Jagannath University Journal of Science
Volume 07, Number I, December 2020, pp. 63-75
https://jnu.ac.bd/journal/portal/archives/science.jsp
ISSN 2224-1698

JnUJSci

Minimum Sample Sizes for Likelihood Ratio Tests: A Simulation Study

Research Article

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Received: 01October 2020
Accepted: 24November 2020

Abstract : The necessity of sample size determination for various research purposes arises due to cost, time or availability of data, and also to offer sufficient statistical power. In this paper, we have tried to determine the minimum sample sizes for which *–2 log* λ *(X)*converges to chi-square distribution with 1 degree of freedom for several discrete and continuous distributions. We have applied a simulation study on 100000 datasets each of size n to calculate *–2 log* λ *(X)* for the considered distributions i.e. Bernoulli, Poisson, Geometric, Exponential and Normal. In order to determine the minimum sample sizes, we have drawn Quantile-Quantile and Probability-Probability plots of*–2 log* λ *(X)* values against the theoretical quantiles and histogram of the generated datasets are plotted with the density curve of chi-square distribution, and finally, sample sizes are determined by careful scrutinization of these three figures. From our study, we have found that sample sizes should be at least 200 for any value of $p > 0$(probability) in Bernoulli distribution so that *–2 log* λ *(X)*$\sim\chi_1^2$. For Poisson and Geometric distributions, the minimum sample sizes are approximately 40 and 80 respectively. Exponential and Normal requires roughly about only 10 samples so that*–2 log* λ *(X)* follows chi-square distribution with 1 degree of freedom.

Keywords: *Sample size determination • Chi-square distribution • Quantile-Quantile plot • Probability-Probability • Histogram • Bernoulli distribution*

1. Introduction

The most important determinant of statistical power of a study is sample size. It is an element of research design and significantly affects the validity and clinical relevance of the findings identified in research studies (Burmeister and Aitken, 2012). Moreover, one of the most fundamental characteristics of a study is sample size. If the sample size is too small, the executed studies may fail to answer the research question. Alternatively, a study with too large sample may be difficult to conduct and waste of time and money. Therefore, sample size calculation is important to make realistic and well researched assumptions before choosing an appropriate sample size accounting for dropouts (Wang *et al*. 2013). However, it becomes very difficult and also time consuming to collect experimental data of gold standard. Also, the evaluation of classification performance requires training sample because the predictive power of any used method strongly depends on sample size (Figueroa *et al*., 2012;Yao *et al*., 2008) Moreover, the quality and size of the training sample greatly influenced the classifiers prediction accuracy (Mukherjee *et al*., 2003; Dobbin *et al*., 2008; Tam*et al*., 2006; kim,2009; Kalayeh and Landgrebe,1983; Nigam *et al*., 2000). Especially for two cases the researcher must need to know the minimal sample size required for their experimental purpose. One case is the diagnostic

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accuracy and another is to obtain a desired significance level of statistical power to identify an effective sample for testing a single modality or a comparative study (Hajian-Tilaki, 2014). Another important reason of sample size determination is to prevent wastage of resources because of unduly large sample size selected for an expensive new diagnostic test (Malhorta and Indrayan, 2010). On the other hand, in medical context a small sample size provides an imprecise estimate of accuracy because a small sample size produces wider confidence interval which is actually non-informative for decision maker (Jones *et al*., 2003).

In an estimation study, the main objective of determining exact sample size is to estimate the parameter with a desired level of precision and confidence. To do a research more precisely a researcher should select a large sample size because as the minimal sample size increases the margin of error decreases that is precision increases. Similarly, level of confidence increases with an increased sample size (Binu*et al*., 2014).

There is a vast literature review for determining sample size in various social, biological, medical etc. fields. Borderer formula was used to calculate sample size for estimating sensitivity and specificity but not for testing (Kim, 2009). Simel *et al.* used sample size based on desired likelihood ratios (LR) confidence interval but not calculate sample size for a wide range of marginal errors around LR (Simel*et al*., 1991). A review of sample size formula had also been provided for various diagnostic test but the practical tables for calculating sample sizes were not provided (Obuchowski, 1998). Several methods had been developed for sample size calculation in diagnostic medicine because their methods were not used frequently due to the lack of available software and it was complex to use for the clinician (Fosgate,2009; Li and Fine, 2004; Steinberg *et al*., 2009; Kumar and Indrayan, 2002). A model-based approach was used to predict the sample size for classifying microarray data (Dobbin et al., 2008). Normal approximations are sometimes used for calculating sample size (Lachin, 1981). Sample size calculations are often based even for data which are not Gaussian and which are analyzed using generalized linear models (GLMs) (Wong *et al*., 2010; Watson-Jones *et al*., 2008; Kessler *et al*., 2009; Holland *et al*., 2005; Kaul *et al*., 2004). Methods have been proposed for sample size determination of logistic (Whittemore, 1981; Hsieh *et al*., 1998; Vaeth and Skovlund, 2004; Alam *et al*., 2010) or Poisson (Signorini, 1991) models or both (Shieh, 2001) or for the negative binomial (Zhu and Lakkis, 2014) and for generalized linear models (Self and Mauritsen, 1988; Shieh, 2000). The maximum likelihood method is a powerful technique and it also provides powerful framework for addressing the aspects of a phylogenetic analysis. Maximum likelihood appears to be both efficient and robust in terms of the estimation of relationship (Kuhner and Felsenstein, 1994; Tateno *et al*., 1994; Huelsenbeck, 1995a, 1995b). However, likelihood provides a natural way of testing hypothesis and this hypothesis is done through the likelihood ratio test (Edwards, 1972).

According to Casella and Berger (2002), for testing $H_0: \theta = \theta_0$versus$H_1: \theta \neq \theta_0$, suppose $X_1, X_2, \cdots, X_n$are i.i.d$f(x|\theta)$, $\hat{\theta}$ is the MLE of θ and $f(x|\theta)$satisfies the regularity conditions. Then under H_0, as $n \to \infty$

$$-2\, log\, \lambda\left(\underset{\sim}{X}\right) \to \chi_1^2$$

The aim of this study is to find minimum sample sizes for which $-2\, log\, \lambda\left(\underset{\sim}{X}\right)$ converges toχ_1^2. Our strategy is to apply simulation study on samples of several important distributions such as Bernoulli, Geometric, Poisson, Normal and Exponential. Here, simulation studies refer to computer experiments and involve creating data by pseudo-random sampli ng. Simulation studies has a key strength and it is the ability to understand the behavior of statistical methods because some parameters of interest are known from the process of generating the data (Morris et al. 2019). In our study, simulation study is applied for finding minimum sample sizes of these populations for which $-2\, log\, \lambda\left(\underset{\sim}{X}\right)$ converges to χ_1^2 under the null hypothesis $H_0: \theta = \theta_0$,versus $H_1: \theta \neq \theta_0$.

In the following section, the likelihood ratio test statistic (LRT) and asymptotic distribution of the LRT are discussed.

2. The Likelihood Ratio Test (LRT) Statistic

Let $X_1, X_2, \cdots, X_n$ be a random sample of size n from $f(x|\theta)$, where $f(x|\theta)$ satisfies the following regularity conditions:

(i) The parameter is identifiable, that is, if $\theta \neq \theta'$, then $f(x|\theta) \neq f(x|\theta')$.

(ii) $f(x|\theta)$ is differentiable in θ.

(iii) The parameter space Ω contains an open set ω of which the true parameter value θ_0 is an interior point.

The likelihood function is

$$L\left(\theta|\underset{\sim}{x}\right) = \prod_{i=1}^{n} f(x_i|\theta).$$

For testing $H_0: \theta \in \Theta_0$ versus $H_1: \theta \in \Theta_0^c$, the value of LRT statistic for a particular sample $\underset{\sim}{x}$ is calculated as (Koch and Karl-Rudolf, 1988)

$$\lambda\left(\underset{\sim}{x}\right) = \frac{\sup_{\Theta_0} L\left(\theta|\underset{\sim}{x}\right)}{\sup_{\Theta} L\left(\theta|\underset{\sim}{x}\right)}.$$

Suppose $\hat{\theta}$, an MLE of θ, exists; $\hat{\theta}$ is obtained by doing an unrestricted maximization of $L\left(\theta|\underset{\sim}{x}\right)$. We can also consider the MLE of θ, call it $\hat{\theta}_0$, obtained by doing a restricted maximization, assuming Θ_0 is the parameter space. That is, $\hat{\theta}_0 = \hat{\theta}_0\left(\underset{\sim}{x}\right)$ is the value of $\theta \in \Theta_0$ that maximizes $L\left(\theta|\underset{\sim}{x}\right)$. Then, the LRT statistic is

$$\boldsymbol{\lambda}\left(\underset{\sim}{X}\right) = \frac{L\left(\theta_0 \middle| \underset{\sim}{X}\right)}{L\left(\hat{\theta}|\underset{\sim}{X}\right)}.$$

2.1 Asymptotic Distribution of the LRT

Theorem: For testing $H_0: \theta = \theta_0$ versus $H_1: \theta \neq \theta_0$, suppose $X_1, X_2, \cdots, X_n$ are i.i.d $f(x|\theta)$, $\hat{\theta}$ is the MLE of θ, and $f(x|\theta)$ satisfies the regularity conditions. Then under H_0, as $n \to \infty - 2\,log\,\lambda\left(\underset{\sim}{X}\right)$ tends to χ_1^2 in distribution (Silvey, 1970)

where χ_1^2 is a χ^2random variable with 1 degree of freedom (Casella and Berger 2002).

Proof: First expand $log\,L\left(\theta|\underset{\sim}{x}\right) = l\left(\theta|\underset{\sim}{x}\right)$ in a Taylor series around $\hat{\theta}$, is giving

$$l\left(\theta \mid \underset{\sim}{x}\right) = l\left(\hat{\theta} \mid \underset{\sim}{x}\right) + l'\left(\hat{\theta} \mid \underset{\sim}{x}\right)\left(\theta - \hat{\theta}\right) + l''\left(\hat{\theta} \mid \underset{\sim}{x}\right)\frac{\left(\theta - \hat{\theta}\right)^2}{2!} + \cdots.$$

Now substitute the expansion for $l\left(\theta_0|\underset{\sim}{x}\right)$ in $-2\,log\,\lambda\left(\underset{\sim}{x}\right) = -2l\left(\theta_0|\underset{\sim}{x}\right) + 2l\left(\hat{\theta}|\underset{\sim}{x}\right)$, and get

$$-2\log\lambda\left(\underset{\sim}{x}\right) \approx \frac{\left(\theta - \hat{\theta}\right)^2}{l''\left(\hat{\theta} \mid \underset{\sim}{x}\right)},$$

where we use the fact that $l'\left(\hat{\theta}|\underset{\sim}{x}\right) = 0$. Since the denominator is the observed information $\hat{I}_n\left(\hat{\theta}\right)$ and $\frac{1}{n}\hat{I}_n\left(\hat{\theta}\right) \to \hat{I}(\theta_0)$ it follows from asymptotic efficiency of MLEs and Slutsky's theorem (Casella and Berger 2002) that $-2\,log\,\lambda\left(\underset{\sim}{X}\right) \to \chi_1^2$.

In order to find minimum sample sizes for various distributions, 100000 datasets each of sample size n are generated and $Y = -2\,log\,\lambda\,(X)$are calculatedfor each 100000 datasets. For each of the sample sizes n,we will drawQuantile-Quantile (Q-Q) plot and Probability-Probability (P-P) plot of *Y* values against the theoretical quantiles. By checking Q-Qand P-P plotsfor various n for each of the considered distribution, the minimum sample size for which $Y = -2\,log\,\lambda\,(X)$converges to χ_1^2 are determined.We will also draw histogram of generated datasets against the density curve of chi-square with 1 degree of freedom to determine the minimum sample sizes. Finally, minimum sample sizes will be determined by cross examination of the three curves. In the following section, we will discuss about various distributions and their likelihood functions.

2.2 Bernoulli Distribution

The likelihood function of a Bernoulli random variable $X$with parameter $p\ (0 < p < 1)$ is

$$L\left(p\middle|\underset{\sim}{x}\right) = p^{\sum_{i=1}^{n} x_i}(1-p)^{n-\sum_{i=1}^{n} x_i}.$$

Thus, for testing $H_0: p = p_0$, the likelihood ratio test statistic is

$$\lambda\left(\underset{\sim}{x}\right) = \frac{(p_0)^{\sum_{i=1}^{n} x_i}(1-p_0)^{n-\sum_{i=1}^{n} x_i}}{(\bar{x})^{\sum_{i=1}^{n} x_i}(1-\bar{x})^{n-\sum_{i=1}^{n} x_i}}$$

Thus, the log-likelihood function is

$$-2\,log\lambda(X) = 2\left[\,log\left\{\frac{\bar{X}(1-p_0)}{p_0(1-\bar{X})}\right\}\sum_{i=1}^{n} X_i + n\,log\left(\frac{1-\bar{X}}{1-p_0}\right)\right]$$

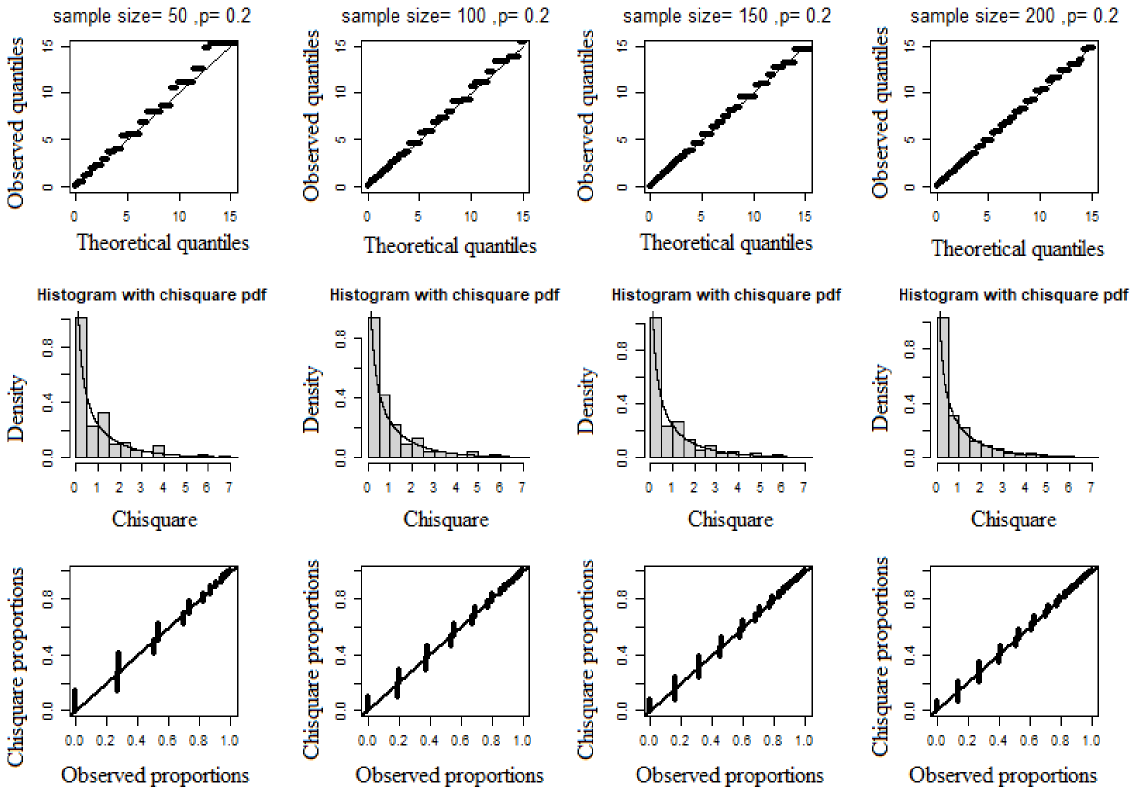

Figure 1: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

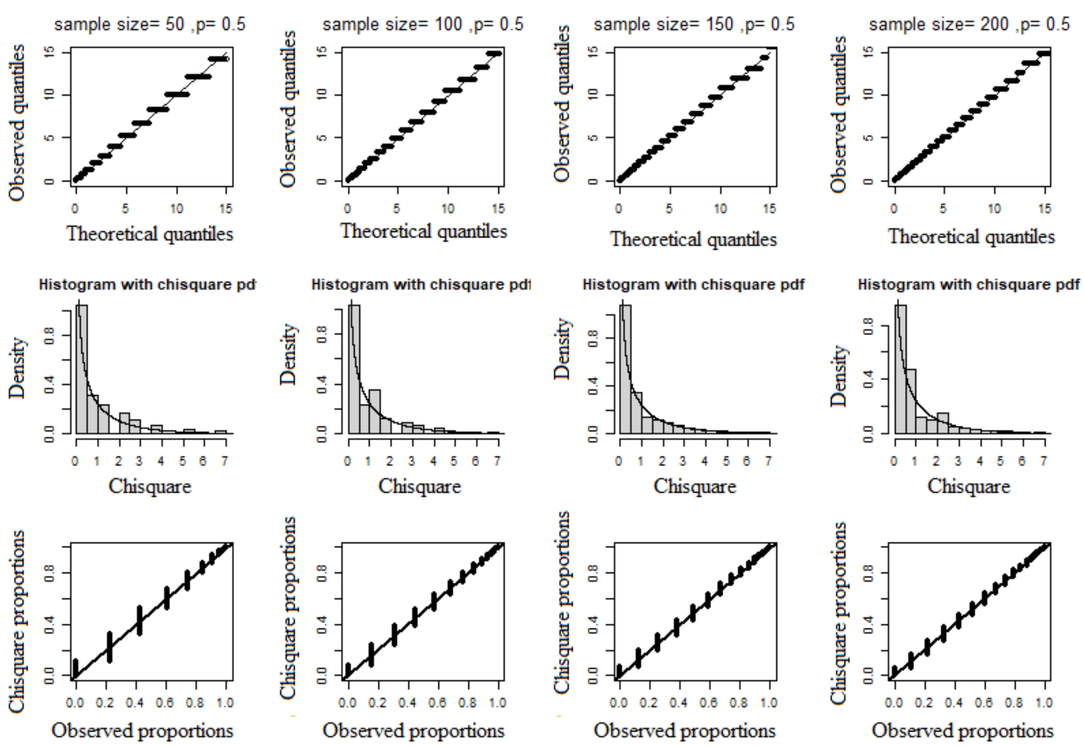

Figure 2: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

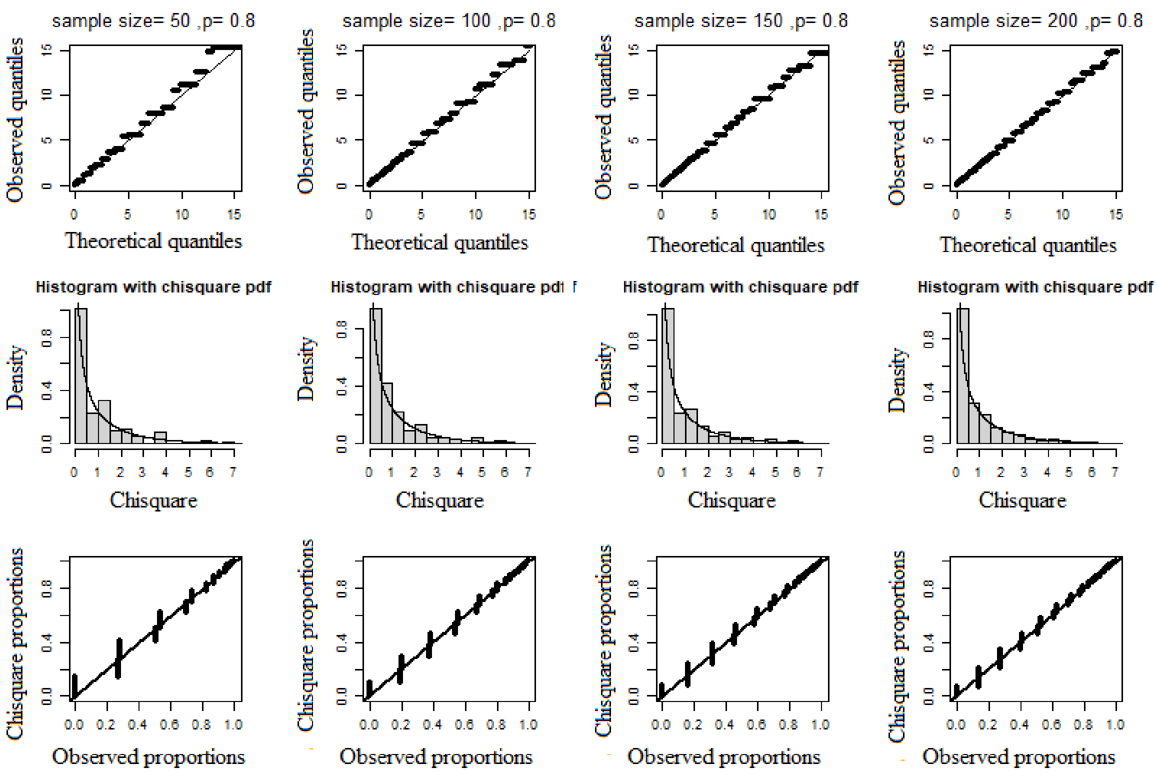

Figure 3: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

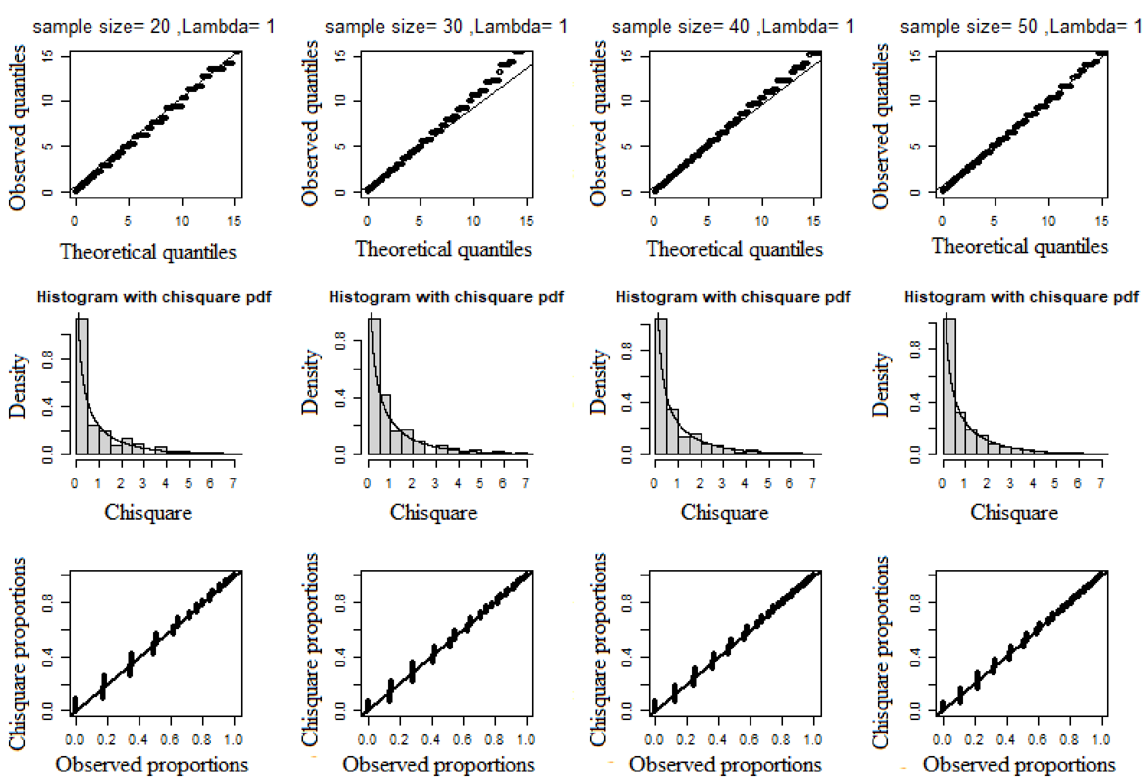

Figure 4: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

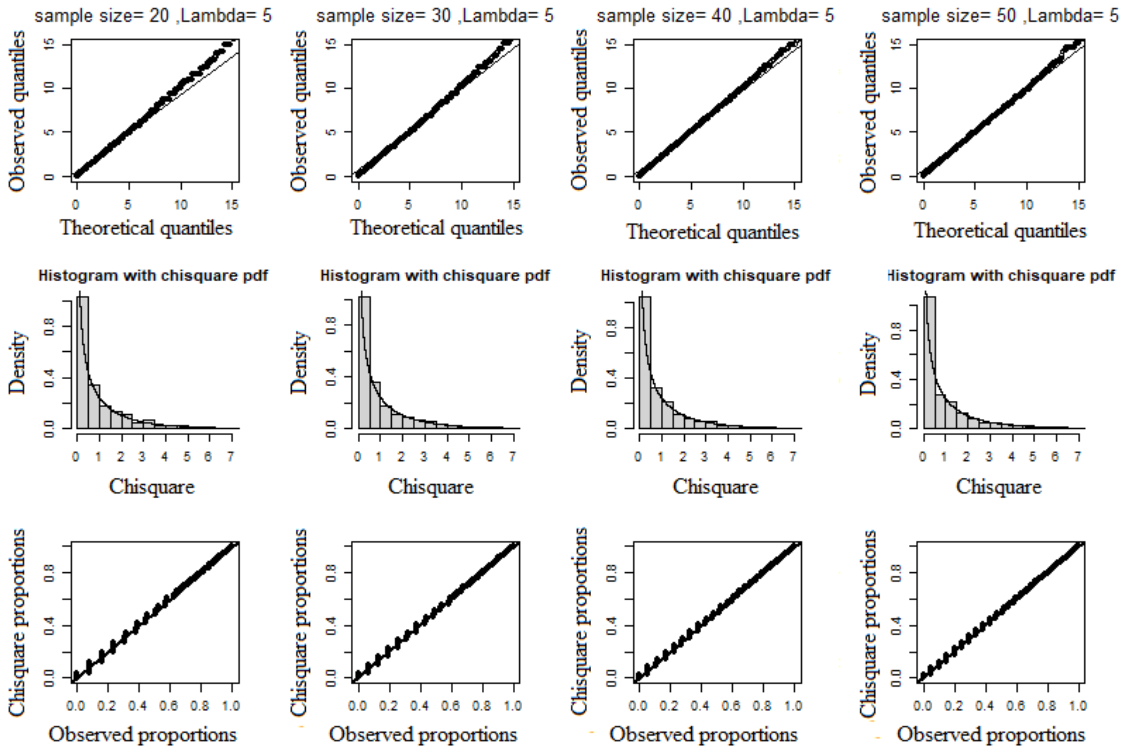

Figure 5: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

From **Fig.1** it is visually clear that approximately for 150 sample size, the observations differ from the fitted line much more than for sample size 200 both in Q-Q and P-P plots. Also, the chi-square curve matches with histogram much better for sample size 200 rather than sample size 150. By cross matching of the three curves, it can be said that for approximately 200 sample size $-2\,log\,\lambda\,(X)$converges to χ_1^2 for testing $H_0: p = 0.2$.

We will consider all possible ways to determine the minimum sample size under the null hypothesis $H_0: p = p_0$. From Fig. 2 it can be seen that for testing $H_0: p = 0.5$, the minimum sample size is 150 for which $-2\,log\,\lambda\,(X)$ converges to χ_1^2 because we can see from Q-Q and P-P plots that the observations vary from the fitted line slightly for sample sizes 150 and 200 compared to sample sizes 50 and 100. Also, plotted histogram coincides with the chi-square curve far better for sample sizes 150 and 200 rather than sample sizes 50 and 100. So, we are about to choose the sample size between 150 and 200. Since our concern is to choose the minimum sample size. So, the minimum sample size will be 150 for which $-2\,log\,\lambda\,(X)$ converges to χ_1^2 under the null hypothesis $H_0: p = 0.5$.

Figure 3 indicates that for approximately 200 sample size, $-2\,log\,\lambda\,(X) \to \chi_1^2$ under $H_0: p = 0.8$ as in the previous two cases.

Minimum sample size should be approximately 200 for which $-2\,log\,\lambda\,(X) \to \chi_1^2$ in Bernoulli distribution for testing $H_0: p = p_0 (p_0 > 0)$ for safe.

2.3 Poisson distribution

The likelihood function of a Poisson random variable *X* with parameter λ > 0is given by

$$L(\lambda|x_i) = \frac{e^{-n\lambda}\lambda^{\sum x_i}}{\prod x_i!}$$

For testing $H_0: \lambda = \lambda_0$, the likelihood ratio test statistic is

$$\lambda(x) = \frac{e^{-n\lambda_0}{\lambda_0}^{\sum x_i}}{e^{-n\hat{\lambda}}\hat{\lambda}^{\sum x_i}} .. = \frac{e^{-n\lambda_0}{\lambda_0}^{\sum x_i}}{e^{-n\bar{x}}\bar{x}^{\sum x_i}}$$

We are going to determine how large will be the sample size *n* for which

$$-2\,log\,\lambda\,(X) = 2n\left[(\lambda_0 - \bar{X}) - \bar{X}\,log\left(\frac{\lambda_0}{\bar{X}}\right)\right] \sim \chi_1^2$$

under $H_0: \lambda = \lambda_0$.

As in Bernoulli distribution we are going to find the minimum sample size by checking three figures simultaneously under the null hypothesis $H_0: \lambda = \lambda_0$.

From Fig.4, we can see that for approximately sample size40,$-2\,log\,\lambda\,(X){\sim}\chi_1^2$ for testing $H_0{:}\,\lambda = 1$ in Poisson distribution. Because the deviations of the observations from the fitted line are smaller for sample size 40 and above compared to sample size 30 and also histogram coincides with chi-square curve suitably for sample size 40 and above. For this reason, sample size 40 will be chosen to fulfill the minimum sample size criteria.

As we increase the value of the parameterλ, it is pretty obvious from Fig. 5 that we will need less sample size to prove the theorem.Forsample size$n = 30$,$-2\,log\,\lambda\,(X){\sim}\chi_1^2$ under $H_0{:}\,\lambda = 5.$ Thus, we can say that in Poisson distribution the minimum sample size is $\max(40, 30) = 40$ because maximum samples should be considered for testing $H_0{:}\,\lambda \geq 1$so that it will cover all possible values of λ.

2.4 Geometric Distribution

The geometric distribution represents the number of failures before one can get a success in a series of Bernoulli trials. This likelihood function of geometric variable X with parameter $p\ (0 < p < 1)$is given by

$$L(p|x_i) = p^n(1-p)^{\sum_{i=1}^{n} x_i}$$

For testing $H_0{:}\,p = p_0$, the likelihood ratio test statistic is:

$$\lambda(x) = \frac{{p_0}^n(1-p_0)^{\sum x_i}}{\hat{p}^n(1-\hat{p})^{\sum x_i}} = \frac{{p_0}^n(1-p_0)^{\sum x_i}}{\left(\frac{1}{1+\bar{x}}\right)^n\left(\frac{\bar{x}}{1+\bar{x}}\right)^{\sum x_i}}$$

Thus,

$$-2\,log\,\lambda\,(X) = 2\left[n\,log\left\{\frac{1}{p_0(1+\bar{X})}\right\} + \sum X_i \log\left\{\frac{\bar{X}}{(1+\bar{X})(1-p_0)}\right\}\right]{\sim}\chi_1^2 \text{ under } H_0{:}\,p = p_0.$$

It is visible from Fig. 6 that the minimum sample size is approximately 20 for testing $H_0{:}\,p = 0.2$in geometric distribution so that$-2\,log\,\lambda\,(X){\sim}\chi_1^2$. For testing $H_0{:}\,p = 0.5$, the sample size is approximately 40 as we can see from Fig. 7. Also, Fig. 8 indicates that approximately 80 sample size, $-2\,log\,\lambda\,(X)$ converges to chi-square distribution with 1 degree of freedom under the null hypothesis $H_0{:}\,p = 0.8$. That is the sample size increases as the probability value increase in geometric distribution. Finally, the minimum sample size for testing $H_0{:}\,p = p_0(p_0 > 0)$should be $max(20, 40, 80) = 80$ as we want to be on the safe side that's why we took the maximum sample size so that it will be true for all values of *p*.

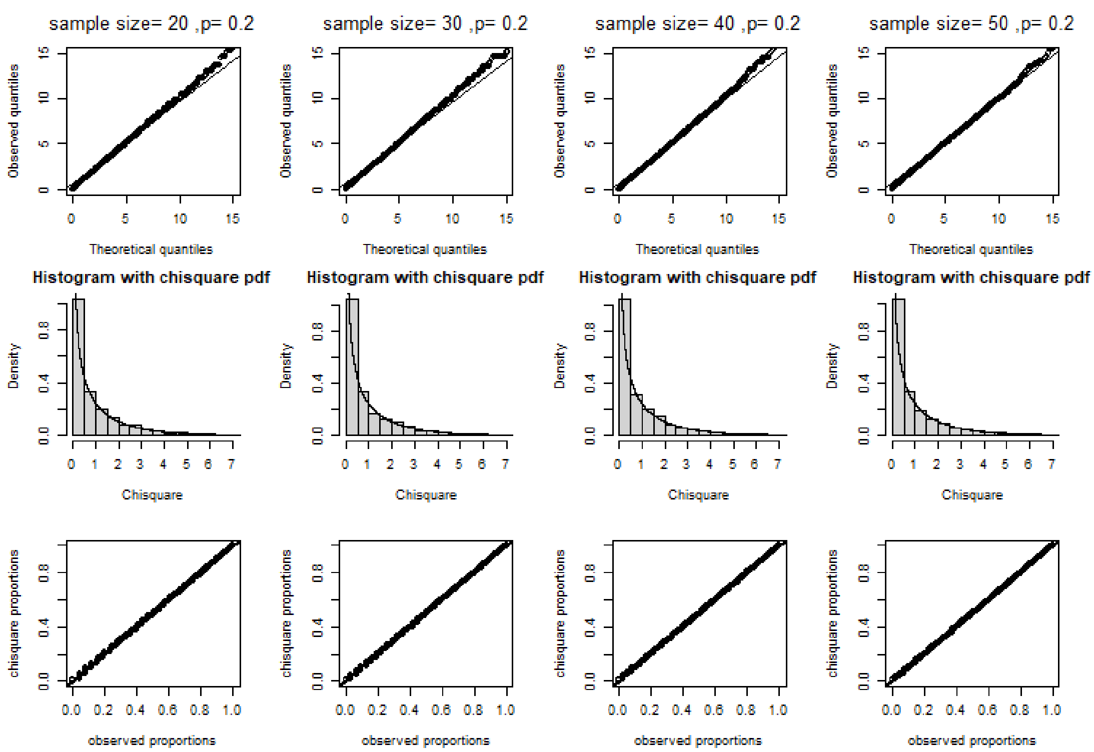

Figure 6: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

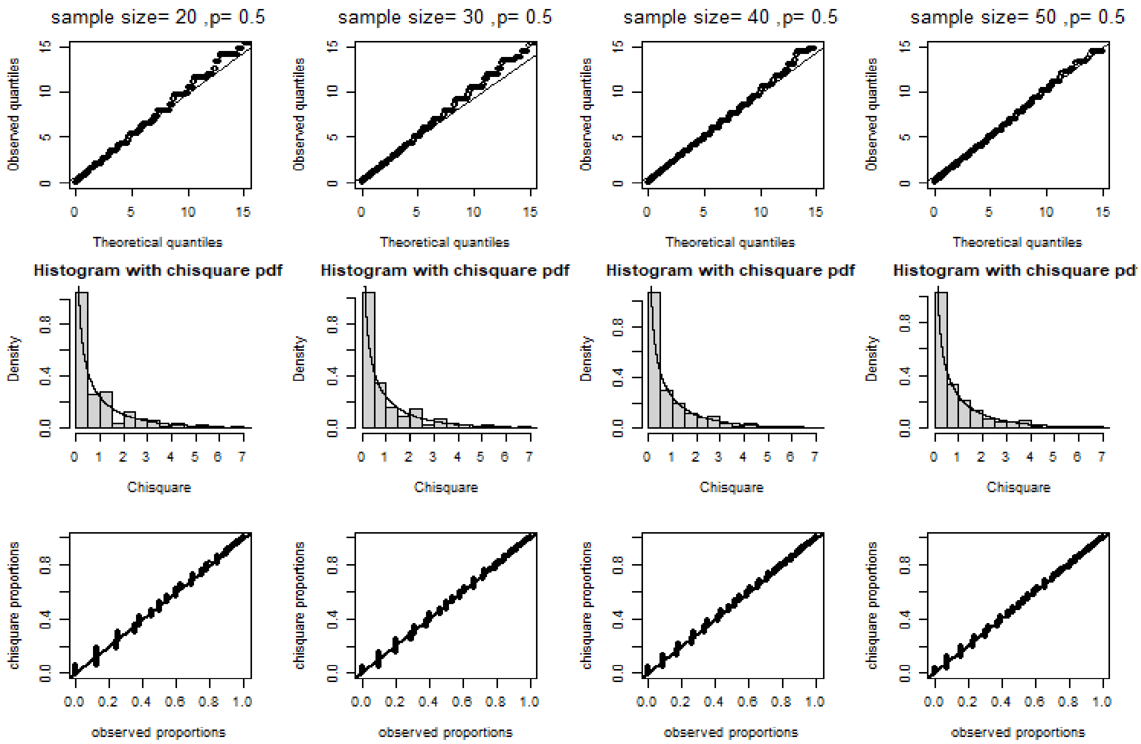

Figure 7: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

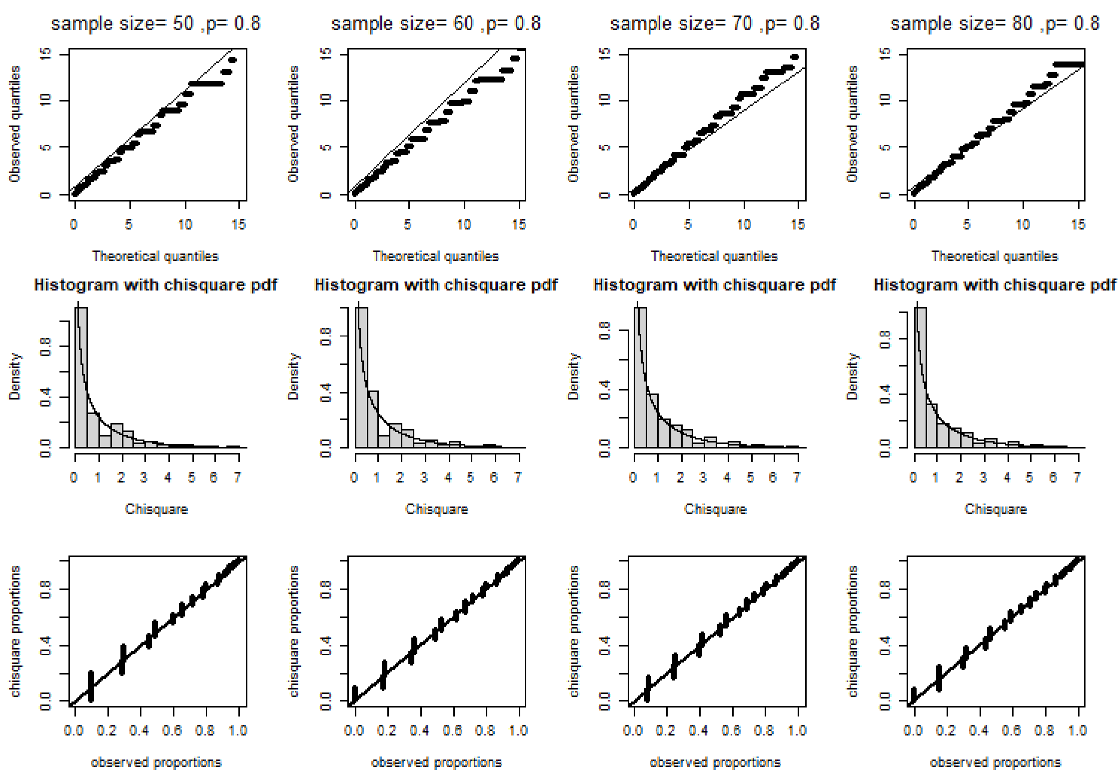

Figure 8: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

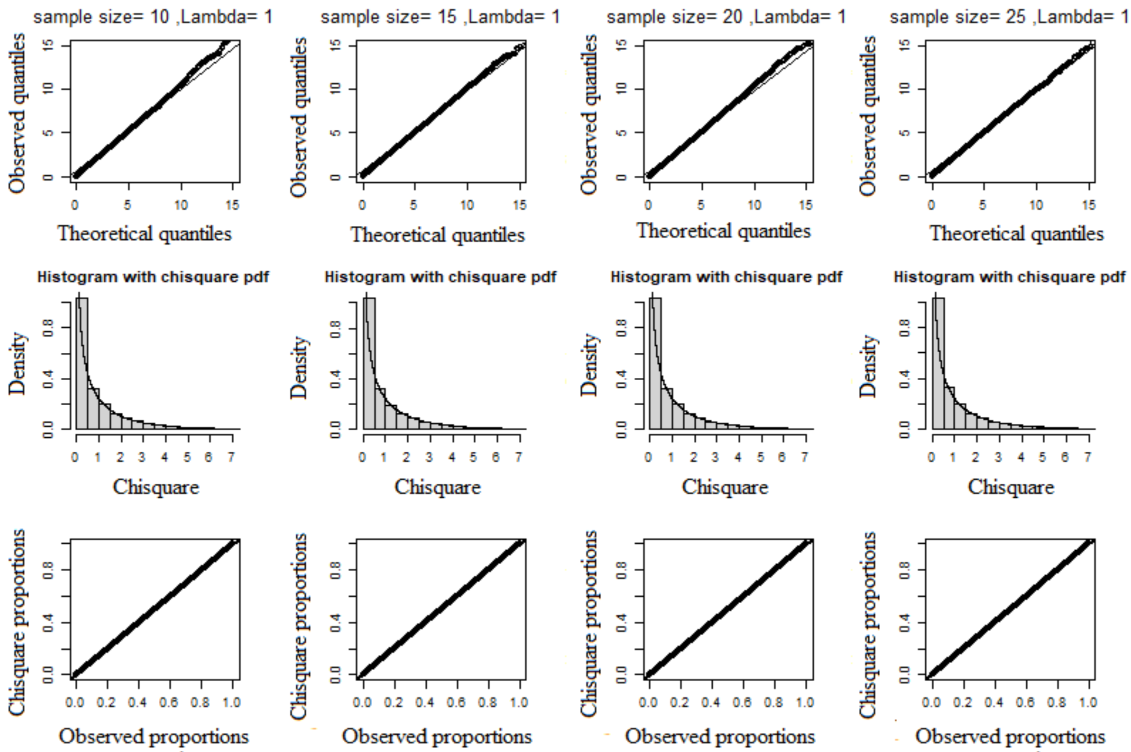

Figure 9: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

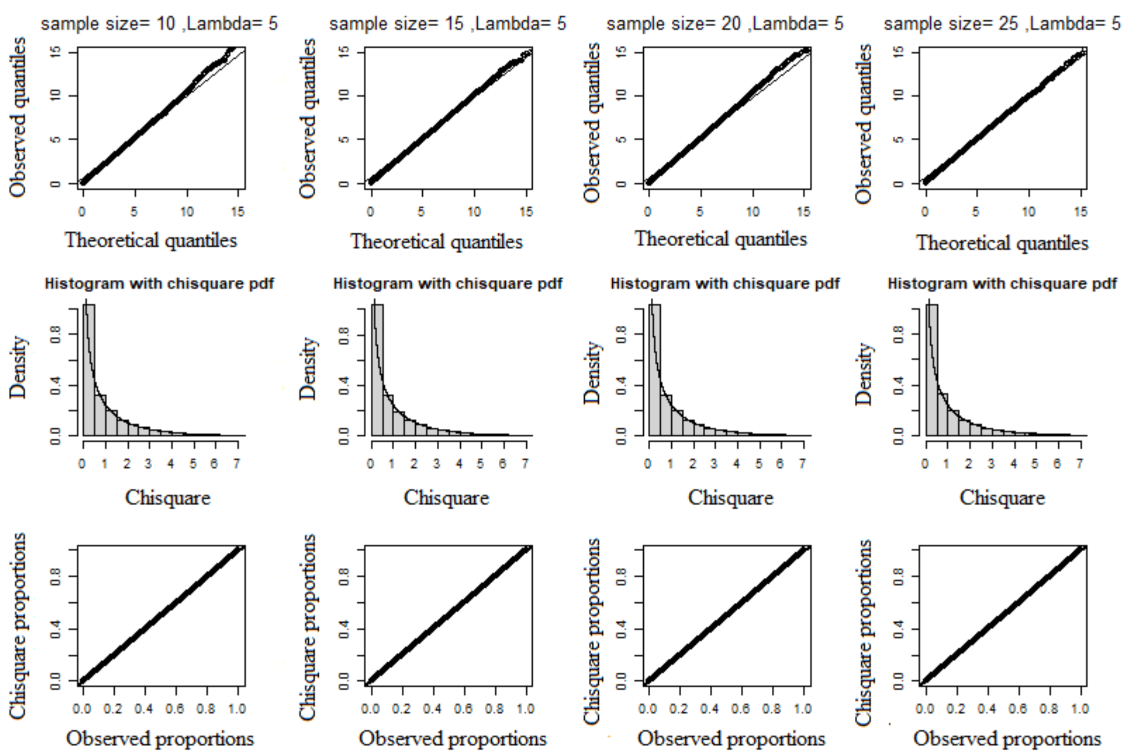

Figure 10: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

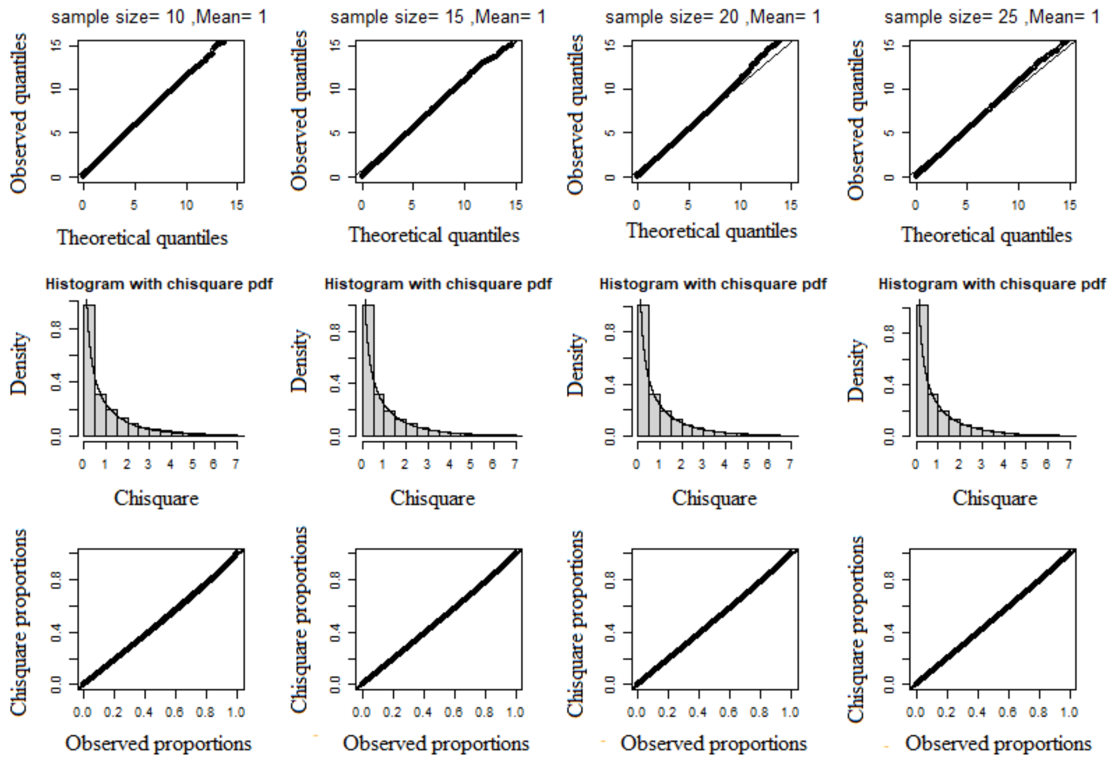

Figure11: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

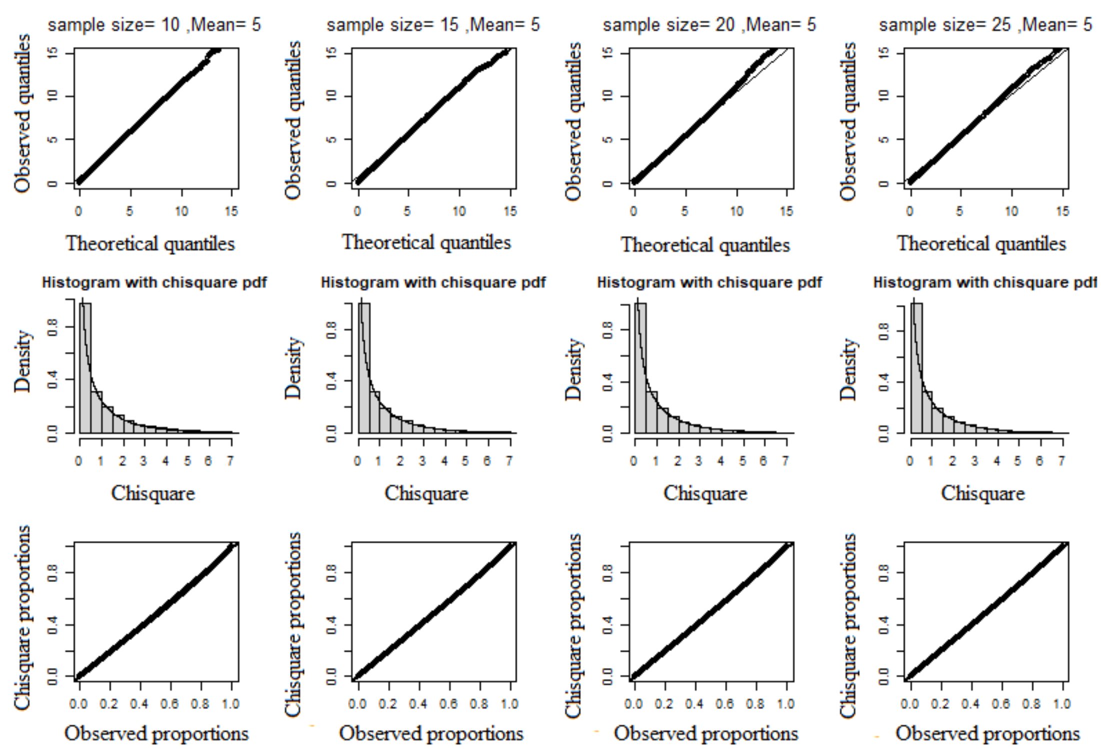

Figure 12: Top panel: Q-Q plot, middle panel: Histogram with pdf, bottom panel: P-P plot

2.5 Exponential Distribution

The likelihood function of an exponential variable X with parameter $\lambda > 0$ is given by

$$L(p|x_i) = \lambda^n e^{-\lambda \sum x_i}$$

The likelihood ratio test statistic for testing $H_0: \lambda = \lambda_0$ is

$$\lambda\left(\underset{\sim}{x}\right) = \frac{\lambda_0^n e^{-\lambda_0 \sum x_i}}{\hat{\lambda}^n e^{-\hat{\lambda} \sum x_i}} = \frac{\lambda_0^n\ e^{-\lambda_0 \sum x_i}}{\left(\frac{1}{\bar{x}}\right)^n\ e^{-n}}$$

The log-likelihood function is:

$$-2\ log\lambda(X) = 2n[1 + \log \bar{X} + \lambda_0 \bar{X} - \log \lambda_0]$$

We want to determine the approximate minimum sample size n for which $-2\,log\,\lambda\,(X)$ converges to χ_1^2 distribution under the null hypothesis $H_0: \lambda = \lambda_0$.
From Fig. 09 it can be said that for approximately 10 size of samples, $-2\,log\,\lambda\,(X)$ converges to χ_1^2 distribution under the null hypothesis $H_0: \lambda = 1$. Similarly, for approximately 10 sample size $-2\,log\,\lambda\,(X)$ converges to χ_1^2 distribution under the null hypothesis $H_0: \lambda = 5$ as we can see from Fig. 10. That is the sample size remains constant as we increase the value of λ. Therefore, the minimum sample size for any value of $\lambda > 0$ should be approximately 10 for safe in exponential distribution.

2.6 Normal Distribution with Unknown Variance

The likelihood ratio test statistic of a normal random variable *X*for testing $H_0: \mu = \mu_0$when σ^2 is unknown is

$$-2\ log\lambda(X) = \frac{n(\bar{X} - \mu_0)^2}{\sum(X_i - \bar{X})^2}$$

From Fig.11and 12 we can see that for approximately 10 size of sample, $-2\,log\,\lambda\,(X)$ converges to χ_1^2 distribution under the null hypothesis $H_0 : \mu = \mu_0$ $(\mu_0 > 0)$.

As we can see from Table01 that minimum sample sizes for which $-2\,log\,\lambda\,(X)$ converges to χ_1^2 distribution in Bernoulli distribution is approximately 200, 40 for Poisson distribution, 80 for geometric distribution, 10 for each of the exponential and normal distributions with unknown variance.

3. Conclusion

In this paper, the main concern was to determine the sample size n so that *–2logλ(X)* converges toχ_1^2distribution. In real fields, we are not sure about the exact or approximate sample size which raises the necessity of sample size determination. Sample size should be as small as possible because of cost and feasibility. In this study, 100000 datasets each of size n are generated from several important distributions such as Bernoulli, Poisson, Geometric, Exponential and Normal with unknown variance, and Y = *–2logλ(X)* are calculated for each of 100000 datasets. We drew quantile-quantile (Q-Q) plot, probability-probability (P-P) plot of Y = *–2logλ(X)*, and then we plot histograms of generated datasets with the density curve of chi-square distribution for the considered distribution to find the minimum sample sizes. Sample sizes should be at least 200 for any value of $p > 0$(probability) in Bernoulli distribution so that *–2 log λ (X)*~χ_1^2. For Poisson distribution, minimum sample size should be approximately 40 and for geometric distribution, it should be roughly 80. But we can see from our analysis that we need only 10 size of samples for exponential and normal distributions with unknown variance.

Table1: Minimum sample sizes for probability distributions

Distribution	Null Hypothesis	Sample Size under H_0	Final Sample Size
Bernoulli	$H_0: p = 0.2$	200	200
	$H_0: p = 0.5$	150	
	$H_0: p = 0.8$	200	
Poisson	$H_0: \lambda = 1$	40	$\max(40, 30) = 40$
	$H_0: \lambda = 5$	30	
Geometric	$H_0: p = 0.2$	20	$\max(20, 40, 80) = 80$
	$H_0: p = 0.5$	40	
	$H_0: p = 0.8$	80	
Exponential	$H_0: \lambda = 1$	10	10
	$H_0: \lambda = 5$	10	
Normal with variance Unknown	$H_0: \mu = 1$	10	10
	$H_0: \mu = 5$	10	

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