

Determining Weights By Entropy Measures In Case Of Heteroscedasticity

Hatice Çiğdem Çin, Atif EVREN

Abstract— In simple regression analysis, the dependent variable is assumed to have constant variance at different levels of independent variable. Whenever the assumption of constant variance fails, some remedies like the weighted least squares, or Box-Cox transformation may be helpful. While Box-Cox approach is based on a nonlinear transformation on the dependent variable, in the weighted least squares methodology, independent variable is rescaled by weights to maintain constant variance. Although there is already a large literature on this issue, determining the weights seems a major problem. In this study, the weights are alternatively calculated by entropy approach, since statistical entropy, and variance conveys similar information about a probability distribution. In this study, by exploiting the normality assumption of linear models, the weights are determined by the reciprocals of Shannon, Tsallis and Rényi entropies of normal distribution. The weighting procedure has been applied on some simulated data having nonconstant variance. In some applications we have shown that weighting by Tsallis and/or Rényi entropies produced better goodness of fit results in terms of coefficient of determination, and the mean square error.

Index Terms— Heteroscedasticity, entropy, weighted least squares, Shannon entropy, Tsallis entropy, Rényi entropy.

I. INTRODUCTION

One of the main assumptions of linear regression model is homoscedasticity. In other words, the variances of dependent variable at each level of independent variable/variables are the same. Heteroscedasticity, or nonconstancy of variances can be detected alternatively. The simplest way is to use visual representation of data, although relying only on visual means may be misleading. Therefore some statistical tools like White Test, or Park's Test are used. Once the heteroscedasticity is detected, to increase the goodness of fit, a kind of weighing procedure is followed. One way is to give more weights to the levels of independent variable/variables whose variabilities are lower. The Box-Cox transformation can also be used to avoid heteroscedasticity. Alternatively, although it's not in common usage, weighting with the reciprocal of entropy can be used. Shannon, Rényi and Tsallis are different types of entropy, and all of them could be used for weighing the data. Indeed, Rényi and Tsallis formulations of entropy bring more flexibility than Shannon entropy, due to their parametric nature.

Hatice Çiğdem Çin, Yildiz Technical University, Faculty of Sciences and Literature, Department of Statistics Davutpasa, Esenler, 34210, Istanbul, Turkey

Atif EVREN, Yildiz Technical University, Faculty of Sciences and Literature, Department of Statistics Davutpasa, Esenler, 34210, Istanbul, Turkey

II. REGRESSION ANALYSIS

The simplest linear model involves only one independent variable, and a constant. The change on the mean of dependent variable is related to only one independent variable. The true mean of Y_i is denoted by $E(Y_i)$. It is stated as below:

$$E(Y_i) = \beta_0 + \beta_1 X_i \quad (1)$$

Here, β_0 is the intercept, and β_1 is the slope. The real Y_i can be found by adding an error item to the true mean of Y_i as

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i \quad (2)$$

The index i indicates the particular observational unit, $i = 1, 2, \dots, n$. X_i 's are observed without any measurement error. The Y_i and X_i are paired observations; both are measured on every observational unit. The random errors ϵ_i 's are assumed to distribute normally with zero mean, and a common variance σ^2 , and to be pairwise independent.

These assumptions imply that the Y_i 's also have common variance σ^2 , and are pairwise independent, since the only random element in the model is ϵ_i . For inferential purposes, the random errors are assumed to be normally distributed, which implies that the Y_i 's are also normally distributed.

III. LEAST SQUARES ESTIMATION

Let $\hat{\beta}_0$ and $\hat{\beta}_1$ be numerical estimates of the parameters β_0 and β_1 , respectively. The least squares principle chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ that minimize the sum of squares of the residuals,

$$SS(\text{Res}) = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2 = \sum \epsilon_i^2 \quad (3)$$

where $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$. In matrix notation, we can find the vector β which is 2×1 matrix, and includes the estimates of β_1 and β_2 . It is as stated below:

$$\hat{\beta} = (X'X)^{-1}(X'Y) \quad (4)$$

where

$$Y_{n \times 1} = \begin{bmatrix} Y_1 \\ Y_2 \\ \dots \\ Y_n \end{bmatrix}, \quad X_{n \times 2} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \dots & \dots \\ 1 & X_n \end{bmatrix}, \quad \hat{\beta}_{2 \times 1} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix}$$

The variances of parameters are given by

$$\text{Var}(\beta) = (X'X)^{-1}\sigma^2 \quad (5)$$

Two general goodness of fit statistics for linear regression models are R^2 , and mean squares error (MSE). R^2 or coefficient of determination is defined as

$$R^2 = 1 - \frac{\sum_{i=1}^n \epsilon_i^2}{\sum_{i=1}^n (Y_i - \bar{Y})^2} \quad (6)$$

Verbally, R^2 measures the proportion or percentage of the total variation in Y explained by the regression model (Rawlings, 1998). Adjusted R^2 is defined similarly as

$$R_{adj}^2 = 1 - \frac{(n-1) \sum_{i=1}^n \epsilon_i^2}{(n-p) \sum_{i=1}^n (Y_i - \bar{Y})^2} \quad (7)$$

Finally, the mean squares error MSE is defined as

$$MSE = \frac{SS(\text{Res})}{n-p} \quad (8)$$

where p is the number of parameters of regression function.

White's and Park's Tests for Heteroscedasticity

The general test of heteroscedasticity proposed by White does not rely on the normality assumption, and is easy to implement. White test can be a test of (pure) heteroscedasticity, or specification error, or both. It has been argued that if cross-product terms are present, then it is a test of both heteroscedasticity, and specification bias. (Gujarati, 2004).

Park formalizes the graphical method by suggesting that σ_i^2 is some function of the explanatory variable X_i . If this relation is found to be statistically significant, it would suggest that heteroscedasticity is present in the data. One may use the Park test as a strictly explanatory method (Gujarati, 2004).

Weighted Least Squares

Let the weights w_i be contained in the diagonal matrix of weights

$$W_{n \times n} = \begin{bmatrix} w_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & w_n \end{bmatrix} \quad (9)$$

The weighted least squares estimators of the regression coefficients are

$$\hat{\beta}_{WLS} = (X'WX)^{-1}X'WY \quad (10)$$

When the variances are not equal, the weights are chosen to be inversely proportional to variances (Neter et al, 1985). The estimated variance-covariance matrix is

$$S_{p \times p}^2 = MSE_W (X'WX)^{-1} \quad (11)$$

where

$$MSE_W = \frac{\sum w_i e_i^2}{n-p} \quad (12)$$

Box-Cox Transformation

Box-Cox transformation aims to convert a set of observations into a set of observations from a normal distribution with constant variance. The transformation involves a parameter estimated from the data using maximum likelihood (Upton&Cook, 2006)). For each real number λ , and positive number Y, the Box-Cox transformation is given by

$$Y_i^{(\lambda)} = \begin{cases} \frac{Y_i^\lambda - 1}{\lambda} & \text{for } \lambda \neq 0 \\ \ln(Y_i) & \text{for } \lambda = 0 \end{cases} \quad (13)$$

In other words, the regression models with the same explanatory variables, but with different values of λ are run to get the best goodness of fit statistics.

Entropy

Entropy is an indicator of reversibility; when there is no change of entropy, the process is reversible. An increase in entropy is a decrease of available energy. In general, an increase in entropy means decrease in order. Disorder in the sense of unpredictability based on a lack of knowledge of the positions and velocities of molecules (Pierce,1980).

The entropy of a statistical experiment, is a measure of uncertainty (Khinchin, 1957). So in a statistical sense, entropy and the amount of information are two closely related concepts. Uncertainty is not present after a statistical experiment is conducted. Therefore entropy is the amount of information that can be provided by sampling. For some concepts and applications of statistical entropy, one can also refer to Cover&Thomas (2006) , Ash (1990), Reza(1994), Kullback(1996), and Rényi (2007).

Shannon Entropy

Let the discrete random variable X takes on the value x_1, x_2, \dots, x_k with respective probabilities p_1, p_2, \dots, p_k Shannon entropy is defined as

$$H_s = - \sum_{i=1}^k p_i \log p_i \quad (14)$$

Let \hat{H} is the estimator of Shannon entropy. It is calculated as

$$\hat{H}_s = - \sum_{i=1}^k \hat{p}_i \log \hat{p}_i \quad (15)$$

Here \hat{p}_i probabilities are estimated by maximum likelihood method. Although this estimator is biased, ncreasing the sample size can reduce the amount of bias . The variance of Shannon entropy is found as (Zhang Xing, 2013).

$$V(\hat{H}) \cong \frac{1}{n} \left(\sum_{i=1}^k p_i \ln^2 p_i - H^2 \right) + \frac{k-1}{2n^2} \quad (16)$$

Rényi Entropy

Rényi entropy is defined as

$$H_R = \frac{\log \sum_{i=1}^k p_i^a}{1-a} \text{ for } a > 0, \text{ and } a \neq 1 \quad (17)$$

Rényi entropy is also called as type of entropy (Ullah, A., 1996). As the parameter approaches unity, Rényi entropy approaches to Shannon entropy. Thus Shannon entropy is a special case of Rényi entropy. The variance of Rényi entropy is given as follows (Pardo, 2006);

$$V(\hat{H}_R) \cong \frac{1}{n} \left[\left(\frac{a}{a-1} \right)^2 \left(\sum_{i=1}^k p_i^{2a-1} - \left(\sum_{i=1}^k p_i^a \right)^2 \right) \right] \quad (18)$$

Tsallis Entropy

Tsallis (or Havrda-Charvat) entropy is known as

$$H_T = \frac{1 - \sum_{i=1}^k p_i^a}{a-1} \text{ for } a > 0 \text{ and } a \neq 1 \quad (19)$$

The variance of this entropy estimator is given by

$$V(H_T) \cong \frac{1}{n} \left[\left(\frac{a}{a-1} \right)^2 \left(\sum_{i=1}^k p_i^{2a-1} - \left(\sum_{i=1}^k p_i^a \right)^2 \right) \right] \quad (20)$$

The formulas of Shannon, Renyi and Tsallis entropy for normal distribution can be calculated as below:

	Normal Distribution
Shannon entropy	$\ln(\sigma\sqrt{2\pi e})$
Renyi entropy	$\ln(\sigma\sqrt{2\pi e}) - \frac{\ln \alpha}{2(1-\alpha)}$
Tsallis entropy	$\frac{\sqrt{\alpha} - (\sigma\sqrt{2\pi})^{1-\alpha}}{\sqrt{\alpha}(\alpha-1)}$

Table1: Entropies for normal distribution

IV. APPLICATION

We have generated and used some artificial heteroscedastic data given in appendix data-1, data-2, data-3 and data-4 We then fitted linear regression models, each having its own weighting methodology. Then we compared the goodness of fit statistics of each linear regression model, after weighting, and performing the weighted least squares technique. Note that initially (as a classical approach) we took the reciprocals of the sample standard deviations calculated at each X-level as the weights. Then we repeated the same procedure by taking the weights as the reciprocals of entropies of normal distribution calculated at the X-levels. Note that since Tsallis, and Rényi entropies have parametric nature, we performed various weighting techniques by giving different values to the α parameter. Finally, as an alternative to the weighted least squares we adopted Box-Cox approach. The three goodness of fit statistics used are R^2 , R_{adj}^2 and MSE .

From Figure1, and Figure 2, the heteroscedastic nature of data is obvious. These data were produced by adding random

numbers whose variances are increasing systematically according to the levels of independent variables. In other words, the bigger the independent variable, the bigger the variance of simulated values. Note that random numbers are generated from normal distributions with different variances. Note too that for the first data set, there are 5 dependent observations for each level of independent variable, and for the second, third, and fourth data sets there are 25 dependent observations generated. By checking regression results summarized in Tables 2-4, we may say that weighing has a positive effect on increasing R^2 , R^2_{adj} and/or decreasing MSE . Besides we have observed that in many cases using the reciprocals of Tsallis, and Rényi entropies as the weights, produced much better goodness of fit statistics.

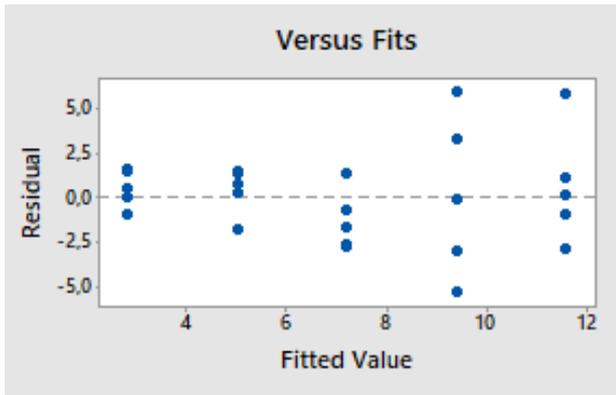


Fig 1: The scatter diagram of data-1

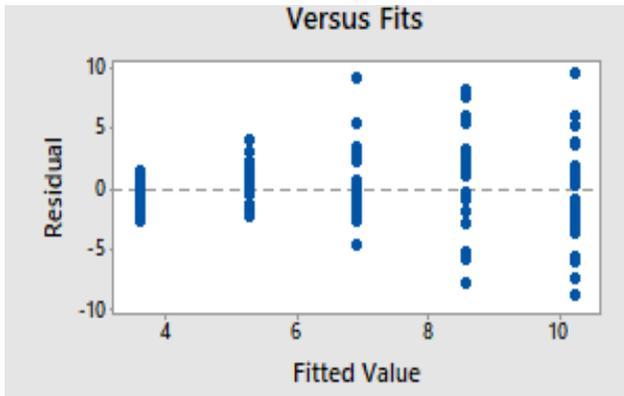


Fig 2: The scatter diagram of data-2

Data-1	R^2	R^2_{adj}	MSE
Classical	59.3%	57.53%	7.173
Weighted with OLS	65.84%	64.35%	1.052
Shannon	63.28%	61.68%	2.881
Rényi $\alpha=0,5$	62.4%	60.77%	2.241
Rényi $\alpha=1,5$	62.71%	61.09%	2.467
Box-cox	63.24%	61.65%	0.094
Tsallis $\alpha=1,5$	61.23%	59.55%	4.064
Tsallis $\alpha=0,5$	63.96%	62.39%	0.027
Tsallis $\alpha=1/9$	66.27%	64.81%	0.021
Tsallis $\alpha=1/10$	66.22%	64.75%	0.068
Rényi $\alpha=1/9$	60.84%	59.14%	1.113

Table I: Goodness of fit statistics model for data-1

Data-2	R^2	R^2_{adj}	MSE
Classical	35.24%	34.71%	10.260
Weighted with OLS	44.63%	44.18%	1.589
Shannon	39.06%	38.57%	4.086
Rényi $\alpha=0,5$	38.25%	37.75%	3.175
Rényi $\alpha=1,5$	38.54%	38.04%	3.497
Box-cox	35.39%	34.87%	0.371
Tsallis $\alpha=1,5$	36.88%	36.37%	5.810
Tsallis $\alpha=0,5$	39.38%	38.89%	0.648
Tsallis $\alpha=1/9$	44.24%	43.79%	0.032
Tsallis $\alpha=1/10$	44.34%	43.89%	0.102
Rényi $\alpha=1/9$	36.77%	36.25%	1.581

Table II: Goodness of fit statistics model for data-2

Data-3	R^2	R^2_{adj}	MSE
Classical	38.48%	37.98%	9.452
Weighted with OLS	52.52%	52.13%	0.952
Shannon	44.29%	43.84%	3.566
Rényi $\alpha=0,5$	42.91%	42.45%	2.816
Rényi $\alpha=1,5$	43.39%	42.93%	3.085
Box-cox	36.67%	36.16%	0.359
Tsallis $\alpha=1,5$	41.12%	40.65%	5.242
Tsallis $\alpha=0,5$	44.44%	43.99%	0.564
Tsallis $\alpha=1/9$	52.3%	51.91%	0.021
Tsallis $\alpha=1/10$	52.41%	52.03%	0.065
Rényi $\alpha=1/9$	40.6%	40.12%	1.435

Table III: Goodness of fit statistics model for data-3

Data-4	R^2	R^2_{adj}	MSE
Classical	56.47%	56.27%	8.150
Weighted with OLS	61.55%	61.38%	0.925
Shannon	60.11%	59.93%	3.180
Rényi $\alpha=0,5$	59.13%	58.95%	2.493
Rényi $\alpha=1,5$	59.46%	59.28%	2.737
Box-cox	56.37%	56.18%	0.279
Tsallis $\alpha=1,5$	58.49%	58.3%	4.570
Tsallis $\alpha=0,5$	59.65%	59.47%	0.508
Tsallis $\alpha=1/9$	62.22%	62.05%	0.020
Tsallis $\alpha=1/10$	62.2%	62.04%	0.064
Rényi $\alpha=1/9$	57.67%	57.48%	1.254

Table IV: Goodness of fit statistics model for data-3

V. CONCLUSION

The simplest model for regression analysis involves one independent variable and a constant. The variances of the equation may be equal for each level of independent variable or not. For equal variances the equation is called homoscedastic, otherwise the equation is called heteroscedastic. The heteroscedasticity could be detected visually when the data is shown in scatter diagram. On the other hand, for the numeric results White Test and Park's Test should be used to be more precise. In order to avoid from

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heteroscedasticity, generally weighting with error squares is one strategy. The Box-Cox transformation is also used to remedy. Alternatively, although it's not in common usage, weighting with reciprocal of entropy can be used, since entropy is a measure of uncertainty. In this study Shannon, Rényi and Tsallis entropies are used for determining the weights of The weighted Least Squares (WLS) procedure. As can be seen on the tables above, introducing Tsallis and Rényi entropies in weighing may improve goodness of test statistics of a regression model like the coefficient of determination, the adjusted coefficient of determination, and the mean squares error.

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APPENDIX:

Data-1

X	Y
1,00	2,70
1,00	1,72
1,00	3,24
1,00	4,28
1,00	4,20
2,00	6,44
2,00	5,64
2,00	6,26
2,00	3,11
2,00	5,13
3,00	8,47
3,00	5,35
3,00	6,32
3,00	4,31
3,00	4,49
4,00	3,89
4,00	15,33
4,00	12,65
4,00	6,24
4,00	9,16
5,00	8,56
5,00	11,61
5,00	12,64
5,00	17,32
5,00	10,49

Data-2

X	Y
1,00	2,46
1,00	4,12
1,00	2,33
1,00	1,81
1,00	0,82
1,00	3,53
1,00	2,81
1,00	3,37
1,00	1,42
1,00	2,60
1,00	2,28
1,00	4,04
1,00	4,93
1,00	3,48
1,00	4,27
1,00	4,59
1,00	1,44
1,00	3,09
1,00	2,65
1,00	2,73
1,00	2,78
1,00	3,28
1,00	1,09
1,00	4,72
1,00	2,91
2,00	2,73
2,00	6,75
2,00	8,11
2,00	5,29
2,00	5,32
2,00	6,59
2,00	4,84
2,00	5,91
2,00	7,24
2,00	5,57
2,00	5,47
2,00	9,15
2,00	4,78
2,00	6,16
2,00	5,19
2,00	6,23
2,00	3,77
2,00	5,61
2,00	3,38
2,00	4,48
2,00	6,94
2,00	4,59
2,00	6,48
2,00	5,27
2,00	6,20
3,00	6,57
3,00	7,42
3,00	5,77
3,00	5,34
3,00	15,82
3,00	5,27
3,00	6,80
3,00	6,79
3,00	4,05
3,00	5,57
3,00	9,65
3,00	2,14
3,00	10,26

Data-3

X	Y
5,00	12,54
5,00	17,02
5,00	13,08
5,00	6,20
5,00	0,93
5,00	6,76
5,00	9,32
5,00	11,55
5,00	4,83
5,00	6,53
5,00	9,75
5,00	14,97
5,00	0,70
5,00	6,86
5,00	13,65
5,00	10,37
5,00	15,28
5,00	10,70
5,00	6,13
5,00	14,25
5,00	8,41
5,00	12,01
5,00	16,71
5,00	5,06
5,00	10,96
4,00	6,42
4,00	5,88
4,00	10,80
4,00	12,96
4,00	10,78
4,00	14,48
4,00	6,78
4,00	7,67
4,00	8,61
4,00	13,07
4,00	6,38
4,00	5,79
4,00	10,36
4,00	8,67
4,00	6,79
4,00	8,74
4,00	9,80
4,00	15,02
4,00	8,49
4,00	14,33
4,00	12,14
4,00	3,63
4,00	12,36
4,00	1,04
4,00	3,49
3,00	7,04
3,00	5,88
3,00	3,78
3,00	9,80
3,00	14,16
3,00	5,37
3,00	3,55
3,00	6,94
3,00	2,82
3,00	10,93
3,00	4,06
3,00	4,20
3,00	5,93

Data-4

X	Y
1,00	2,89
1,00	3,19
1,00	2,01
1,00	4,76
1,00	2,43
1,00	2,94
1,00	4,30
1,00	3,33
1,00	4,12
1,00	1,47
1,00	3,63
1,00	2,99
1,00	3,68
1,00	2,37
1,00	3,67
1,00	2,02
1,00	5,51
1,00	3,66
1,00	4,08
1,00	3,32
1,00	4,00
1,00	3,22
1,00	4,31
1,00	3,39
1,00	3,53
2,00	6,14
2,00	5,58
2,00	5,14
2,00	5,89
2,00	7,85
2,00	5,40
2,00	4,96
2,00	3,91
2,00	3,64
2,00	7,75
2,00	8,80
2,00	2,89
2,00	5,26
2,00	3,17
2,00	4,22
2,00	4,56
2,00	6,87
2,00	4,00
2,00	5,51
2,00	3,98
2,00	5,03
2,00	3,78
2,00	4,79
2,00	3,46
2,00	2,81
3,00	9,18
3,00	6,01
3,00	4,36
3,00	6,30
3,00	7,17
3,00	13,33
3,00	5,90
3,00	12,44
3,00	6,67
3,00	0,25
3,00	9,77
3,00	9,09
3,00	11,89

