\Theta = \{c < \theta \leq 0\}$, and also that the sample mean \bar{x} has a bounded density for some n . This assumption can also be expressed in terms of integrability of the characteristic function (Kolassa 1994, Chapter 6). In this situation, we will derive high-order properties for the likelihood ratio test. The saddlepoint approximation does not always exist for the whole range of the distribution, as noted in the pioneering paper of Daniels (1954). Fortunately, it exists in cases which are useful in our situation.

Following Daniels (1954), when $\bar{x} < \mu_0$ we have the saddlepoint approximation to the probability density function of the sample mean

$$f_{\bar{x}}(\bar{x}) = \sqrt{n} \frac{\exp\{-n(\hat{\theta}\bar{x} - \kappa(\hat{\theta}))\}}{\sqrt{2\pi\sigma(\hat{\theta})}} \{1 + \mathcal{O}(n^{-1})\}, \tag{3.1}$$

where $\hat{\theta}$ is defined by $\kappa'(\hat{\theta}) = \bar{x}$, and $\sigma(\hat{\theta})^2 = \kappa''(\hat{\theta})$ is the variance of X with the probability density function $f(x; \hat{\theta})$. In particular, $\sigma_0^2 = \kappa''(0)$ is the variance with respect to $f(x)$.

From the likelihood ratio statistic, w , let us consider the one-to-one transform of \bar{x} , for $\bar{x} \leq \mu_0$, given by the *signed log-likelihood ratio statistic*

$$r = \text{sgn}(\hat{\theta})\sqrt{w}, \tag{3.2}$$

extended by zero when $\bar{x} \geq \mu_0$.

When $\bar{x} < \mu_0$, we easily deduce from (3.1) and the Jacobian $\partial r / \partial \bar{x} = n\hat{\theta} / r$, an approximation to the probability density function of r ,

$$f_r(r) = \frac{1}{\sqrt{2\pi u}} \frac{r}{r} e^{-r^2/2} \{1 + \mathcal{O}(n^{-1})\}, \tag{3.3}$$

where $u = \sqrt{n\hat{\theta}\sigma(\hat{\theta})}$.

The last expression suggests we should look for a modified version of r with dominant term equal to the standard normal density. Such a modified version was suggested in Barndorff-Nielsen (1986):

$$r^* = r + \frac{1}{r} \log\left(\frac{u}{r}\right). \tag{3.4}$$

Hence, the modified likelihood ratio test statistic will be

$$w^* = (r^*)^2. \tag{3.5}$$

In the next result the probability density function of r^* is found.

Theorem 1. *Let \mathcal{F} be a model given by (2.1), with $\Theta = \{c < \theta \leq 0\}$, where $E[X^4] < \infty$ and the sample mean \bar{x} has a bounded density for some n .*

(i) *The probability density function of r^* , when $\bar{x} < \mu_0$, is given by*

$$f_{r^*}(r^*) = \frac{1}{\sqrt{2\pi}} e^{-(r^*)^2/2} \{1 + \mathcal{O}(n^{-1})\}.$$

(ii) *The asymptotic distributions of $\sqrt{n}\sigma_0\hat{\theta}$, r and r^* are the same.*

Proof. First of all we consider the expressions

$$u = \sqrt{n}\theta\kappa''(\theta)^{1/2}, \quad r = -\sqrt{2n}(\theta\kappa'(\theta) - \kappa(\theta))^{1/2}.$$

From Lemma 1 we have the expansions

$$u = \sqrt{n} \left\{ \sqrt{\kappa_2} \theta + \frac{\kappa_3 \theta^2}{2\sqrt{\kappa_2}} + \frac{2\kappa_2 \kappa_4 - \kappa_3^2}{8\kappa_2^{3/2}} \theta^3 + o(|\theta|^3) \right\}, \tag{3.6}$$

$$r = \sqrt{n} \left\{ \sqrt{\kappa_2} \theta + \frac{\kappa_3 \theta^2}{3\sqrt{\kappa_2}} + \frac{9\kappa_2 \kappa_4 - 4\kappa_3^2}{72\kappa_2^{3/2}} \theta^3 + o(|\theta|^3) \right\}. \tag{3.7}$$

From the definition of r^* in (3.4) we can compute that

$$r^* - r = \frac{1}{\sqrt{n}} \left\{ \frac{\kappa_3}{6\kappa_2^{3/2}} + \frac{9\kappa_2 \kappa_4 - 14\kappa_3^2}{72\kappa_2^{5/2}} \theta + o(|\theta|) \right\}. \tag{3.8}$$

It follows that

$$\Delta r = r^* - r = \mathcal{O}(n^{-1/2}), \quad \frac{\partial \Delta r}{\partial \theta} = \mathcal{O}(n^{-1/2}), \quad \frac{\partial \theta}{\partial r} = \mathcal{O}(n^{-1/2}).$$

Hence

$$e^{(\Delta r)^2/2} = 1 + \mathcal{O}(n^{-1})$$

and

$$\frac{\partial r^*}{\partial r} = 1 + \frac{\partial \Delta r}{\partial \theta} \frac{\partial \theta}{\partial r} = 1 + \mathcal{O}(n^{-1}).$$

Finally, from (3.3),

$$f_{r^*}(r^*) = \frac{1}{\sqrt{2\pi}} e^{-(r^*)^2/2} e^{\Delta r^2/2} \{1 + \mathcal{O}(n^{-1})\} \left| \frac{\partial r^*}{\partial r} \right| = \frac{1}{\sqrt{2\pi}} e^{-(r^*)^2/2} \{1 + \mathcal{O}(n^{-1})\}.$$

We are now considering r and r^* as functions of the maximum likelihood estimator $\hat{\theta}$. In Section 2 we showed that $\hat{\theta} \xrightarrow{p} 0$, hence from (3.7) we find that $r - \sqrt{n}\sigma_0\hat{\theta} = o_p(1)$, where $\sigma_0 = \sqrt{\kappa_2}$. Clearly from (3.8), $r^* - r = o_p(1)$. □

The last result shows that r^* has the same properties as the saddlepoint method. That is, we have control over the relative error of the probability density function with respect to the standard normal, and the relative error is of order $\mathcal{O}(n^{-1})$.

From the Theorem 1 and the Proposition 2 we have:

Proposition 3. *Let \mathcal{F} be an exponential model under the assumptions of Theorem 1. Then the asymptotic convergence*

$$r^* \xrightarrow{d} \frac{1}{2} N_-(0, 1) + \frac{1}{2} \delta_0$$

has relative error $\mathcal{O}_p(n^{-1})$.

Finally, from this last result (3.5) improves the convergence of Corollary 2.

Corollary 3. *Let \mathcal{F} be an exponential model under the assumptions of Theorem 1. Then the asymptotic convergence of w^* to $\bar{\chi}_1^2$ has relative error $\mathcal{O}_p(n^{-1})$.*

4. Applications in reliability theory and survival analysis

The results of the previous sections extend to some more general situations. For instance, let X be a continuous random variable with probability density function $f(x)$. Assume that $T(X)$ is a statistic with cumulant generating function $\kappa_T(\theta) = \log E[e^{\theta T(x)}]$ that converges for θ in Θ . We can construct by *exponential tilting* the set of all distributions

$$f(x; \theta) = e^{\theta T(x) - \kappa_T(\theta)} f(x), \quad \theta \in \Theta, \tag{4.1}$$

which is a full exponential model. If $T(x)$ is a one-to-one function of x , this model reduces to (2.1) by considering the distribution of the random variable $T = T(X)$. Moreover, since the asymptotic distribution is a local property, the results of the previous sections apply when $T(x)$ is simply a one-to-one function of x in a neighbourhood of the boundary point. Hence, in order to apply Corollary 3 in this case we need to assume $E[T(X)^4] < \infty$.

The most important distributions in reliability and survival analysis are increasing failure rate (IFR) distributions. A relevant particular case is the exponential distribution which has constant failure rate. It can be seen that the convexity of the negative logarithm of the density ensures that a distribution belongs to the IFR class. Here we consider two-parameter exponential models with probability density function on $x \geq 0$, of the form

$$p(x; \alpha, \beta) = \exp(-\alpha x - \beta S(x)) / C(\alpha, \beta), \tag{4.2}$$

where S is a convex function and C is the normalizing constant. Moreover, if we assume that

$$\lim_{x \rightarrow \infty} \frac{S(x)}{x} = \infty, \quad (4.3)$$

then the model is only defined for $\beta \geq 0$, hence all the distributions are IFR, because convexity is invariant under linear transforms; see del Castillo and Puig (1999b). Hence, clearly (4.2) is an exponential model with boundary points. The boundary, $\beta = 0$, corresponds to the exponential distribution. Hence, a likelihood ratio test can be used to test exponentiality against alternatives in IFR.

The possible choices for the function S that lead to the model (4.2) being scale invariant are $\log x$, $x \log x$, and x^q for any real number q ; again see del Castillo and Puig (1999b). When $S(x) = \log(x)$ the model (4.2) is the gamma distribution and there are no boundary points. With the assumption (4.3) only the functions $x \log x$ and x^q , for $q > 1$, are admissible. Because the function $x \log(x)$ is not a one-to-one transformation we do not consider this case.

Under the null hypothesis of exponentiality we have that $E[X^k]$ are finite for $k \geq 0$. Hence, the model (4.2) with $S(x) = x^q$ ($q > 1$) has moments of all orders and $S(x)$ is a one-to-one transformation of x in the sample space ($x > 0$).

If α is fixed the model (4.2) is a particular case of (4.1) and the saddlepoint approximation for the likelihood ratio test $\beta = 0$, given by Corollary 3, can reasonably be used. In general, α is a nuisance parameter. However, since (4.2) is scale invariant and the likelihood ratio test, w , is also invariant, its distribution conditional on α does not depend on α . Hence, as in the no nuisance parameter case, we can apply the w^* transform.

Example 2. In an example discussed by Lee (1992), the remission times in weeks of 21 patients with acute leukaemia were as follows:

1, 1, 2, 2, 3, 4, 4, 5, 5, 8, 8, 8, 8, 11, 11, 12, 12, 15, 17, 22, 23.

Del Castillo and Puig (1999b) showed that the fits obtained by the Weibull distribution, proposed by Lee (1992), in this example can be improved by the model (4.2) with $S(x) = x^3$. The maximum likelihood estimators are $\hat{\alpha} = 0.031334$ and $\hat{\beta} = 0.00012846$.

We can consider testing exponentiality with the likelihood ratio test. In this example

$$w = 2\{l(\hat{\alpha}, \hat{\beta}) - l(\tilde{\alpha}, 0)\} = 2.68367,$$

where l is the log-likelihood function and $\tilde{\alpha} = 1/\bar{x} = 0.11538$ is the maximum likelihood estimator of α under the null hypothesis.

The asymptotic distribution of w is a $\tilde{\chi}_1^2$ distribution, as Corollary 2 shows. The same asymptotic distribution works for the saddlepoint correction w^* , from Corollary 3, but with a smaller relative error. In this case, the critical point of the asymptotic distribution is $\tilde{\chi}_1^2(0.05) = 2.70554$. Hence $w = 2.68367$ leads to the rejection of the null hypothesis. However, our saddlepoint correction with higher accuracy gives $w^* = 1.5255$, suggesting the acceptance of exponentiality. The nominal p -values, using the asymptotic distribution for w and w^* , are 0.057 and 0.1048, respectively. However, the issue is whether a sample size of $n = 21$ is enough to accept these results.

Table 1. Empirical critical points for the distribution of w and w^* for sample size $n = 21$, to test exponentiality with a nuisance parameter α based on 100 000 samples. $n = \infty$ corresponds to the theoretical critical points for their asymptotic distributions

	$\alpha = 0.1$	$\alpha = 0.05$	$\alpha = 0.01$
w	2.829 51	4.108 65	7.111 14
w^*	1.644 95	2.725 68	5.385 18
$n = \infty$	1.642 37	2.705 54	5.411 89

Since the model is scale invariant and the likelihood ratio test is also invariant, we can check these results by simulation, taking a fixed value for the nuisance parameter. The results are based on 100 000 samples with $\alpha = 1$. The p -value obtained from simulation is 0.1069, very close to that corresponding to w^* , and it also leads us to not reject the null hypothesis. Taking the result obtained by simulation as the exact value, we see that the likelihood ratio test, w , has a relative error of 53% and its saddlepoint correction, w^* , less than 1.4%; this shows the high improvement obtained by saddlepoint correction.

Table 1 shows the empirical critical points for the distribution of the statistics w and w^* as well as the nominal critical points for the asymptotic distribution. We can see that for a sample size as small as 21, the empirical critical points for w^* are close to the nominal ones.

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