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COMPUTER-INTENSIVE METHODS IN AGRICULTURAL STATISTICS*

JAGDISH S. RUSTAGI
International Business Machines Corporation
San Jose, California, U.S.A.

1. Introduction

Modern practice of statistics has been going through a revolutionary change due to the use of computer-intensive methods in many areas. Whether one is testing hypotheses or one is estimating fundamental statistical quantities, computer-intensive methods such as those of Monte Carlo sampling, jackknife and bootstrap are playing an important role. In agricultural statistics, especially where extensive use is made of sample survey and design of experiment methodology, these methods provide improved procedures. Their use in econometrics, statistical genetics and various other agricultural sciences is likely to make important contributions to the solution and understanding of fundamental scientific questions.

Most of the computer-intensive methods in statistics can be implemented on desk top computers such as an IBM PC or an Apple computer. These computers not only are capable of running a large variety of statistical software but also have built in capability for many procedures in statistical graphics. Due to the easy accessibility of desk-top computers, the use of computer-intensive methods in statistical practice is very likely to grow in the future.

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Some of the modern applications in agricultural statistics require huge data bases. For example, in processing satellite data to estimate acreage under a specified crop and in other areas of image processing, computer-intensive methods are necessary. An important problem in the analysis of images is that of classification through extraction of features. Without considerable amount of computational power, statistical procedures in image analysis cannot be made.

In this paper, computer-intensive techniques in statistics are introduced through illustrations of the jackknife, bootstrap and Monte Carlo procedures. Their use will be made in examples of density estimation for bias reduetion, confidence interval estimation and testing of hypotheses. Numerical procedures, so commonly used in statistics are not discussed. They include computer-intensive procedures especially in optimization, essential in statistical practice. We give a brief introduction to Quinouille-Tukey method of jackknife and apply it to reduction of bias in the non-parametric estimates of density. An elementary introduction to the bootstrap resampling procedure of Efron is given. There are numerous applications of bootstrap in statistics, a recent conference on bootstrap was held at Michigan State University in May, 1990. Examples are given for estimating p-values for testing hypotheses through Monte Carlo simulation procedures.

In this period of fast and cheap computation, there is a bright future for computer–intensive methods to be of special benefit to the applied scientist. For the agricultural sciences, these methods are bound to provide easy access to statistical techniques needed in experimentation, inference and other decision making situations. In this short survey, it is difficult to point out the large variety of cases in which computer-intensive methods have made significant contributions. This is indicated by including many interesting applications and advances of these methods in the references at the end of the paper.

2. Jackknife Method

Suppose a random sample $X_1, X_2, \ldots . . X_n$ is given from a population with unknown parameter θ, say, the mean or the median. Now if $\hat{\theta}$ is the mean, the sample average $\bar{X}$ and the sample standard deviation s, provide not only its estimate but also its measure of precision. However, if θ is the median, then the precision of the sample median is not so obvious from the sample. The delete-one jackknife procedure is to obtain the value of the statistic from various subsamples, deleting one observation at a time.

Let $\hat{\theta}_n$ be any estimate of θ, and let $\hat{\theta}^i_{n-1}$ = estimate of θ, after X_i, is deleted from the sample.

Let $\hat{\theta}^i_{PS} = n\,\hat{\theta}_n - (n-1)\,\hat{\theta}^i_{n-1}$, be the "pseudo-value". The average of the pseudo-values is the 'delete-one jackknife' estimate of θ, given by

$$\hat{\theta}_J = \frac{1}{n} \sum_{i=1}^{n} \theta^i_{PS}.$$

An estimate of the precision of $\hat{\theta}_J$, can be obtained with the help of the estimate of its variance, given by

$$\hat{\text{Var}}\,(\hat{\theta}_J) = \frac{\sum_{i=1}^{n} (\theta^i_{PS} - \hat{\theta}_J)^2}{n-1}.$$

If $\hat{\theta}_n = \overline{X}_n$, notice that

$$\hat{\theta}^i_{PS} = n\,\overline{X}_n - n\,\overline{X}^i_{n-1} = X_i,$$

and $\hat{\theta}_J = \overline{X}_n$

That is, the jackknife procedure recovers the sample mean. The following motivation is provided for the above technique and its use in bias reduction of order $1/n$. Suppose, in general, the statistic $\hat{\theta}_n$ leads to representation of $E(\hat{\theta}_n)$ by

$$E\,(\hat{\theta}_n) = \theta + \frac{a}{n} + \frac{b}{n^2} + \ldots \tag{2.1}$$

where $a, b, \ldots$ are constants not dependent on the sample size. Then,

$$E(\hat{\theta}^i_{n-1}) = \theta + \frac{a}{n-1} + \frac{b}{(n-1)^2} + \ldots$$

and $$E(\hat{\theta}^i_{PS}) = \theta + \frac{b}{n(n-1)} + \ldots.$$

so that, $$E(\hat{\theta}_J) = \theta + \frac{b}{n(n-1)} + \ldots$$

That is, the bias of $\hat{\theta}_J$ is of order $1/n^2$ whereas the bias of $\hat{\theta}_n$ was of order $1/n$. In small sample size problems, this leads to considerable improvement of the estimate.

Quenouille (1949) introduced the technique of jackknife (so named by John Tukey) and there exists an extensive literature on the subject.

Extensions to deleting more than one observation as well as, deleting a group of observations at a time when the sample has been divided among several groups, are available. When the expansion of the expectation of the estimate $\hat{\theta}_n$ has a different form than (2.1), modifications for defining jackknife can be made. Also using robust methods, such as the trimmed mean of the pseudo-values in place of the average sometimes improves the behaviour of the jackknife estimate, Rustagi (1990).

We give here an example of delete-one-jackknife estimate of the probability density function. A common estimate of the density function is given by histogram, a term carried by Karl Pearson in 1890's. This estimate is not always desirable since, besides the arbitrariness in the choice of number of intervals, the choice of origin, and the length of intervals, it is not easy to visualize it in higher dimensions. A class of nonparametric estimates of density have been proposed in the literature. Here we discuss the kernel method and its improvement through jackknife. This fundamental statistical quantity not only is important in data analysis but also leads to developing the right model for statistical inference.

The jackknife method for density estimation was used by Schucany and Sommers (1977) and Rustagi and Dynin (1989) for reduction of bias.

A recent application of jackknife kernel estimate was made to data on tumors of breast cancer, Rustagi and Dynin (1988). Rustagi, Javier and Victoria (1989) applied a robust jackknife procedure developed by Hinkley and Wang (1984) to density estimation. It has been shown that the jackknife and trimmed jackknife estimates preserve the asymptotic properties of the density estimates while reducing bias.

Let $X_1, X_2, \ldots, X_n$ be a random sample from a population with cumulative distribution function $F(x)$ and probability density function $f(x)$. Let $K(x)$ be a given kernel function with the following properties, Parzen (1958).

(i) $\sup \mid K(x) \mid < \infty$,

(ii) $\int K(x)dx = 1$,

(iii) $\lim\limits_{|x| \to \infty} \mid xK(x) \mid = 0$,

(iv) $\int_{-\infty}^{\infty} x^i K(x)dx = 0, \quad i = 1, 2, \ldots, r-1, \int x^r K(x)\, dx \neq 0,$

and $\int | x^r K(x) | \, dx < \infty$.

Let $F_n(x)$ be the empirical distribution function based on the random sample, and let $[h_n]$ be a sequence of constants. Then the kernel density estimate of $f(x)$ as given by

$$\hat{f}_{nh_n}(x) = \frac{1}{nh_n} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h_n}\right) = \frac{1}{h_n} \int_{-\infty}^{\infty} K\left(\frac{x-y}{h_n}\right) dF_n(y).$$

The expectation of the estimate is

$$E[\hat{f}_{nh_n}(x)] = \frac{1}{h_n} \int K\left(\frac{x-y}{h_n}\right) dF(y) \neq f(x).$$

However,

$$E[\hat{f}_{nh_n}(x)] \to f(x) \text{ as } n \to \infty \text{ and } h_n \to 0.$$

That is, the kernel density estimate is asymptotically unbiased. The variance of $\hat{f}_{nh_n}(x)$ also approaches zero if in addition we assume $nh_n \to \infty$.

Let $F_{n,i}(x)$ be the empirical distribution function of the random sample $X_1, \ldots, X_n$ with the observation X_i removed, and let

$$\hat{f}^{i}_{n-1\, h_{n-1}}(x) = \frac{1}{h_{n-1}} \int K\left(\frac{x-y}{h_{n-1}}\right) dF_{n,i}(y),$$

where h_{n-1} are constants based on $n-1$ observations. The notation h_{n-1} does not mean that it is the previous value to h_n, rather h_n, h_{n-1} are function of n.

We define the pseudo-values as follows:

$$\hat{f}^{i}_{S}(x) = \frac{h_n^{-r}}{h_n^{-r} - h_{n-1}^{-r}} \hat{f}_{nh_n}(x) - \frac{h_{n-1}^{-r}}{h_n^{-r} - h_{n-1}^{-r}} \hat{f}^{i}_{n-1}\, h_{n-1}(x).$$

The jackknifed estimate of $f(x)$ is then given by $\hat{f}_J(x)$,

$$\hat{f}_J(x) = \frac{1}{n} \Sigma \hat{f}^{i}_{S}(x) = \gamma \hat{f}_{nh_n}(x) + (1-\gamma)\hat{f}_{n-1\, h_{n-1}}(x)$$

where $\gamma = \dfrac{h_{n-1}^{-r}}{h_n^{-r} - h_{n-1}^{-r}}$.

$$\text{and } \hat{f}_{n-1\, h_{n-1}}(x) = \frac{1}{n} \sum_{i=1} \hat{f}^{i}_{n-1\, h_{n-1}}(x)$$

That is, the jacknife estimate is simply a linear function of the classical estimate based on n observations and an average of estimates based on $n - 1$ observations.

Rustagi and Dynin (1983) provided expressions for bias and variance of the jackknife estimate of the density. For finding asymptotic properties of the jackknife estimate, we need the following additional assumptions.

(v) The rth derivative of the density satisfies a Lipschitz condition,

$| f^{(r)}(x) - f^{(r)}(y) | < C | x - y |^{\alpha}$,

C is a constant, and $0 \leqslant \alpha \leqslant 1$ for all x and y,

(vi) $\int | x^{r+\alpha} K(x) | \, dx < \infty$,

(vii) $\{h_n\}$ and $\{h_{n-1}\}$ are sequences of constants such that

$$\frac{h_n}{h_{n-1}} \to 1 \text{ as } h_n \to 0 \text{ and } nh_n \to \infty.$$

It is known that bias of $\hat{f}_n(x)$ is of order h_n^r. Under condition (i)—(vii), it was shown by that Rustagi and Dynin (1983) that

$$\text{Bias } [\hat{f}_J(x)] = 0(h_n^{r+\alpha}).$$

They also gave the Berry-Esseen bounds showing that asymptotic distribution of $\hat{f}_J(x)$ is normal.

A trimmed jackknife estimate of the probability density function is obtained by

$$\hat{f}_{J\beta}(x) = \frac{1}{n - 2 r_\beta} \sum_{i = r\beta + 1}^{n - r\beta} \hat{f}^{i}_{S}(x),$$

where β is the trimming proportion and r_β is the integral part of $n\beta$. $\hat{f}_{J\beta}(x)$ also has asymptotic normal distribution, Rustagi, Javier and Victoria (1990).

The estimate of hazard function,

$$\lambda(x) = \frac{f(x)}{1 - F(x)},$$

where $f(x)$ is the probability density function and $F(x)$, the cumulative distribution function of time to failure, can be obtained in terms of estimate of the density as well. Consider the case of censored data, where not all items are observed until failure. Such situations usually arise in clinical trials where the failure is death of the subject as well as in reliability testing where all items on test need not be observed until failure. The following situation prevails.

$t_1, t_2, \ldots, t_n$ are failure times having probability density function $f_T(x)$, with cumulative distribution function $F_T(x)$.

Let $C_1, C_2, \ldots, C_n$ be the censoring variable having probability density $f_C(x)$ and cumulative distribution function $F_C(x)$.

Observations are $X_i = \min(X, C_i)$, $i = 1, 2, \ldots, n$,

$$\text{and} \quad \delta_i = \begin{cases} 1 & \text{if } t_i < C_i \\ 0 & \text{if } t_i > C_i \end{cases}$$

That is, based on (X_i, δ_i), $i = 1, 2 \ldots, n$, we wish to estimate the hazard function for the random variable X, denoted by $H_T(x)$.

Note that the hazard rate has the representation,

$$\lambda_T(x) = -\frac{d}{dx}(\log H_T(x)).$$

Let $R_1, R_2, \ldots, R_n$ be the ranks of $X_1, \ldots, X_n$, then, estimate of $\lambda_T(x)$ is given by

$$\hat{\lambda}_T^n(x) = \frac{1}{h_n} \sum_{i=1}^{n} \frac{\delta_i K\left(\frac{x - X_i}{h_n}\right)}{n - R_i + 1}$$

where h_n, and kernel K have the same meaning as before, Tanner and Wong (1983). This estimate is biased and can be improved through the jackknife technique. Defining the pseudo-values as

$$\hat{\lambda}_S^i(x) = \frac{h_n^{-r}\,\hat{\lambda}_T^n(x) - h_{n-1}^{-r}\,\hat{\lambda}_T^{n-1}(x)}{h_n^r - h_{n-1}^{-r}}$$

the jackknife estimate is

$$\hat{\lambda}_J(x) = \frac{1}{n}\sum_{i=1}^{n} \hat{\lambda}_s^i(x)$$

It has been shown by Rustagi and Dynin (1988) that

$$\sup_x \left| \hat{\lambda}_J(x) - \lambda(x) \right| \to 0 \text{ as } n \to \infty$$

and the central limit theorem applies for $\hat{\lambda}_J(x)$ under certain conditions on h_n, h_{n-1} and kernel K.

The small sample behaviour of the jackknife and trimmed jackknife estimates of the density can only be studied through simulations. A few examples are given here. Consider a bimodal density which is a mixture of two normal distributions, given by

$$f(x) = .4\,N(1, 4) + \cdot 6N(8, 4),$$

where $N(\mu, \sigma^2)$ gives the normal distribution with mean μ and variance σ^2. Figure 1 gives the graph of the true, kernel estimate and corresponding jackknife and trimmed jackknife estimates of the density $f(x)$ with

$$h_n = \frac{7}{(500)^{1/5}}$$

for $n = 500$ observations using the standard normal density as the kernel. Figure 2 gives the same using the biweight kernel,

$$K(x) = \frac{15}{16}(1 - x^2)^2, \; -1 \leqslant x \leqslant 1, \; 0, \text{ elsewhere},$$

and $h_n = 10/(500)^{0\cdot 2}$, when $n = 500$

The mean integrated squared error of the estimates (MISE) is calculated for the above two cases in Table 1.

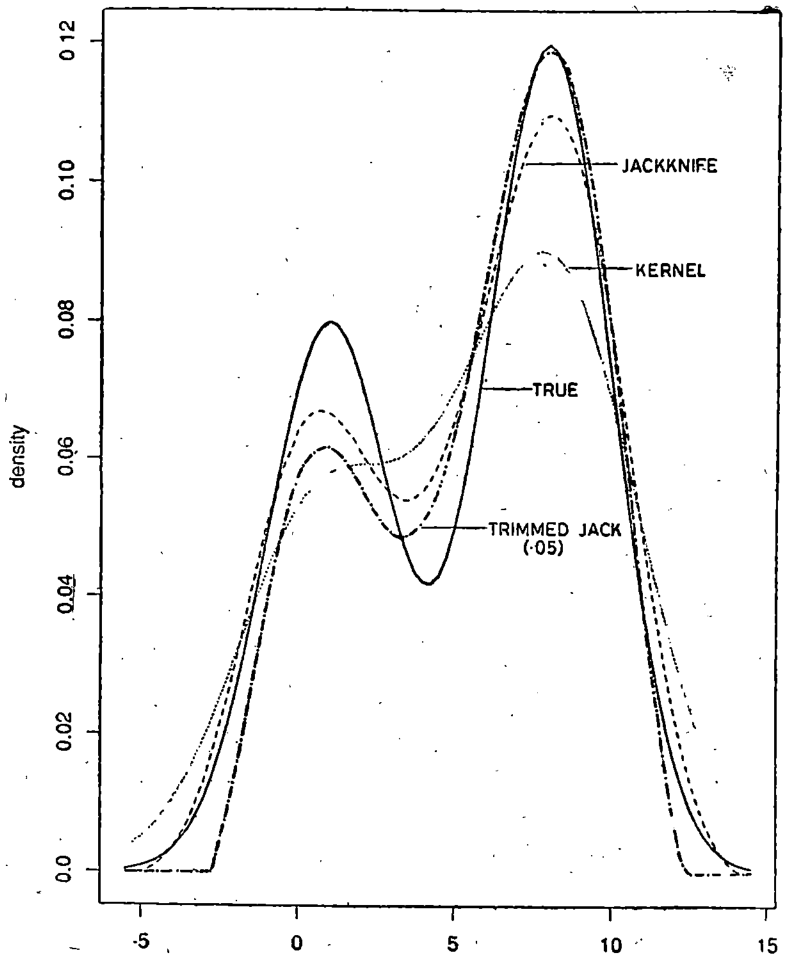

Figure I.

TABLE 1

	Kernel est.	*Jackknife est.*	*Trimmed Jack. est.*
Standard Normal Kernel	0.00435	0.00116	0.00705
Biweight Kernel	0.00825	0.00396	0.00393

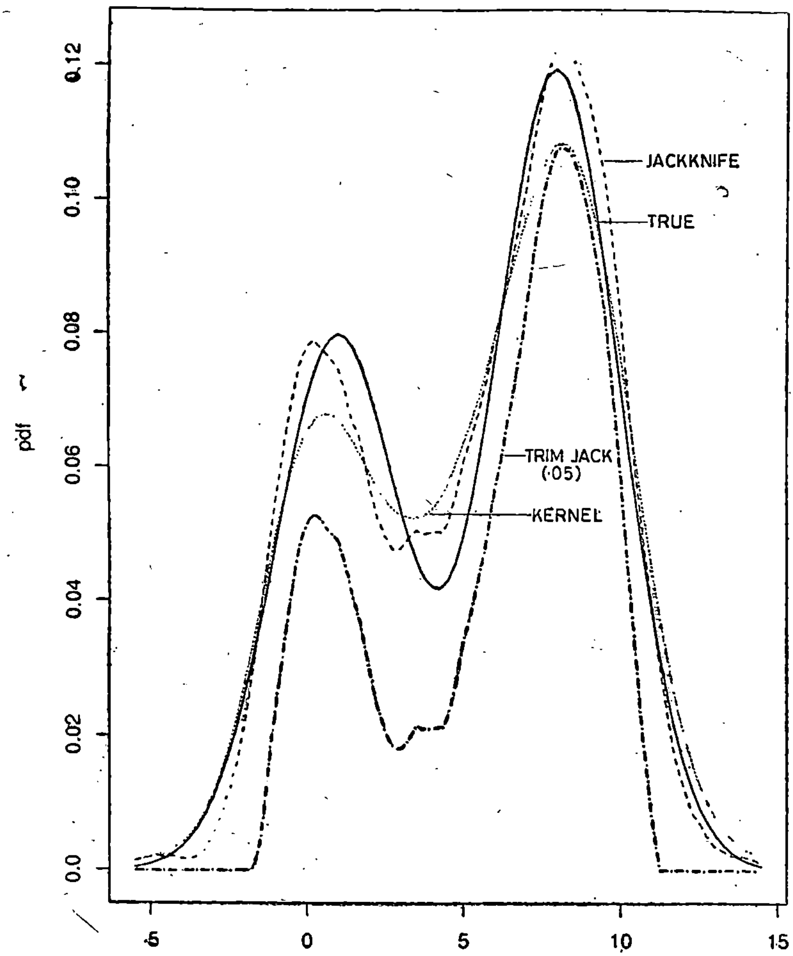

Figure 2.

When samples are generated from the bimodal density

$$f(x) = .5\, N(1, 4/9) + .5\, N(-1, 4/9),$$

eresults are given Figure 3 for

$$h = 1/(25)^{\cdot 2}, \text{ sample size } n = 25$$

and standard normal kernel.

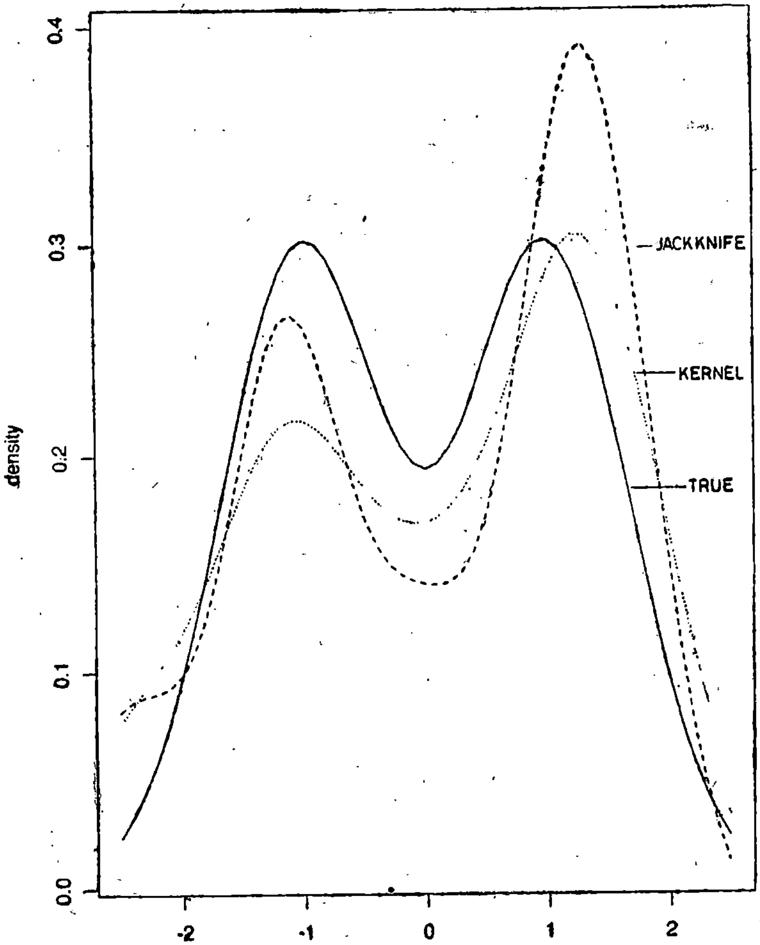

Figure 3

In Figure 4, comparison is made for kernel and jackknife estimate for sample size 50, $h = 1/(50)^{0.2}$, for the standard normal kernel.

Results for small samples are not very good since density estimates require large number of observations.

The choice of bandwidth for estimating a density function has been based alone on the theoretical justification of Rosenblatt (1956) and Parzen (1958), who showed that

$$h = \alpha(K)\, \beta(f)\, n^{-1/5}$$

where $\alpha(K) = [\int K^2(y)\, dy / (\int y^2 K(y)\, dy)^2]^{1/5}$

$$\beta(f) = [\int f''(y)^2\, dy]^{-1/5}.$$

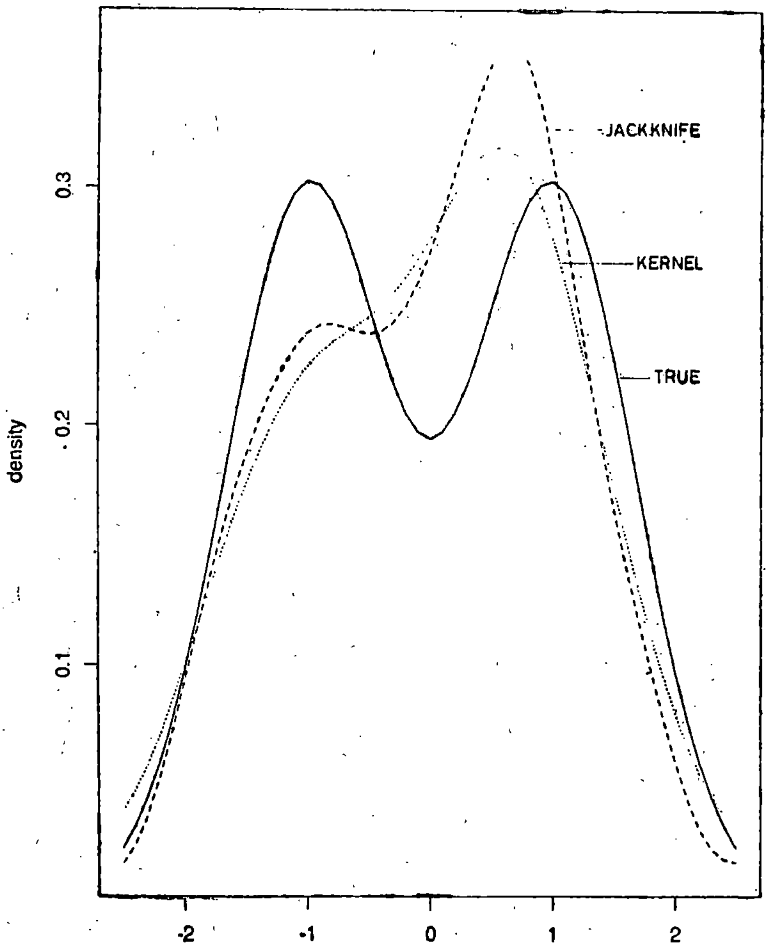

Figure 4

minimizes the asymptotic mean integrated squared error. Obviously f is unknown and hence β (f) cannot be determined. Several suggestions have been made, the recent are by Marron (1990), and others, utilize bootstrap method for its determination. We shall consider bootstrap resampling procedure later in the paper.

Use of jackknife technique has been made in many other areas of statistics. For example, jackknife has been used in reducing bias of ratio estimates in sample surveys, Durbin (1959) and Cochran (1977), for parameter estimation in dilution series, Does, Strijbosch and Albers (1988), in assessing competition among skewed distributions of plant biomass, Higgins, Bendel and Mack (1984), in breast cancer data analysis, Rustagi and Dynin (1988), and estimating species richness, Heltsche and Forrester (1983) among many others. Recently Efron (1990) has applied jackknife-after-bootstrap for getting more information out of bootstrap analysis especially about the accuracy of the bootstrap estimates.

3. Computer-intensive Methods in Hypotheses Testing

Using fairly general assumptions about the population from which sample is taken, computer-intensive methods can be used to test hypotheses about the distribution. Usually normal distribution theory is needed to test hypotheses about equality of means of two or more groups such as for using F-test in analysis of variance. With the help of randomization tests, which use hardly any distributional assumptions, all the above tests can be performed and their p-values can be computed using the computed distribution from the sample. We illustrate the computer-intensive procedure with an example. For a comprehensive review, the book of Noreen (1989) may be consulted.

Randomization test was introduced by Fisher (1935) and its properties have been studied extensively in the literature. Due to the computational requirement, the test was seldom used. This practical difficulty is now easily removed by fast and cheap computing. Also the test is easy to implement even on a personal computer.

As an example of randomization, consider the problem of deciding whether variety A of a cereal gives better yield than variety B, other things remaining the same. If we assume that yields are normally distributed with common variance, the test is made comparing the means of the populations using t-statistic, However, if no assumptions are made about the distribution, we can consider the problem as that of testing the hypothesis that the yield is unrelated to the variety. Let m observations be made on variety A and n on variety B. Consider the statistic, the absolute difference between their sample averages. The sample value of the statistic is obtained as $u = | \bar{x} - \bar{y} |$, say, where $\bar{x}$, $\bar{y}$ are the averages of samples from variety A and B respectively. The distribution of the statistic u can be obtained by randomization procedure under the null hypothesis. Consider the sample of $m + n$ observations, choosing m items at random from this sample will lead to various values of the statistic u. The frequency distribution of u, given a large number of values of u provides a mechanism to give the p-value of the test. Let u_0 be the sample observed value. Then the estimate of the probability that $u > u_0$ is obtained giving us the p-value of the test. Figure 5 gives the upper tail value, for example as the p-value of the test. Based on this value the hypothesis can be rejected or accepted. The procedure can be extended to several groups or to the use of any other statistic and is very general. The computer-intensive nature of these tests is obvious. Many other tests are given by Noreen (1989).

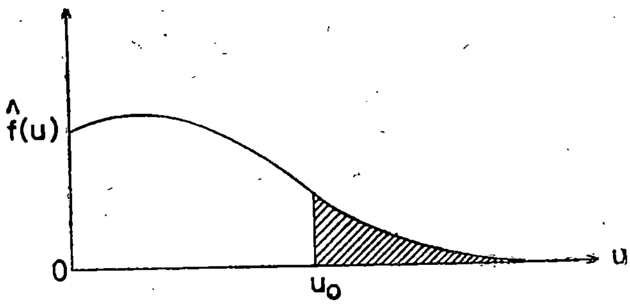

Figure 5

Methods using simulation are needed to compute power of many tests where the test statistic does not lead to a closed form distribution under the alternative hypothesis. Such procedures are commonly used in the nonparametric case, Hollander and Wolfe (1973).

Randomization tests can be used for contingency tables as well as for nominal data. Many times we can use the permutation of the observations for finding the distributions of the statistics and hence randomization tests are generally known as permutation tests in such cases.

4. Bootstrap Method

An ingeneous method using resampling recently introduced by Efron (1982), is that of bootstrap. This computer-intensive technique has received extensive attention in the statistical community. A recent conference on bootstrap was held at the Michigan State University in May, 1990 where recent advances in many statistical areas based on bootstrap, were discussed.

The bootstrap method provides the distribution of statistics and other important measures such as standard deviation of a statistic through resampling from a given sample. Let $X_1, X_2, \ldots, X_n$ be a random sample from a population having cumulative distribution function $F(x)$. Let the sampling empirical distribution function be denoted by

$$\hat{F}(x) = \frac{1}{n}\left\{ \# X_i < x \right\}$$

which puts probability $1/n$ at each observation X_i.

Let $X_1^*, X_2^*, \ldots, X_n^*$ be a random sample(obtained through simulation) from $\hat{F}(x)$. That is, $X_1^*, X_2^*, \ldots, X_n^*$ is a random sample drawn with replacement from $X_1, X_2, \ldots, X_n$. Several such samples will provide the sampling distribution of any statistic obtained from the sample. For example, let $\theta(F) = E(X)$, the mean of F.

$$\text{Let } \bar{X} = \hat{\theta}, \text{ Let } \bar{X}^* = \frac{\Sigma X_i^*}{n}.$$

$$\text{The variance of } \bar{X}^* \text{ is } \frac{1}{n}\left(\frac{\Sigma (X_i - \bar{X})}{n}\right).$$

In general, for a statistic $\hat{\theta}(X_1, X_2, \ldots, X_n)$, the standard error can be obtained from the bootstrap sample. That is

$$\text{S.E (bootstrap)} = \{\text{Var}\,(\hat{\theta}\,(X_1^*, X_2^*, \ldots, X_n^*)\}^{1/2}$$

In general, let F^* be the sampling distribution of the bootstrap samples. Then F^* can be used to provide various quantities needed for the use of statistic $\hat{\theta}(X_1, \ldots, X_n)$ such as prediction error, confidence intervals and bias. Many asymptotic properties of this procedure have been studied, and show the versatility and power of bootstrap procedure.

There is a deep connection between jackknife and bootstrap procedure. The resampling in bootstrap is the procedure which assigns probability $1/n$ with each observation in the sample. That is, the resampling procedure requires the weights

$$\left(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}\right)$$

on the observed vector. The jackknife procedure instead requires that the resampling procedure assign weight according to

$$\left(\frac{1}{n-1}, \frac{1}{n-1}, \ldots, 0, \frac{1}{n-1}, \ldots, \frac{1}{n-1}\right)$$

with 0 at the ith observation X_i. It can be shown that in some case, such as the estimate of the standard deviation, bootstrap and jackknife procedure lead to approximately the same estimate of the standard deviation, Efron (1982).

Relation with Cross-validation

Cross-validation is a general procedure in which half the sample is used to fit a given model and the other half is used to verify the model. This second phase is known as cross-validation. It is not necessary that sample be divided in two equal parts. One could leave an observation from a sample of size n and fit the model to $n-1$ data points. The cross-validation procedure then will predict the left out observation. This form looks like a jackknife procedure but we are not "jackknifing" a statistic here. For a comprehensive discussion of the interrelationships among bootstrap jackknife and cross-validation, see Efron (1982).

For obtaining more information on the accuracy of bootstrap estimates, bootstrap-after-bootstrap or iterative bootstrap has been used by many authors, e.g. Hall (1986). However, it has been shown by Efron (1990), that jackknife-after-bootstrap provides a more economic method for obtaining information on the accuracy of the bootstrap estimates.

5. Monte Carlo Simulation

Simulations by nature are computer-intensive. Computer simulations are used in variety of ways in statistics. In studying theoretical properties of various statistical procedures recourse is made to simulations when mathematical tractability is remote. Applications to multivariate simulation procedures has been reviewed and collected in a book by Johnson (1987). There are hardly any areas of statistics where simultions are not applied In auditing by Biddle, Bruton and Siegel (1986), in modelling by Catchpole, Morgan and O'Dowd (1987), in optimization by Rustagi (1981), in Michaelis-Menten analysis, Currie (1982), and Rustagi and Yang (1979), in testing hypotheses, Hope (1968) etc., simulations have been extensively utilized.

It should be remarked that compter-intensive methods discussed above have a high potential for use in applied statistics. With the improvement and accessibility of cheap and fast computing power, computer-intensive methods will allow the applied scientist to use powerful statistical techniques in data analysis and statistical decision making in future.

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