On the proper use of Box-Cox transformation method: a note on a Taguchi case study

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Summary

In studying the role of transformation in the Taguchi method, Logothetis (1990) analyzed the data from a plasma etching process and concluded that the Box-Cox method can induce a mean bias in the variability performance measure which can inhibit the production of clearcut results. This paper points out that the above conclusion is in part due to an inappropriate application of the Box-Cox method where the transformation parameter is determined from one model but the analysis is done on the other. Further, it may not be appropriate to state that Box-Cox method induces a mean bias, but rather that there exists an intrinsic nonlinear relationship between the trial means and the trial variances and the Box-Cox transformation applied to the original data is just unable to transform it away. However, if the Box-Cox transformation is applied to the original trial means and standard deviations, the dependence vanishes and clearcut results are obtained.

Key words: β-technique; Box-Cox transformation; Heteroscedasticity; Noise performance measure; Target performance measure

Introduction

In studying the capability of Box-Cox transformation in simplifying and validating a 'Taguchi analysis', Logothetis (1990) analyzed the data from a plasma etching process that was used to define the interconnect tracks on an integrated circuit. He concluded that Box-Cox method can induce a mean bias in the variability performance measure which can inhibit the production of clearcut separation between target control factors (TCF) and variability control factors (VCF). This paper points out that the above conclusion is partially due to an inappropriate application of the Box-Cox method where the transformation parameter is determined from one model that contains only linear effects but the analysis is done on the other that contains both linear and quadratic effects. To reduce the mean bias and to achieve clear separation, new target performance measure (TPM) and noise performance measure (NPM) are introduced. Analysis of the same data set shows that the newly defined TPM and

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NPM work very well. It achieves a clearcut separation of the two types of factors, reduces the heteroscedasticity of TPMs, and gives a high sensitivity of the model analysis.

We first present briefly the original analysis and a simple remedy of it, then an alternative analysis that contains an analysis of outliers, and then some discussions. For details of the Box-Cox method, the Taguchi method, and the original Taguchi case study, refer to Box and Cox (1964), Logothetis and Wynn (1989) and Logothetis (1990), respectively.

Analysis and Remedy

In the experiment, an $L_{18}(3^6)$ orthogonal array was used to study the effect of six design factors F1-F6, each with three levels, on the response y, the etch rate of the alloy layer. Each of the 18 trials were assigned to two wafers to study the effect of overetch time OE. Five measurements were taken at different locations on each of the 36 wafers to enable study of within wafer variabilities. Since each factor takes three different levels with equal distance, it can be separated into a linear and a quadratic part, called the linear and quadratic effect, respectively.

Logothetis employed TPM(λ) = $\bar{y}(\lambda)$ and NPM(λ) = $-10\log_{10}(s^2(\lambda))$ as measures of target performance and noise performance, where $\bar{y}(\lambda)$ and $s^2(\lambda)$ are the trial mean and variance in $y^{(\lambda)}$ scale with $y^{(\lambda)}$ denoting the power transformation (Box and Cox, 1964). He considered two methods for choosing λ: the Box-Cox transformation method and the β-method, yielding $\lambda = -1$ and 0.5, respectively. When estimating the Box-Cox transformation, he used a model with only linear effects and obtained $\lambda = -1$, but when analyzing TPM(-1) and NPM(-1), he switched to the full additive model with both linear and quadratic effects. Obviously, the correct application of the Box-Cox transformation technique should be that once a transformation (model) being selected the post transformation analysis should be based on the selected model. Thus, if one does want to analyze the TPMs and NPMs using the full additive model, the correct value for λ should be -0.675 instead of -1 as in Logothetis (1990).

Table 1 summarizes the p-values of the F tests for the effects and for the model (M) and R^2 of the four models with $\lambda = 1$, 0.5, -1 and -0.675, respectively. The effects and the models that are significant at 10% level are highlighted by bold-face letters. The reason for adding the results with $\lambda = 1$ (no transformation) is for comparison and to see the effect of transformation.

Table 1. Analysis based on the full additive models: linear and quadratic effects separated

	$\bar{y}(1)$	$\bar{y}(.5)$	$\bar{y}(-.675)$	$\bar{y}(-1)$	NPM(1)	NPM(.5)	NPM (-.675)	NPM(-1)
L1	**0.0001**	**0.0001**	**0.0001**	**0.0001**	0.6526	0.4314	**0.0011**	**0.0002**
Q1	0.1307	**0.0369**	**0.0018**	**0.0010**	0.9176	0.9513	0.6555	0.5828
L2	0.8807	0.3850	**0.0033**	**0.0008**	**0.0875**	0.1081	0.1805	0.2076
Q2	**0.0001**	**0.0001**	**0.0030**	**0.0099**	0.2116	0.3157	0.6921	0.8212
L3	0.8117	0.6311	0.3366	0.2921	0.8876	0.8593	0.7954	0.7787
Q3	**0.0013**	**0.0014**	**0.0034**	**0.0052**	0.3820	0.2764	0.1182	**0.0924**
L4	**0.0002**	**0.0003**	**0.0007**	**0.0010**	0.5433	0.3869	0.1495	0.1120
Q4	0.1008	0.1425	0.2899	0.3358	0.5187	0.5641	0.6853	0.7214
L5	**0.0001**	**0.0001**	**0.0001**	**0.0001**	**0.0077**	0.1257	0.1287	**0.0232**
Q5	0.6779	0.6659	**0.0236**	**0.0083**	**0.0458**	**0.0507**	**0.0685**	**0.0753**
L6	**0.0001**	**0.0001**	**0.0001**	**0.0001**	0.1241	**0.0318**	**0.0008**	**0.0003**
Q6	**0.0178**	**0.0405**	0.2065	0.2872	0.9926	0.9036	0.7020	0.6507
OE	0.2049	0.1155	**0.0230**	**0.0150**	0.6586	0.7551	0.9992	0.9331
M	**0.0001**	**0.0001**	**0.0001**	**0.0001**	0.1235	0.2067	**0.0067**	**0.0012**
R^2	0.9774	0.9789	0.9806	0.9805	0.5060	0.4645	0.6609	0.7214

From the analysis of $\bar{y}(-1)$ and NPM(−1) based on the full additive models, we see that the linear effects of F1, F5 and F6, and the quadratic effects of F3 and F5 are significant to both $\bar{y}(-1)$ and NPM(−1). Logothetis also claimed the significance of L4 after pooling. Thus five out of six controllable factors significantly affect both the TPM and the NPM, which lead him the main conclusion:

> 'Box-Cox transformation can induce mean bias in the variability performance measure which can inhibit the production of clearcut result'.

He then went on to analyze $\bar{y}(0.5)$ and NPM(0.5) with the $\lambda = 0.5$ selected by his β-method and found that only F5 and F6 significantly affect both the TPM and the NPM. He thus concluded that the β-method ensures the determination of simple, valid and independent performance measures for the mean response and the variability in response.

We argue that Logothetis' conclusion needs more attention if not correction. First, in the inverse scale, L4 is not significant on NPM after pooling and Q3 becomes insignificant after pooling. In fact if we look at the pooled results (Table 2) we found only F1, F5 and F6 are significant on both TPM and NPM. Second, the way that he chose the Box-Cox transformation is inappropriate as argued earlier. If the correct Box-Cox transformation $\lambda = -.675$ (for the full additive model) is used, we found that only the linear effects of F1 and F6 and the quadratic effect of F5 are significant on both TPM and NPM. The pooled results in Table 2 also show that F1, F5 and F6 are significant on both TPM and NPM. Thus, the Box-Cox method actually produces only three overlapped significant factors instead of five (as claimed by Logothetis), compared with the two overlapped significant factors produced by the β-method. This is certainly not a strong evidence to support Logothetis' conclusion.

The above discussions are based on the idea of separating the TCFs and NCFs. If one looks at the results from the goodness of fit point of view, the advantage definitely goes to the Box-Cox method as evidenced by the model p-values (0.0067 vs 0.2067). No doubt, the large model p-value will make it questionable the reliability of the analysis based on the β-method.

Furthermore, a comparison between the $\lambda = 1$ models with the $\lambda = 0.5$ models shows that the $\lambda = 1$ models perform as good as (in fact better than if looking at the combined results of Table 2) the $\lambda = 0.5$ models in terms of separating the TCFs and NCFs but better in terms of model fit. Hence, it seems that the β-transformation has offered more harms than helps, whereas the Box-Cox model improves the model fit significantly and the same time gives a reasonably good separation between the TCFs and NCFs.

Table 2. Analysis based on the full additive models:
linear and quadratic effects are combined

	$\bar{y}(1)$	$\bar{y}(.5)$	$\bar{y}(-.675)$	NPM(1)	NPM(.5)	NPM (-.675)
F1	**0.0001**	**0.0001**	**0.0001**	0.8967	0.7273	**0.0041**
F2	**0.0001**	**0.0002**	**0.0005**	0.1116	0.1690	0.3711
F3	**0.0048**	**0.0052**	**0.0091**	0.6698	0.5373	0.2783
F4	**0.0004**	**0.0006**	**0.0019**	0.6714	0.5786	0.3202
F5	**0.0001**	**0.0001**	**0.0001**	**0.0059**	**0.0516**	**0.0661**
F6	**0.0001**	**0.0001**	**0.0001**	0.2985	**0.0941**	**0.0030**
OE	0.2049	0.1155	**0.0230**	0.6586	0.7551	0.9992
M	**0.0001**	**0.0001**	**0.0001**	0.1235	0.2067	**0.0067**
R^2	0.9774	0.9789	0.9806	0.5060	0.4645	0.6609

The Logothetis' β-method aims to reduce the dependence between trial means and trial standard deviations. From Figure 1, we see that his method indeed improves the linear independence between $s(0.5)$ and $\bar{y}(0.5)$), but is still unable to remove nonlinear dependence. In fact, it does not make much difference in terms of heteroscedasticity as which transformation is applied to the original data if the TPM is defined as the trial mean. Although the Box-Cox method is also unsuccessful in reducing the heteroscedasticity, it may be successful in achieving other goals such as normality of error distributions and simplicity of the model structure. The simplicity is illustrated by the results in Table 3.

Figure 1. Scatter plots of trial standard deviations vs trial means.

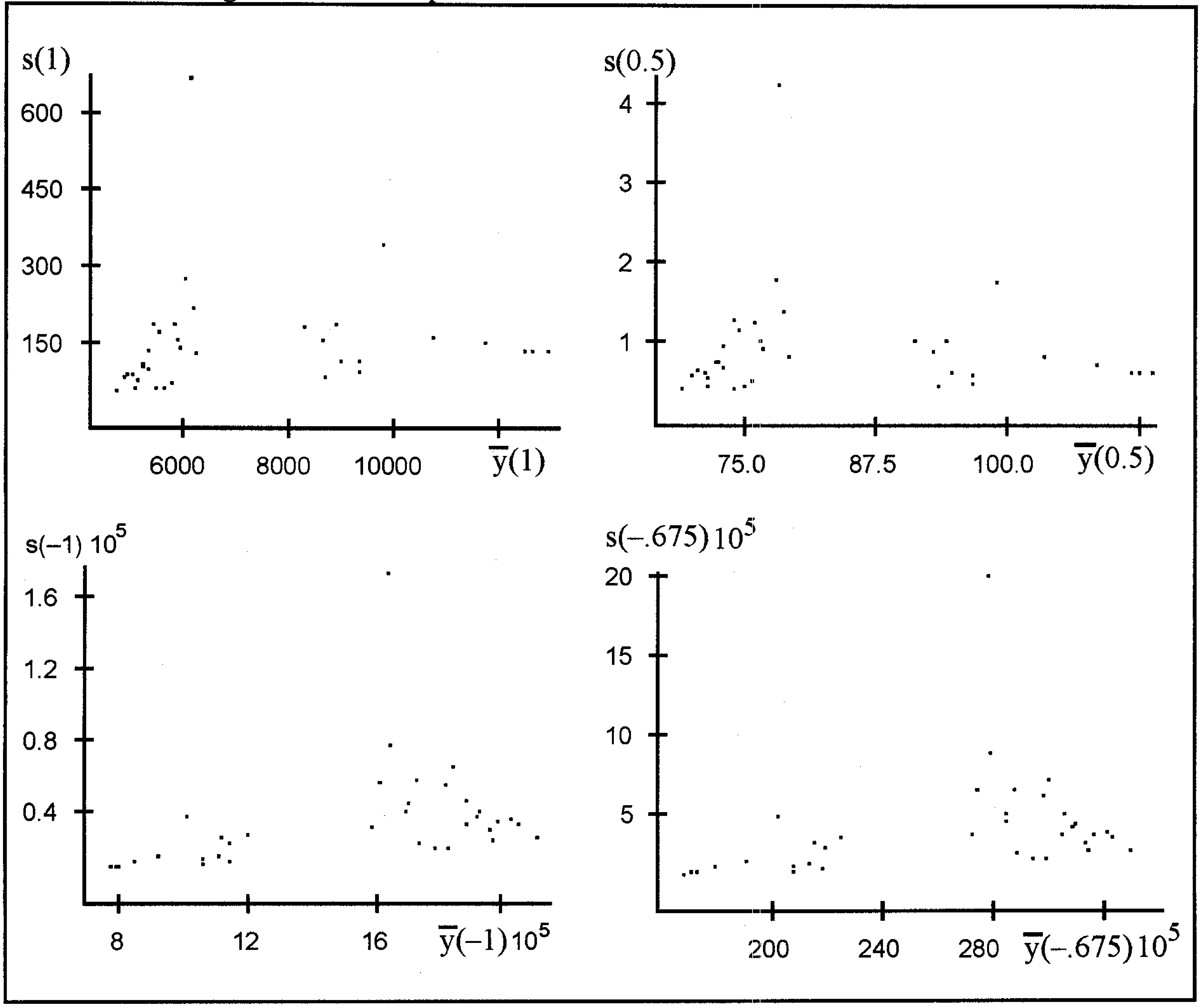


Table 3. Analysis based on models with only linear effects

	$\bar{Y}(1)$	$\bar{Y}(.5)$	$\bar{Y}(-1)$	NPM(1)	NPM(.5)	NPM(−1)
L1	**0.0001**	**0.0001**	**0.0001**	0.6594	0.4370	**0.0001**
L2	0.9277	0.5838	**0.0168**	**0.0918**	0.1106	0.2147
L3	0.8855	0.7630	0.4834	0.8900	0.8613	0.7830
L4	**0.0122**	**0.0111**	**0.0184**	0.5515	0.3926	0.1167
L5	**0.0001**	**0.0001**	**0.0001**	**0.0079**	0.1287	**0.0240**
L6	**0.0001**	**0.0001**	**0.0001**	0.1298	**0.0321**	**0.0002**
OE	0.4375	0.3144	**0.0934**	0.6652	0.7583	0.9344
M	**0.0001**	**0.0001**	**0.0001**	**0.0817**	0.1548	**0.0001**
R^2	0.9208	0.9313	0.9426	0.3403	0.2958	0.6291

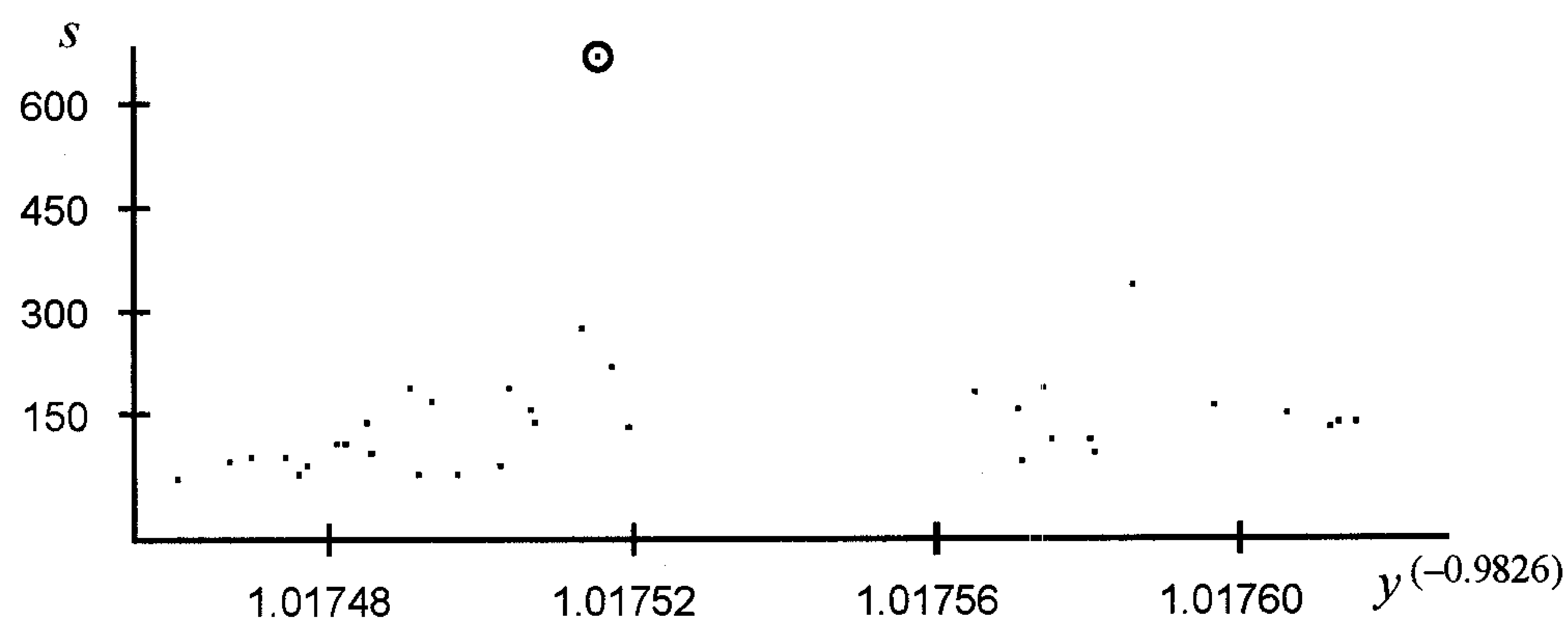
An Alternative Analysis

In terms of both separation of the TCFs and NCFs and model fit, we have found in previous sections that neither the β-method nor the Box-Cox transformation are quite satisfactory. Since the objective variables of analysis are the TPMs that are related to the trial means and the NPMs that are related to the trial standard deviations, it is necessary that they satisfy the linear model assumptions if we decide to analyze them using a linear model technique. The Box-Cox transformation technique aims to transform non-normal variables to normal with constant variances and simple model structure, hence it is natural to define the TPM and NPM as the Box-Cox transformed trial mean ($\bar{y}$) and trial standard deviation (s), respectively,

$$\bar{y}^{(\lambda)} = \begin{cases} (\bar{y}^{\lambda} - 1)/\lambda, & \lambda \neq 0, \\ \log \bar{y}, & \lambda = 0. \end{cases} \qquad s^{(\delta)} = \begin{cases} (s^{\delta} - 1)/\delta, & \delta \neq 0, \\ \log s, & \delta = 0. \end{cases}$$

The parameters λ and δ are estimated from linear models fitted to $\bar{y}^{(\lambda)}$ and $s^{(\delta)}$, respectively. Since λ is estimated in the way that $\bar{y}^{(\hat{\lambda})}$'s are homogeneitic, it is expected that $\bar{y}^{(\hat{\lambda})}$ does not depend much on s. Plots in Figure 2 reflect this point. The results, summarized in the second and third columns of Table 3, show that only factor F5 is highly significant on both the TPM and NPM. Also the model for $s^{(\delta)}$ is significant at 10% level. Hence the analysis based on the new TPM and NPM gives the greatest separation between the TCF and NCF while preserving the goodness of model fit for both models. Separating the effects into linear and quadratic parts shows that only L5 and Q5 are highly significant on both the TPM and NPM. This is consistent with, but sharpens, the analysis of NPM(1) in the last section.

Figure 2. Plot of trial standard deviation vs target performance measure



Analysis of Outliers

The plots of Figures 1 and 2 clearly indicate the existent of a possible outlying value for the trial standard deviation. This value corresponds to trial 3 with OE=90's. Indeed the standard deviation for this trial is unusually large, almost twice as large as the second largest value. A modification of the values in this trial (the two 6880s are changed to 5880s to make them conformable to the other three values 5750, 5750 and 5500 in the trial) improves the analysis significantly with p-values for F5 and for model reduced to almost half of their original values. The major conclusions are kept unchanged. The results after modifying the outlier are listed in the last two columns of Table 3.

Notice that the effect of the outlier on the estimation of the transformation parameters λ and δ is quite significant, especially on the estimation of δ. The $\hat{\lambda}$ value is changed from −0.9826 to −1.1160, whereas the $\hat{\delta}$ value is changed from −0.5007 to −0.0314. However, the analysis of factor effects are very robust against the outliers. After modification of the outlier, we again found that only F5 (or L5 and Q5) are highly significant on both TPM and NPM.

Notice also that after the modification of the outlier, the transformation value −0.0314 (close to zero and hence corresponding to the log transformation) reveals that the two NPM measures NPM(1) and $s^{*(-0.0314)}$ are equivalent, which is confirmed by the actual analysis. This is only a coincidence. It doesn't tell that the original NPM measure performs well when the original data are normal. In fact, we found that after modifying the outlier, the original data still need to be transformed with transformation parameter −0.85.

Table 3. Analysis based on new TPM and NPM before and after modification of outlier

	$\bar{y}^{(-0.9826)}$	$s^{(-0.5007)}$	$\bar{y}^{*(-1.1160)}$	$s^{*(-0.0314)}$
F1	**0.0001**	0.6784	**0.0001**	0.3489
F2	**0.0004**	0.1315	**0.0005**	0.2084
F3	**0.0138**	0.7744	**0.0062**	0.6725
F4	**0.0033**	0.6693	**0.0012**	0.4551
F5	**0.0001**	**0.0030**	**0.0001**	**0.0015**
F6	**0.0001**	0.3377	**0.0001**	0.4540
OE	**0.0151**	0.8046	**0.0174**	0.9285
M	**0.0001**	**0.0955**	**0.0001**	**0.0589**
R^2	0.9802	0.5242	0.9818	0.5552

Discussions

Fearn (1992) provided an alternative analysis for this Taguchi case study and reached a substantial different conclusion from that of Logothetis (1990). In particular, his analysis suggested that an inappropriate treatment of components of error variance plus the overlooking of a large two factor interaction may have let to the identification in the original analysis of too many significant TCFs. His results showed that only L1, L5 and their interaction L1 $\times$L5 are significant TCFs. He also pointed out a misprint in the raw data in Logothetis' paper. Our conclusion differs from that of Logothetis in NCFs. Both Logothetis and Fearn concluded that there is basically no factor that is a significant NCF, but the results of our analysis show that the factor F5 is a highly significant NCF.

Analysis so far has shown that none of transformation is able to remove heteroscedasticity in the analysis of TPM. Our view is that there exists a natural heteroscedasticity in the Taguchi type of data. This is explained as follows: before the experiment, one believes that there are some factors that will significantly affect the TPM and there are some factors that will significantly affect the NPM. An experiment is then designed to model all the potential factors and the data are thus collected. The data that come from an experiment with such a nature would have to be heteroscedastic if there were some significant NCFs. In fact, there are many practical situations where a transformation induces normality and simple model structure, but fails to stabilize the variance. Hence the analysis of the trial means or TPM should be done by combining transformations and weighting (Carroll and Ruppert, 1988).

Logothetis indicated that analysis of variability could be also carried out in terms of the log of the signal-to-noise ratio. Box (1988), in a important article, commented that the log of the signal-to-noise ratio is appropriate as an NPM only when the standard deviation is proportional to the mean of the response (clearly not the case for this example). He then introduced a general transformation approach to suite the other forms of dependence.

Besides transformations to handle the non-normal quality characteristics, there is a rising trend of using generalized linear model (GLM). Myers and Montgomery (1997) presented an excellent tutorial on GLM in connection with off-line quality control. Hamada and Nelder (1997) explained and illustrated how non-normal data can be analyzed alternatively by GLM.

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