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Jackknife Method to Estimate the Confidence Intervals about an R-squared statistic Using SAS Software

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ABSTRACT Re-sampling methods cover a range of ideas. All of them involve taking a sample and using it as our basis for drawing new samples, hence the name 'Resampling'. We sample from our sample, in one way or another. There are several ways in which we can 'resample'. We can draw 'randomly' from our sample, or we can draw designed subsets from our sample. Also, we can pull the data but exchange the labels on the data points. For example in bootstrapping, we want to approximate the entire sampling distribution of some estimator. We can do that by resampling from our original sample.

In this dissertation we focus on generating samples by resampling techniques by jack-knifing, perform regression analysis for generated samples and then estimate the confidence intervals about an R squared statistic by using SAS software[1].

KEYWORDS :

1-Introduction to Resampling:

It is often relatively simple to plan a statistic that measures the property of interest, but is almost always difficult or impossible to determine the distribution of that statistic. The classical statistical methods concentrated mainly on the statistical properties of the estimators that have a simple closed form and which can be analysed mathematically. Except for a few important but simple statistics, these methods involve often unrealistic model assumptions. These limitations have been overcome in the last two decades of the 20th Century with advances in electronic computers. A class of computationally intensive procedures known as resampling methods provide inference on a wide range of statistics under very general conditions. Resampling methods involve constructing hypothetical populations derived from the observations, each of which can be analysed in the same way to see howthe statistics depend on possible random variations in the observations. Resampling the original data preserves whatever distributions are truly present, including selection effects such as truncation and censoring[3].

Perhaps the half-sample method is the oldest resampling method, where one repeatedly chooses at random half of the data points, and estimates the statistic foreach resample. The inference on the parameter can be based on the histogram of there sampled statistics. It was used by Mahalanobisin 1946 under the name interpenetrating samples. An important variant is the Quenouille-Tukey jack-knife method For a dataset with n data points, one constructs exactly n hypothetical datasets each with n-1 points, each one omitting a different point. For the main tasks in statistical inference hypothesis testing and confidence intervals - the appropriate resampling test often is immediately obvious. For example, if one wishes to inquire whether baseball hitters exhibit behavior that fits the notion of a slump, one may simply produce hits and outs with a random-number generator adjusted to the batting average of aplayer, and then compare the number of simulated consecutive sequences of either hits or outs with the observed numbers for the player. The procedure is also straightforward for such binomial situations as the Arbuthnot birth-sex case.

2. Re-sampling Procedures:

Re-sampling is done to test model statistics. There are several resampling methods available like bootstrapping, jackknifing, permutation tests and cross validation. Bootstrapping is a method of taking samples randomly with replacement while ensuring the sample statistics are in conformity with super set.

Resampling is useful when we do not have enough real data. It can also be used when we do not have any data at all, only some understanding of some event. In later case we can generate enough data which in theory would be similar to what we would expect in practice if we had data[8].

Resampling has its limitations; you cannot keep on generating additional data. Generating a lot of data in resampling can be time consuming. While resampling and Monte Carlo simulation are mostly same, in Monte Carlo simulation you can restrict number of samples to generate and also in this you need to have at least some real data.

Using resampling methods, “you're trying to get something for nothing. You use the same numbers over and over again until you get an answer that you can't get any other way. In order to do that, you have to assume something, and you may live to regret that hidden assumption later on”.

- A method of Resampling: creating many samples from a single sample
- Generally, resampling is done with replacement
- Used to develop a sampling distribution of statistics such as mean, median, proportion, others.

Re-sampling is any of a variety of methods for doing one of the following:

- Estimating the precision of sample statistics (medians, variances, percentiles) by using subsets of available data (jackknifing) or drawing randomly with replacement from a set of data points (bootstrapping)
- Exchanging labels on data points when performing significance tests (permutation tests, also called exact tests, randomization tests, or re-randomization tests)
- Validating models by using random subsets (bootstrapping, cross validation)

2.1. Jackknife Method:

This method is also known as the Quenouille-Tukey Jackknife; this tool was invented by Maurice Quenouille (1949) and later developed by John W. Tukey (1958). As the father of EDA, John Tukey attempted to use Jackknife to explore how a model is influenced by subsets of observations when outliers are present. The name "Jackknife" was coined by Tukey to imply that the method is an all-purpose statistical tool.

The jackknife or “leave one out" procedure is a crossvalidation technique first developed by Quenouille to estimate the bias of an estimator. John Tukey then expanded the use of the jackknife to include variance estimation and tailored the name of jackknife because like a jackknife - a pocket knife akin to a Swiss army knife and typically used by boy scouts - this technique can be used as a “quick and dirty" replacement tool for a lot of more sophisticated and specific tools. Curiously, despite its remarkable influence on the statistical community, the seminal work of Tukey is available only from an abstract (which does not even mention the name of jackknife) and from an almost impossible to and unpublished note (although some of this note found its way into Tukey's complete work).

The jackknife estimation of a parameter is an iterative process. First the parameter is estimated from the whole sample. Then each element is, in turn, dropped from the sample and the parameter of interest is estimated from this smaller sample. This estimation is called a partial estimate (or also a jackknife replication). A pseudo-value is then computed as the difference between the whole sample estimate and the partial estimate. These pseudo-values reduce the bias ofthe partial estimate (because the bias is eliminated by the subtraction betweenthe two estimates). The pseudo-values are then used in lieu of the original valuesto estimate the parameter of interest and their standard deviation is used to estimate the parameter standard error which can then be used for null hypothesistesting and for computing confidence intervals. The jackknife is strongly related tothe bootstrap (i.e., the jackknife is often a linear approximation of the bootstrap)which is currently the main technique for computational estimation of populationparameters.

As a potential source of confusion, a somewhat different (but related) method,also called jackknife is used to evaluate the quality of the prediction of computational models built to predict the value of dependent variable(s) from a set ofindependent variable(s). Such models can originate, for example, from neural networks, machine learning, genetic algorithms, statistical learning models, or anyother multivariate analysis technique. These models typically use a very largenumber of parameters (frequently more parameters than observations) and aretherefore highly prone to overfitting (i.e., to be able to perfectly predict the datawithin the sample because of the large number of parameters, but being poorlyable to predict new observations). In general, these models are too complex to beanalyzed by current analytical techniques and therefore the effect of over-fitting is difficult to evaluate directly. The jackknife can be used to estimate the actual predictive power of such models by predicting the dependent variable values of eachobservation as if this observation were a new observation. In order to do so, thepredicted value(s) of each observation is (are) obtained from the model built onthe sample of observations minus the observation to be predicted. The jackknife,in this context, is a procedure which is used to obtain an unbiased prediction (i.e.,a random effect) and to minimize the risk of over-fitting.

2.2. Generating Jack-knife Samples:

The Jack-knife samples are computed by leaving out one observation xi from $x = (x_1, x_2, \cdot\cdot, x_n)$ at a time:

$x_{(i)} = (x_1, x_2, \cdots, x_{i-1}, x_{i+1}, \cdots, x_n)$

- The dimension of the jack-knife sample x(I) is m = n – 1 .
- n different Jack-knife samples : {x(I) }i=1···n.
- No sampling method needed to compute the n jack-knife samples.

2.3. Jackknife Replications:

The i[th] jack-knife replication $\hat{\theta}_{(i)}$ of the statistic $\hat{\theta} = s(x)$ is

$\hat{\theta}_{(i)} = s(x_{(i)}), \forall i = 1,2, \ldots.n$ (1)

Jackknife replication of the mean,

$$s(x_{(i)}) = \frac{1}{n-1}\sum_{j\neq i} Xj$$

$$= \frac{n\bar{x} - xi}{n-1}$$

$$s(x_{(i)}) = \bar{x}(i)$$

2.4. Assumptions of the Jack-knife:

Although the jackknife makes no assumptions about the shape of the underlyingprobability distribution, it requires that the observations are independent of eachother. Technically, the observations are assumed to be independent and identicallydistributed (i.e., in statistical jargon: "i.i.d."). This means that the jackknife isnot, in general, an appropriate tool for time series data. When the independenceassumption is violated, the jackknife underestimates the variance in the datasetwhich makes the data look more reliable than they actually are.

Because the jackknife eliminates the bias by subtraction (which is a linear operation), it works correctly only for statistics which are linear functions of theparameters or the data, and whose distribution is continuous or at least "smooth enough" to be considered as such. In some cases, linearity can be achieved by transforming the statistics (e.g., using a Fisher Z-transform for correlations, or a logarithm transform for standard deviations), but some non-linear or non-continuousstatistics, such as the median, will give very poor results with the jackknife nomatter what transformation is used[14].

2.5. Advantages:

- The jackknife can be used to estimate standard errors in a non-parametric way.
- The jackknife can also be used to obtain nonparametric estimates of bias[21].

2.6. Bias estimation:

The jackknife was originally developed by Quenouille as a nonparametric way to estimate and reduce the bias of an estimator of a population parameter. The bias of an estimator is defined as the difference between the expected value of this estimator and the true value of the population parameter. So formally, the bias, denoted B, of an estimation T of the parameter θ is defined as

$B = E\{T\} - \theta$ (2)

with E{T} being the expected value of T.

The jackknife estimate of the bias is computed by replacing the expected value of the estimator (i.e., E{T}) by the biased estimator (i.e., T) and by replacing the parameter (i.e., θ) by the "unbiased" jackknife estimator (i.e., T.). Specifically, the jackknife estimator of the bias, denoted B_{jack} is computed as[14]:

$B_{jack} = T - T^*$ (3)

2.7 Jackknife estimate of the Standard Error:

Compute the n jackknife subsamples $x_{(1)}, \cdots, x_{(n)}$ from x.

Evaluate the n jackknife replications $\hat{\theta}_{(i)} = s(x_{(i)})$.

The jackknife estimate of the standard error is defined as below,

$$\hat{se}_{Jack} = \left[\frac{n-1}{n}\sum_{i-1}^{n}(\hat{\theta}(.) - \hat{\theta}(i))2\right]^{1/2} \quad (4)$$

$$\text{Where, } \hat{\theta}_{(.)} = \frac{1}{n}\sum_{i-1}^{n}(\hat{\theta}(i))$$

2.8. The Jackknife estimate of Variance:

Tukey (1958) suggested how the recomputed statistics $\hat{\theta}_{(i)}$ could also provide a non-parametric estimate of variance. Let

$Var = E_F[\hat{\theta}(X_1, X_2, \ldots. X_n) - E_F\hat{\theta}]^2$ (5)

Whereas E_F indicates expectation with $X_1, X_2, \ldots..X_n \sim F$, F an unknown probability distribution on some space χ.

In general, 'E_F' means that all random variables involved in the expectation are independently distributed according to F.

Tukey's formula for estimating Variance is

$$\widehat{VAR} = \frac{n-1}{n}\sum_{i=1}^{n}[\hat{\theta}(i) - \hat{\theta}(.)]^2 \quad (6)$$

$$\text{Where } \hat{\theta}_{(.)} = \sum \hat{\theta}_{(i)}/n$$

We will often be more interested in standard deviations than variances, since the standard deviation relates directly to accuracy statements about $\hat{\theta}$, in which case we will use the notation

$$\text{Sd} = \sqrt{Var}$$

$$\text{SD} = \sqrt{Var^{\wedge}}$$

Considerable effort has gone into verifying, and in some cases diversifying, the usefulness of $\widehat{VAR}$ as an estimate of var[6].

2.9. Jackknife Confidence Intervals:
The jack-knife suggests the following approach to constructing confidence intervals[14]

$$\text{Mean } (\hat{\theta}_{(i)}) \pm t_{1-\alpha/2;n-1}SE_{jack} \quad (7)$$

Let ∅ n(X) = ∅ n(X1, X2, ……,Xn)be an estimator defined for samples X = (X1, X2, ……, Xn). The ithpseudo value of ∅ n(X) is

$P_{si}(X) = n\varnothing_n(X_1, X_2, \ldots\ldots, X_n) - (n-1)\,\varnothing_{n-1}((X_1, X_2, \ldots\ldots, X_n)_{[i]})$(8)

In the above equation, $X_{[i]}$ means the sample $X = (X_1, X_2, \ldots\ldots, X_n)$ with the ith value X_i deleted from the sample, so that $X_{[i]}$ is a sample of size n-1

$P_{si}(X) = \varnothing_n(X) + (n-1)\,(\varnothing_n(X) - \varnothing_{n-1}(X_{[i]}))$ (9)

So that psi(X) can be viewed as a bias-corrected version of $\varnothing_n(X)$ determined by the trend in the estimators $\varnothing_n(X)$ from $\varnothing_{n-1}(X_{[i]})$ to $\varnothing_n(X)$.

The basic jack-knife recipe is to treat the pseudovalues $ps_i(X)$ as if they were independent random variables with mean θ. One can then obtain confidence intervals and carry out statistical tests using the Central Limit Theorem.

Specifically, let

$$Ps(X) = \frac{1}{n}\sum_{i=1}^{n} psi(X) \quad \text{and} \quad V_{ps}(X) = \frac{1}{n-1}\sum_{i=1}^{n}(psi(X) - ps(X))^2 \quad (10)$$

Be the mean and sample variance of the pseudovalues. The sample mean ps(X) was Quenouille's (1949) bias-corrected[15] version of $\emptyset_n(X)$. The jack-knife 95% confidence interval for θ is

$$\left(ps(X) - 1.960\sqrt{\tfrac{1}{n}Vps(X)},\ ps(X) + 1.960\sqrt{\tfrac{1}{n}Vps(X)}\right) \quad (11)$$

2.11. Jackknifing Linear Regression Model:
One of the most important and frequent types of statistical analysis is regression analysis, in which we study the effects of explanatory variables on a response variable. The use of the jackknife and bootstrap to estimate the sampling distribution of the parameter estimates in linear regression model was first proposed by Efron (1979) and further developed by Freedman (1981); Wu (1986). There has been considerable interest in recent years in the use of the jackknife and bootstrap in the regression context. In this study, we focus on the accuracy of the jackknife and bootstrap resampling methods in estimating the distribution of the regression parameters through different sample sizes and different bootstrap replications.

For the linear regression model

$Y = X\beta + e$ (12)

where Y denotes the n×1 vector of the response, $X = (x_1, x_2, \ldots, x_k)$ is the matrix of regressors with n × k, and e is an n×1 vector of error which has normal distribution with zero mean and variance σ^2_e[22]. The least squares estimator is given by

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

The variance Covariance matrix of $\hat{\beta}^{ols}$ is

$$\text{Var-cov}(\hat{\beta}^{ols}) = \hat{\sigma}^2(X'X)^{-1}$$

If β is estimated by $\hat{\beta}$, then θ is estimated by $\hat{\theta} = g(\hat{\theta})$, with respective jackknife values $\hat{\theta} = g(\hat{\beta})$. The jackknife estimation of the variance and bias of the $\hat{\theta}_{ols} = g(\hat{\beta}_{ols})$, delete the pair (yi , x'i), (i =1,2,..., n) and calculate $\hat{\theta}_{ols}(J)$, the least squares estimate of θ based on the rest of the data set [23]. The estimation of the $\hat{\beta}_J$, bias and variance with pseudo-values are,

$$\hat{\beta}_J = \frac{1}{n}\sum_{i=1}^{n} \tilde{\beta}_{Ji}$$

$$\text{bias}(J) = \left(\frac{1}{n}\right)\sum_{i=1}^{n} (\hat{\beta}ols - \tilde{\beta}_{Ji}) \quad (13)$$

$$V(\hat{\beta}_J) = \frac{1}{n(n-1)}\sum_{i=1}^{n} (\tilde{\beta}_{Ji} - \hat{\beta}_J)(\tilde{\beta}_{Ji} - \hat{\beta}_J)' \quad (14)$$

Respectively, where the $\tilde{\beta}_{Ji}$ is the pseudo value[24] and equals to

$$\tilde{\beta}_{Ji} = n\hat{\beta}_{ols} - (n-1)\tilde{\beta}_{Ji} \quad (15)$$

The following are the steps of jackknifing linear regression model [25].

1. Draw n sized sample from population randomly and label the elements of the vector wi = (yi ,xji)'.
2. Delete the first row of the vector wi = (yi ,xji)' and label the remaining n −1 sized observation sets and estimate the ols regression coefficients $\hat{\beta}_{J1}$ from w_1. Then, omit second row of the vector wi = $(y_i , x_{ji})'$ after that bring back the deleted first row, label remaining n-1 sized observation sets and estimate the ols regression coefficients $\hat{\beta}_{J2}$ from w_2. Similarly, omit each one of the n observation sets and estimate the regression coefficients as $\hat{\beta}_{Ji}$ alternately, where $\hat{\beta}_{Ji}$ is jackknife regression coefficient vector estimated after deleting of ithobservation set from w_i.
3. Calculate the jackknife regression coefficient, bias, and standard error for each coefficient from above mentioned equations.

3. Introduction to Data:
Data was collected through a pilot survey on Hybrid Jowar Crop on yield and biometrical characters. The biometrical characters were average plant population (PP), plant height (PH), average number of green leaves (NGL) and yield (kg/plot).

4. Data Analysis:
The data looks as below[5]; in the data we have 4 variables with 46 records. In this paper we have used SAS software for data analysis.

PP	Plant Population
PH	Plant Height
NGL	Number of Green Leaves
YLD	Yield (kg/plot)

Fitting Regression model for the original data.

The regression results are as follows,

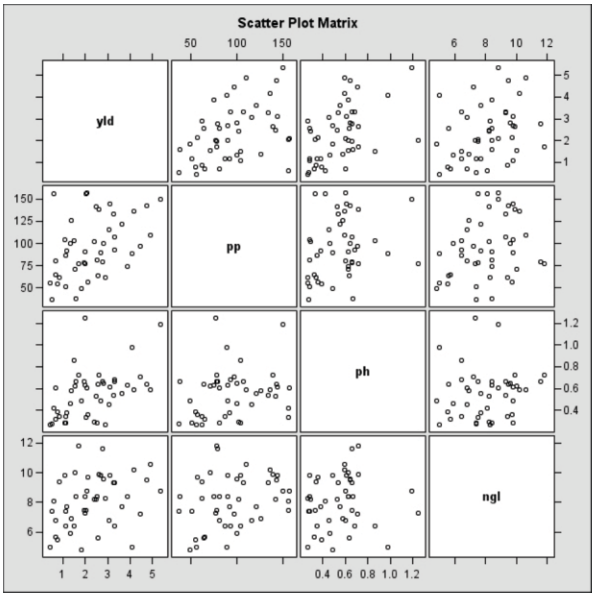
Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr> F
Model	3	27.74654	9.24885	8.67	0.0001
Error	42	44.80696	1.06683		
Corrected Total	45	72.55350			

Root MSE	1.03288	R-Square	0.3824
Dependent Mean	2.32978	Adj R-Sq	0.3383
CoeffVar	44.33357		

In our model the R squared value is 0.39, which means that approximately 39% of variation can be explained by our model, in other words 39% of variation can be explained by those independent variables which we included in our regression model.

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr> |t|
Intercept	1	-1.13798	0.81766	-1.39	0.1713
Pp	1	0.01041	0.00487	2.14	0.0385 *
Ph	1	2.31100	0.71255	3.24	0.0023 *
Ngl	1	0.14797	0.09260	1.60	0.1175

From the below scatter plot, we can observe that the dependent variable is moderately correlated with all other independent variables.



Generating Jack-knife samples:

Now we will generate (n-1=46-1) jack-knife samples. That is we will get 45 jack-knife samples and each sample will have 45 observations.

```
Dataorigjack; /*create a new data set which contains observation */
set data1 end=eof; /* numbers 1 to &nobs (no. obs in data set) */
obsnum=_n_;
ifeofthencallsymput('nobs', put(obsnum, 2.));
run;

/* GeneratingJackknife samples*/

%macrojackdata; /* use macro for %do processing utility */
Datajackdata;
set
%doi=1%to&nobs; /* do loop to create all samples */
origjack (in=in&i
where=(obsnum ne &i)) /* remove a different value each time */
%end;;
%doi=1%to&nobs;
Ifin&i then repeat=&i; /* add repeat number for each sample */
%end;
run;
%mend;
%jackdata;
```

Performing Regression analysis separately for each jack-knife sample.

```
/* Performing Regression Analysis for generated Jackknife samples*/

OdsoutputFitStatistics=t (where=(label2="R-Square"));
Odshtml;
Odsgraphicson;
Procregdata=jackdata;
by repeat;
modelyld=pp phngl;
run;
quit;
odshtmlclose;
odsgraphicsoff;

data t1;
set t;
 r2=cvalue2+0;
run;
```

The below is the sample output for each jack-knife sample.

The REG Procedure
Model: MODEL1
Dependent Variable: yld
repeat=1

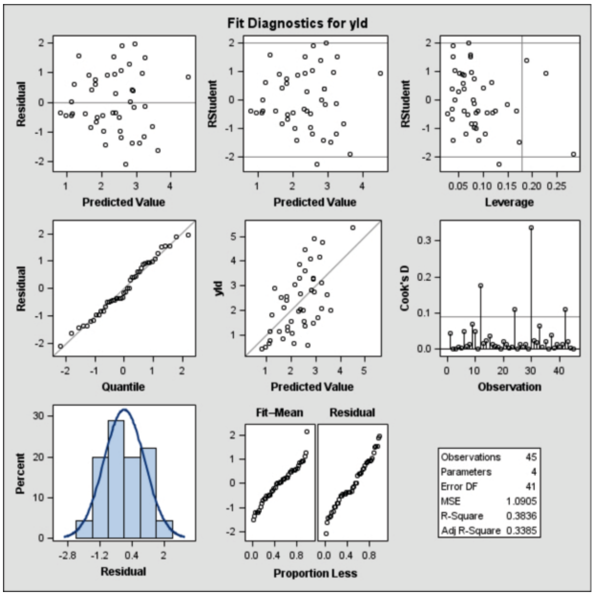
Number of Observations Read	45
Number of Observations Used	45

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr> F
Model	3	27.82166	9.27389	8.50	0.0002
Error	41	44.71174	1.09053		
Corrected Total	44	72.53340			

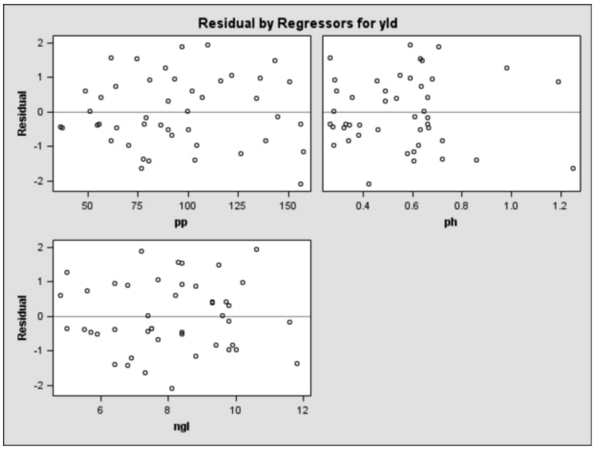
Root MSE	1.04428	R-Square	0.3836
Dependent Mean	2.32667	Adj R-Sq	0.3385
CoeffVar	44.88329		

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr> |t|
Intercept	1	-1.14333	0.82689	-1.38	0.1742
Pp	1	0.01075	0.00505	2.13	0.0396 *
Ph	1	2.29576	0.72227	3.18	0.0028 *
Ngl	1	0.14660	0.09374	1.56	0.1255

The REG Procedure
Model: MODEL1
Dependent Variable: yld
repeat=1



Plot for Regressors Vs Residuals:



5.Confidence Intervals:

SAS code for calculating Confidence intervals for estimated R^2 values from 45 Jack-knife samples.

```
/* Confidence Intervals */
ODSHTML;
ODSgraphicson;
%letalphalev=.05;
Odslisting;
Procsql;
Select&r2bar as r2,
mean(r2) - &r2bar as bias,
                              std(r2) asstd_err,
&r2bar - tinv(1-&alphalev/2, &rep-1)*std(r2) aslb,
&r2bar + tinv(1-&alphalev/2, &rep-1)*std(r2) ashb
from t1;
quit;
odshtmlclose;
odsgraphicsoff;
```

Confidence intervals from the above jack-knife samples will be as below.

R2	Bias	std_err	LB	UB
0.3824	0.00095	0.019779	0.34354	0.42126

6. Conclusions:

From the above correlation plot, we can observe that the dependent variable is moderately correlated with all other independent variables.

By looking at Regression results from original data we can observe that, the overall model fit is significant. The variables PP and PH are highly significant variable which are having high impact for predicting the yield.

The fitted regression equation is,

Yield = -1.138 + 0.0104(PP) + 2.311(PH) + 0.148(NGL)

The coefficient of determination R^2 values is 0.38, so it means that approximately 38% of variation in yield can be explained by the included independent variables PP, PH and NGL.

The coefficient of determination R^2 value from Jack-knife methods are 0.3824, this is close to original R^2 value (which we got from original data). The bias and standard error values from jack-knife method are lesser than the other methods as (Bootstrap method), indicating that Jack-knife gives better estimates than (Bootstrap estimation.).

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