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Power Transformations when the Choice of Power
is Restricted to a Finite Set

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Abstract

We study the family of power transformations proposed by Box and Cox (1964) when the choice of the power parameter λ is restricted to a finite set Ω_R . The two cases in which obvious answers obtain are when the true parameter λ is an element of Ω_R and when λ is "far" from Ω_R . We study the case in which λ_0 is "close" to Ω_R , finding that the resulting methods can be very different from unrestricted maximum likelihood and that inference depends on the design, the values of the regression parameters, and the distance of λ to Ω_R .

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A. D. BLOSE

Technical Information Officer

1. Introduction

Box and Cox (1964) suggested the power family of transformations, wherein for some unknown λ ,

$$(1.1) \quad y_i^{(\lambda)} = x_i \beta + \sigma \epsilon_i = \tau_i + \sigma \epsilon_i, \quad i=1, \dots, N.$$

Here the design vectors $x_i = (1 \ c_{i2} \ \dots \ c_{ip})'$, $\beta = (\beta_0 \ \dots \ \beta_{p-1})'$, the ϵ_j are independent and identically distributed with mean zero, variance one and distribution F , and

$$\begin{aligned} y^{(\lambda)} &= (y^{(\lambda)} - 1)/\lambda & \lambda \neq 0 \\ &= \log y & \lambda = 0. \end{aligned}$$

They studied both maximum likelihood and Bayes inference when F is the normal distribution. There is now a substantial literature on the problem, an incomplete list of which includes Andrews (1971), Atkinson (1973), Hinkley (1975), Bickel and Doksum (1980, denoted B-D), Carroll (1980), and Carroll and Ruppert (1980, denoted C-R).

B-D developed an asymptotic theory for estimation. If the normal theory MLE is $\hat{\beta}$ when λ is known and $\beta^* = \hat{\beta}(\hat{\lambda})$ when λ is unknown and estimated by $\hat{\lambda}$, they compute the asymptotic distributions of $N^{1/2}(\hat{\beta} - \beta)/\sigma$ and $N^{1/2}(\beta^* - \beta)/\sigma$ as $N \rightarrow \infty$, $\sigma \rightarrow 0$. These distributions are different, with the latter having a covariance matrix at least as large and often very much larger than that of the former; the estimates $\hat{\lambda}$ and β^* are highly variable and highly correlated in general. This suggests that there is a large "cost" due to estimating the power parameter λ . Unfortunately, these results (and independent Monte-Carlo work by Carroll (1980)) suggest that unconditional inference concerning β can be very difficult for, except in certain balanced designs, inference without taking into account the variability of $\hat{\lambda}$ will be incorrect while β^* is itself too variable to be much help. A theory for conditional inference might prove useful.

It is relevant to note that when $\beta=0$ and $\sigma=1$ are known, the curvature (Efron (1975)) for λ at $\lambda=0$ is $\gamma_0^2 = 10.67$; Efron suggests that a value $\gamma_0^2 \geq 1/8$ is "large".

C-R study the prediction problem in the sense of estimating the conditional median of Y given a design point x_0 ; this is inference in the original scale of the data. Their results are much more encouraging; while there is a cost due to estimating λ , it is generally not severe. For example, if $\beta = (\beta_0 \beta_1 \dots \beta_{p-1})'$, the cost averaged over the distribution of the design is $(1+p)^{-1}$ (asymptotically as $N \rightarrow \infty$ and $\sigma \rightarrow 0$).

We are concerned with the following point which has been raised concerning the applicability of the B-D and C-R theories. In practice, one may be uncomfortable using an estimate such as $\hat{\lambda} = .037$, then the much more common log scale ($\hat{\lambda}=0$) is "just as good". Thus it is reasonable to restrict the estimate of λ to a finite set Ω_R and to study the consequences of such a decision. Asymptotically, as $N \rightarrow \infty$ but λ and Ω_R stay fixed, one has the trivial results that if $\lambda \in \Omega_R$ one is almost always in the right scale so there are no difficulties, while if $\lambda \notin \Omega_R$ bias dominates and no useful results are obtainable.

In Table 1 we present the results of a Monte-Carlo study for estimating the conditional median of Y given x_0 . The model is simple linear regression based on a uniform design with $\beta_0=5$, $\beta_1=2$ and

$$(1.2) \quad N^{-1} \sum_{i=1}^N x_i' x_i = I_2.$$

The errors were normally distributed with mean 0 and variance σ^2 , and there were 500 replications of the experiment. The restricted power set was $\Omega_R = \{0, \pm 1/2, \pm 1\}$, and we made decisions in this set on the basis of the likelihood. For a given $\hat{\lambda}$, our estimator is

$$(1.3) \quad \begin{aligned} & (1 + \hat{\lambda} x_0 \beta^*)^{1/\hat{\lambda}} & (\hat{\lambda} \neq 0) \\ & \exp(x_0 \beta^*) & (\hat{\lambda} = 0) \end{aligned}$$

The numbers listed in the Table 1 are the "relative mean square errors (MSE)", i.e., the mean square error of (1.3) divided by the MSE when λ is known. We list results for the origin $x_0 = (1 \ 0)$ and

when x_0 is a randomly chosen number of the design; the latter is in effect an average relative MSE over the distribution of the design.

In Table 1 we see that the restricted estimator (RE) dominates the MLE when $\lambda=0$ (hence $\lambda \in \Omega_R$), while the MLE dominates when $\lambda \notin \Omega_R$. In this latter case note that increasing N or decreasing σ results in improved performance of the MLE relative to the RE.

In Table 2 we repeat the above experiment with the changes $\beta_0=7$, $\beta_1=4$. The slightly worse behavior of the MLE relative to the λ -known case is expected from the C-R theory. Note here that the change in parameter values causes the RE to be much worse than the MLE if $\lambda \notin \Omega_R$. Also, the effect of changing N or σ is highlighted.

From the Monte-Carlo, we see that the performance of the RE relative to the MLE depends on λ , N , σ and β . One purpose of the rest of this paper is to propose and investigate a simple theory which gives a somewhat more systematic understanding of this performance. More generally, we also investigate the question of the feasibility of constructing procedures for which the choice of λ is restricted but which also give performance comparable to the MLE.

Table 1

The MSE behavior of the MLE and RE relative to the λ -known estimate of the conditional median of Y given x_0 . Here $\Omega_R = \{0, \pm 1/2, \pm 1\}$, $\beta_0 = 5$ and $\beta_1 = 2$.

			ORIGIN ($x_0 = (0 \ 1)$)			AVERAGE (x_0 random member of design)		
N	σ	λ	MLE	RE	Ratio (High/Low)	MLE	RE	RATIO
20	1	0	1.17	1.05	1.11	1.07	1.01	1.06
20	1/2	0	1.28	1.18	1.08	1.17	1.01	1.16
40	1		1.13	1.00	1.13	1.08	1.00	1.08
40	1/2		1.22	1.00	1.22	1.16	1.00	1.16
20	1	1/8	1.13	1.26	1.12	1.07	1.15	1.07
20	1/2	1/8	1.25	1.43	1.14	1.13	1.24	1.10
40	1		1.12	1.29	1.15	1.03	1.10	1.07
40	1/2		1.25	1.53	1.22	1.05	1.24	1.18
20	1	1/4	1.12	1.17	1.04	1.06	1.10	1.04
20	1/2	1/4	1.24	1.34	1.08	1.12	1.24	1.11
40	1		1.10	1.29	1.17	1.04	1.10	1.06
40	1/2		1.23	1.52	1.24	1.06	1.14	1.08

Table 2

The MSE behavior of the MLE and RE relative to the λ -known estimate of the conditional median of Y given x_0 . Here $\Omega_R = \{0, \pm 1/2, \pm 1\}$, $\beta_0 = 7$ and $\beta_1 = 4$.

N	σ	λ	ORIGEN ($x_0 = (0 \ 1)$)			AVERAGE (x_0 random member of design)		
			MLE	RE	Ratio (High/Low)	MLE	RE	RATIO
20	1	0	1.34	1.00	1.34	1.25	1.00	1.25
20	1/2	0	1.43	1.00	1.43	1.27	1.00	1.27
40	1	0	1.23	1.00	1.23	1.32	1.00	1.32
40	1/2	0	1.37	1.00	1.37	1.27	1.00	1.27
20	1	1/8	1.25	1.72	1.38	1.15	1.61	1.40
20	1/2	1/8	1.37	2.24	1.64	1.18	2.30	1.95
40	1	1/8	1.24	1.80	1.45	1.04	1.59	1.53
40	1/2	1/8	1.38	2.47	1.79	1.07	2.33	2.18
20	1	1/4	1.24	1.65	1.33	1.13	1.49	1.32
20	1/2	1/4	1.36	2.52	1.85	1.16	2.19	1.89
40	1	1/4	1.22	2.11	1.73	1.05	1.42	1.35
40	1/2	1/4	1.36	3.41	2.51	1.09	2.20	2.02

2. A large sample theory

Any reasonable theory must have λ "close" to Ω_R for large sample sizes. We choose to do this by letting the cardinality of Ω_R increase with increasing sample size N and by letting $\lambda = \lambda_N$ converge to a fixed element of Ω_R . For ease of calculation we focus on the important special case that the log scale is "almost" correct, i.e., Ω_R always contains zero and

$$\lambda = b\sigma/N^{1/2}.$$

Of course, when $b = 0$ the data truly have a log-normal distribution.

Let $\hat{\lambda}_R$ and $\hat{\lambda}_M$ denote the restricted and ML estimates of λ , let $\hat{\beta}_R$ or β^* be the estimate of β having chosen the power $\hat{\lambda}_R$ or $\hat{\lambda}_M$, and let

$$\begin{aligned} f(\lambda, x_0 \beta) &= (1 + \lambda x_0 \beta)^{1/\lambda} & (\lambda \neq 0) \\ &= \exp(x_0 \beta) & (\lambda = 0), \end{aligned}$$

which is the conditional median of Y given x_0 , with estimate (1.2). We assume the errors are normally distributed. Letting $e = (1 \ 0 \ \dots \ 0)$, we assume

$$\begin{aligned} \underline{x}_i' e' &= 1 & (\text{there is an intercept}) \\ N^{-1} \sum \underline{x}_i' \underline{x}_i &= I : \end{aligned}$$

Then, for any value of b , when λ is known the limit MSE is

$$(2.2) \quad \text{MSE}(\lambda \text{ known}) = \|\underline{x}_0\|^2 \exp(2 \underline{x}_0 \beta).$$

For fixed σ the computations are very difficult, so we will follow the lead of Bickel and Doksum and consider only the case that $\sigma = \Gamma \eta$, where $\Gamma = \Gamma(N) \rightarrow 0$ is a known sequence; it simplifies notation to make the convention $\eta = 1$.

We are now in a position to define the restricted estimate $\hat{\lambda}_R$ of λ , which we take by convention to satisfy $|\hat{\lambda}_R| \leq 1$. Let $\mathcal{D} = \{d_k\}$ be a finite or countably infinite subset of the extended real line with $d_0 = 0$, $d_{-k} = -d_k$, and $\sup\{d_k\} = \infty$. Define intervals midway between these points:

$$B_k = \left[(d_{k-1} + d_k)/2, (d_k + d_{k+1})/2 \right].$$

Our restricted estimate $\hat{\lambda}_R$ satisfies $|\hat{\lambda}_R| \leq 1$ and maximizes the likelihood over the admissible set with $N^{1/2} \hat{\lambda}_R / \Gamma \in \mathcal{D}$.

Asymptotically, the procedure becomes

Choose $N^{1/2} \hat{\lambda}_R / \Gamma = d_k$ if $N^{1/2} \hat{\lambda}_M / \Gamma \in B_k$ and $|\hat{\lambda}_R| \leq 1$.

If not possible, choose $\hat{\lambda}_R = \pm 1$ on the basis of the likelihood.

The resulting estimate of β is $\hat{\beta}_R$ and the estimate of the conditional median of Y given x_0 is $f(\hat{\lambda}_R, x_0 \hat{\beta}_R)$.

The above procedure is asymptotically the same as a restricted maximum likelihood method and is quite intuitive as it chooses the point in $\mathcal{D}$ closest to $N^{1/2} \hat{\lambda}_M / \Gamma$. Note also that as N increases, the number of possible choices for scale also increases, as desired. Make the definitions:

$$q_N = N^{-1} \sum_{i=1}^N \tau_i^2 x_i \rightarrow q$$

$$a_1 = [x_0 q' - (x_0 \beta)^2] / 2$$

$$c_N = (-\tau_1^2 / 2 \dots -\tau_N^2 / 2)$$

$$x_N' = (x_1' \dots x_N')$$

$$e_N = (1/4) \{ N^{-1} \sum_{i=1}^N \tau_i^4 - \|q_N\|^2 \} \rightarrow e_0 > 0.$$

Theorem. Using the B-D asymptotics, the limit distribution of the restricted estimator of the conditional median

$$(2.1) \quad N^{1/2} \left[f(\hat{\lambda}_R, x_0 \hat{\beta}_R) - f(\lambda = b\sigma/N^{1/2}, x_0 \beta) \right]$$

is given by

$$(2.2) \quad \exp(x_0 \beta) \left[\|x_0\| Z_1 + a_1 \sum_k (d_k - b) I(c_0^{-1/2} Z_2 + b \in B_k) \right],$$

where Z_1 and Z_2 are independent standard normal random variables. The proof is in the appendix.

The Theorem shows that the estimate of the conditional median of Y given x_0 based on a restricted choice of λ is not necessarily asymptotically normally distributed.

Example #1. Suppose that for any sample size we restrict our choice of $\hat{\lambda}_R$ to a fixed set, say

$$\Omega_R = \{0, \pm 1/2, \pm 1\}.$$

In this case we eventually have $\hat{\lambda}_R = 0$ so that $\mathcal{D} = \{0, \pm \infty\}$ and

(2.3) MSE (fixed finite set)

$$\rightarrow \exp(2 x_0 \beta) \left[\|x_0\|^2 + b^2 a_1^2 \right].$$

In simple linear regression with a symmetric design and fourth moment μ_4 satisfying (1.2), we find that at the origin $x_0 = (1, 0)$, $a_1^2 = \beta_1^4/4$ and $c_0 = \beta_1^4(\mu_4 - 1)/4$. In this case, while (2.3) does not serve as a very good method for predicting the individual values in Tables 1 and 2, it does, however, lead to the following qualitative conclusions, all of which are satisfied by the simulations:

(i) Changing the value of N from 20 to 40 while fixing Ω_R and λ basically increase b by a factor of $\sqrt{2}$. Hence, larger values of N will result in a worse performance for the RE when $\lambda \notin \Omega_R$.

(ii) Changing σ from 1 to $1/2$ increases b by a factor of 2 and should result in worse performance for the RE.

(iii) Changing p_1 from 2 to 4 increases the term β_1^4 by a factor of sixteen. Such a large change should cause much worse performance in Table 2.

(iv) The increase in (iii) above should make the changes in the RE when one changes N or σ much more dramatic in Table 2 than in Table 1.

Example #2. The theory includes the MLE $\hat{\lambda}_M$ by choosing $\mathcal{V}$ dense. In this case we get

(2.4a) MSE (MLE of λ)

$$+ \exp(2x_0\beta) \left[\|x_0\|^2 + a_1^2/e_0 \right] .$$

In the simple linear regression, at the origin this becomes

$$(2.4b) \quad \exp(2\beta_0) \left[1 + (u_4-1)^{-1} \right] .$$

Note that (2.4b) is independent of the value of b .

Example #3. An interesting example in which the number of possible values of $\hat{\lambda}_R$ increases with N occurs when $\mathcal{V} = \{\text{all integers}\}$. It is not too unreasonable to suspect that this restricted estimate will be at least comparable to the MLE, perhaps somewhat better when $b=0$ and hence $\lambda \in \Omega_R$, but not too much worse when $b = 1/2$ and $\lambda \notin \Omega_R$. In this case

(2.5) MSE (restricted procedure)

$$+ \exp(2x_0\beta) \left[\|x_0\|^2 + (a_1^2 e_0^{-1}) \sum_k (k-b)^2 e_0 P\{e_0^{-1/2}Z + b \in B_k\} \right] .$$

The only important difference between (2.4a) and (2.5) is the term

$$\sum_k (k-b)^2 e_0 P\{e_0^{-1/2}Z + b \in B_k\} .$$

In Table 3 we compare the values of (2.4b) and (2.5) for the uniform simple linear regression design of the introduction with $\mu_4 = 1.79$; all comparisons are at the origin $x_0 = (1 \ 0)$.

Table 3

Comparison of MSE for a simple linear regression design with moments $\mu_1 = \mu_3 = 0$, $\mu_2 = 1$, $\mu_4 = 1.79$, $x_0 = (1 \ 0)$

b	β_1	$\frac{\text{MSE(ML\ddot{E})}}{\text{MSE}(\lambda \text{ known})}$	$\frac{\text{MSE(RE)}}{\text{MSE}(\lambda \text{ known})}$	$\frac{\text{MSE(RE)}}{\text{MSE(ML\ddot{E})}}$
0	1.5	2.27	2.37	1.04
0	2.0	2.27	2.59	1.14
0	4.0	2.27	1.03	.45
1/2	1.5	2.27	2.37	1.04
1/2	2.0	2.27	2.61	1.15
1/2	4.0	2.27	129.42	57.01

The results are somewhat surprising. First note that the case $b=0$ corresponds to situations in which λ truly belongs to the set Ω_R . The restricted estimate does not always outperform the MLE, although it does for large β_1 . What is even more interesting is the case $b=1/2$, which is one of the simplest cases in which λ is not in the set Ω_R although it is quite close. Here we see that the restricted procedure can perform very badly indeed.

Tables 1-3 and the Theorem thus suggest that if the number of possible choices of scale is only on the order of $N^{1/2}$, the performance of the resulting estimates will differ from estimates based on the MLE of λ , in some cases being better but in others being very much worse. If one has no prior belief or evidence that only a finite number of values of λ are possible, but rather in estimating the conditional median of Y given x_0 one wants to make only "reasonable" choices of λ while retaining MLE-type behavior, the number of possible choices of λ will have to be

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Appendix

We will use contiguity techniques (Hajek and Sidak (1978)). Let L_1 be the log-likelihood when $b=0$ and let L_2 be the log-likelihood for fixed $b \neq 0$. Somewhat detailed calculations show that as $N \rightarrow \infty$, $\sigma \rightarrow 0$, under the distribution L_1 with $\lambda = 0$,

$$(A.1) \quad -(L_2 - L_1) = (b^2/8N) \sum_{i=1}^N \tau_i^4 + (bN^{-1/2}) \sum_{i=1}^N \epsilon_i \tau_i^2/2 + o_p(1).$$

This shows that the case $b \neq 0$ is contiguous to the case $b=0$.

Proof of the Theorem: When $\lambda = b = 0$ it follows by a Taylor expansion in λ_R that as $N \rightarrow \infty$, $\sigma \rightarrow 0$

$$(A.2) \quad S_N = N^{1/2} \left[f(\hat{\lambda}_R, \hat{\beta}_R) - f(\lambda=0, \beta) \right] \exp(-x_0' \beta) \\ = N^{-1/2} \sum_{i=1}^N x_0 x_i' \epsilon_i + a_1 N^{1/2} \hat{\lambda}_R / \sigma + o_p(1).$$

Also, B-D show that when $\lambda = 0$,

$$(A.3) \quad 2e_0 N^{1/2} \hat{\lambda}_M / \sigma = N^{-1/2} \sum_{i=1}^N (\tau_i^2 - x_i' q') \epsilon_i + o_p(1).$$

It is easy to check that the r.h.s. of (A.3) is asymptotically independent of the first term on the r.h.s. of (A.2). We now use the definition of $\hat{\lambda}_R$ and the convention $\sigma = r(N)\eta = r(N)$ to obtain that when $\lambda = 0$, as $N \rightarrow \infty$ and $\sigma \rightarrow 0$,

$$(A.4) \quad S_N = N^{-1/2} \sum_{i=1}^N x_0 x_i' \epsilon_i + a_1 \sum_k d_k I(N^{1/2} \hat{\lambda}_M / \sigma \in B_k) + o_p(1).$$

We are now in a position to use Theorem 7.2 of Roussas (1972, page 38). In his notation,

$$(A.5) \quad T_N' = N^{-1/2} \sum_{i=1}^N (x_0 x_i' \epsilon_i \quad q x_i' \epsilon_i \quad \tau_i^2 \epsilon_i) \\ \Gamma = E T_N T_N' \\ h' = (0 \quad 0 \quad -b/2).$$

One can show that the terms in (A.5) satisfy the conditions of Roussas' Theorem 7.2 so that when $\lambda = b \sigma N^{-1/2}$, as $N \rightarrow \infty$ and $\sigma \rightarrow 0$, T_N is asymptotically normally distributed with mean Γh and covariance Γ . Because of (A.3), this means that $N^{1/2} \hat{\lambda}_N / \sigma$ and the first term on the r.h.s. of (A.2) are, when $\lambda = b \sigma N^{-1/2}$, jointly asymptotically normally distributed with means $(h - b x_0 q/2)$, variances $(c_0^{-1}, \|x_0\|^2)$ and zero covariance. From this we obtain that (2.1) is asymptotically distributed with the same distribution as

$$\|x_0\| Z_1 - b a_1 + a_1 \sum_k d_k (c_0^{-1/2} Z_2 + b \in B_k),$$

where Z_1 and Z_2 are as in the Theorem. This completes the proof. □