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RESEARCH COMMUNICATIONS

An algorithm for conducting hypotheses testing based on Neyman–Pearson Lemma. I. The case of continuous univariates

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Neyman–Pearson Lemma provides a method for constructing the best critical region in hypotheses testing problems involving two simple hypotheses H_0 and H_1. In many applications H_0 and H_1 are expressed as probability density functions $f_0(x)$ and $f_1(x)$. In practical situations the functions $f_0(x)$ and $f_1(x)$ are either too complicated to be amenable for straightforward theoretical treatment by Neyman–Pearson Lemma or given only as a table of numerical values. An algorithm to conduct the Neyman–Pearson test for such a complicated situation is proposed. A Fortran program, called NPTEST, for implementing the algorithm has also been developed and tested.

In many hypotheses testing problems one has to decide between two probability density functions (PDF) $f_0(x)$ and $f_1(x)$ and the Neyman–Pearson Lemma[1] can be used to construct the best critical region for the test. In many practical situations the PDF $f_0(x)$ defining the null hypothesis H_0 and the PDF $f_1(x)$ defining the alternative hypothesis H_1 are either too complicated to be amenable for straightforward theoretical treatment by Neyman–Pearson Lemma or are given only as a table of numerical values. For example, in statistical tests for determining the space group symmetry of a crystal one meets with such a situation. It would therefore be quite useful to develop an algorithm for conducting the Neyman–Pearson test for such complicated situations and in this paper we shall describe one such algorithm. A Fortran program, called NPTEST, for implementing the algorithm has also been developed and tested using random samples generated from a few known probability distributions. NPTEST has also

been tested in a few crystallographic situations related to space group determination. The details of these tests are also presented.

In the present paper we shall assume x to be a 1-dimensional continuous random variable. For the convenience of numerical calculation we shall assume $f_0(x)$ and $f_1(x)$ to be defined in a finite interval $a<x<b$. If the PDF's under H_0 and H_1 are themselves defined on a finite interval, the choice of a and b are trivial. However if the PDF's under H_0 and H_1 are defined on an infinite interval, the user has to specify a suitable finite interval (a, b) for conducting the test. In this case it is advisable to choose a and b such that the probability mass of the original distributions included in that interval is as large as possible. If the PDF's under H_0 and H_1 are defined on an infinite interval, then NPTEST computes the truncated distributions applicable to the interval (a, b) and uses them in the calculation.

Consider the following hypotheses testing problem:

$$H_0: f(x)=f_0(x)$$
$$H_1: f(x)=f_1(x) \qquad (1)$$

Let $\{x_1, x_2, \cdots, x_n\}$ be a random sample used in the test. We shall assume that, for any given value of x, the values of $f_0(x)$ and $f_1(x)$ can be calculated to a desired accuracy. In view of the Neyman–Pearson Lemma[1], the best critical region (BCR) is determined by

$$\prod_{j=1}^{n}\left[\frac{f_1(x_j)}{f_0(x_j)}\right] \geq k, \qquad (2)$$

where k is a non-negative constant. Taking the natural logarithms of (2) and then dividing both sides by n, we obtain

$$(1/n)\sum_{j=1}^{n} t_j \geq (\ln k)/n, \qquad (3)$$

where t is defined to be

$$t=\ln\left[\frac{f_1(x)}{f_0(x)}\right]. \qquad (4)$$

Defining T and c by

$$T=\left\langle \ln\left[\frac{f_1(x)}{f_0(x)}\right]\right\rangle = \langle t\rangle, \quad c=(\ln k)/n, \qquad (5)$$

we can rewrite (3) compactly as

$$T\geq c. \qquad (6)$$

T defined in (5) is the test statistic of the Neyman–Pearson test. Let $f(T|H_0)$ be the PDF of T when H_0 is true. The BCR of size α (i.e., the level of significance α) is given by the inequality

$$T\geq T_c, \qquad (7)$$

where the value of T_c is to be chosen such that

$$P(T\geq T_c|H_0)=\alpha. \qquad (8)$$

Thus the best test for the present situation is the one that is based on the statistic T with the region $T\geq T_c$ as the critical region. For a given α, the value of T_c satisfying (8) can be obtained by Monte Carlo Method as shown below.

To obtain the critical value T_c for a given $\alpha(=0.05$, say), we must first obtain the sampling distribution of T under the null hypothesis H_0. This can be done numerically using the technique of inverse transform[2] by the Monte Carlo method and it involves the following steps: (i) Generating a value of the random variable x from the distribution given by the PDF $f_0(x)$ by the inverse transform method (see the next paragraph for more details); (ii) Using this value x compute the value of $t(x)$ defined in (4); (iii) Repeating steps (i) and (ii) r times ($r=500$, say) and obtaining r values of t (denoted by $t_1, t_2, \cdots, t_r$). (iv) Computing the average value $\left(\sum_{j=1}^{r} t_j\right)/r$ and denoting it by T_1. T_1, thus obtained, is a sample value from $f(T|H_0)$; (v) Repeating the steps (i)–(iv) p times ($p=500$, say) and obtaining the values $T_1, T_2, \cdots, T_p$. These represent a random sample of size p from $f(T|H_0)$; (vi) Arranging the values $T_1, T_2, \cdots, T_p$ in decreasing order and obtaining the set of values $T'_1, T'_2, \cdots, T'_p$, where $T'_1\geq T'_2\geq\cdots\geq T'_p$; (vii) Since there are 500 values of T in all, it follows that $(T'_{25}+T'_{26})/2$ may be taken to be the solution of (8) corresponding to $\alpha=0.05$.

Step (i) in the above procedure needs some explanation and we shall consider this aspect presently. Let $F_0(x)$ be the cumulative distribution function of x for the truncated PDF of x valid for the finite interval $a\leq x\leq b$. According to the principle of probability integral transformation[3], the random variable u defined by

$$u=F_0(x) \qquad (9)$$

is uniformly distributed in the interval $0\leq u\leq 1$. For any given value u' of u the value of the inverse of the function in (12) can be obtained numerically by solving the equation

$$F_0(x)-u'=0 \qquad (10)$$

by the Newton–Raphson method[4] as

$$x_{m+1} = x_m - \frac{\{F_0(x_m) - u'\}}{f_0(x_m)}, \quad m = 0, 1, 2 \cdots, \tag{11}$$

where we have used the fact that $f_0(x)$ is the deviation of $F_0(x)$. The initial approximation x_0 needed for the Newton–Raphson algorithm in (11) may be obtained by the following steps: (i) Generating 501 equally spaced values of x in $[a, b]$ and letting these be denoted by x_j, $j = 1$ to 501. Computing the values of $F_0(x_j)$ $(= u_j$, say), $j = 1$, 501. The ordered pairs (x_j, u_j), $j = 1$ to 501, provide a discrete representation of the function defined in (9). Evidently the ordered pairs (u_j, x_j), $j = 1$ to 501, provide a discrete representation of the inverse of the function defined in (12); (ii) For the v $(= 43$, say) numbers* $u_k' = 0, 0.05, 0.1, \cdots, 0.9, 0.905, 0.910, \cdots, 0.98, 0.9825, 0.9850, \cdots, 1.0$ computing the corresponding x_k', $k = 1$ to v, by using linear interpolation on the set $\{(u_j, x_j), j = 1$ to $501\}$ obtained in step (i). The ordered pairs (u_k', x_k'), $k = 1$ to v, thus obtained also provide a discrete representation of the inverse of the function defined in (9). This smaller set (i.e., $v \ll 501$) is more convenient for obtaining the value of x for any given value of u by linear interpolation: (iii) Finding the interval in which the number u' lies and using it to find x_0 by linear interpolation on the set $\{(u_k', x_k'), k = 1$ to $v\}$.

A Fortran program, called NPTEST, has been written incorporating the above numerical calculations**. The program requires the following information as input: (i) A table of values of $f_0(x)$ and $f_1(x)$ for different values of x, (ii) The sample values $\{x_i\}$ for the test. It computes tables of values of the PDFs of x under H_0 and H_1 at 50 equally-spaced grid points in the interval (a, b). It then fits these two truncated PDFs with interpolating cubic splines. It calculates the cumulative function of x for the truncated distributions of x under H_0 and H_1 at the 50 grid points by numerical integration. It then computes the critical value of the test statistic T by Monte Carlo method. The program then conducts the test and prints out the unique decision arrived at.

The algorithm was tested for 3 hypothetical cases. In each case (see Table 1) a random sample of size 700 was generated from a specific distribution using the principle of random variable generation[3]. While the

*The grid-point-spacings, in the u'-space are taken to be 0.05, 0.005, 0.0025 for $0 \leq u' \leq 0.9$, $0.9 \leq u' \leq 0.98$ and $0.98 \leq u' \leq 1$ respectively. Such a choice has been made to obtain sufficiently accurate values for x_0 in the numerical process.

**The listing of NPTEST can be had from the authors on request.

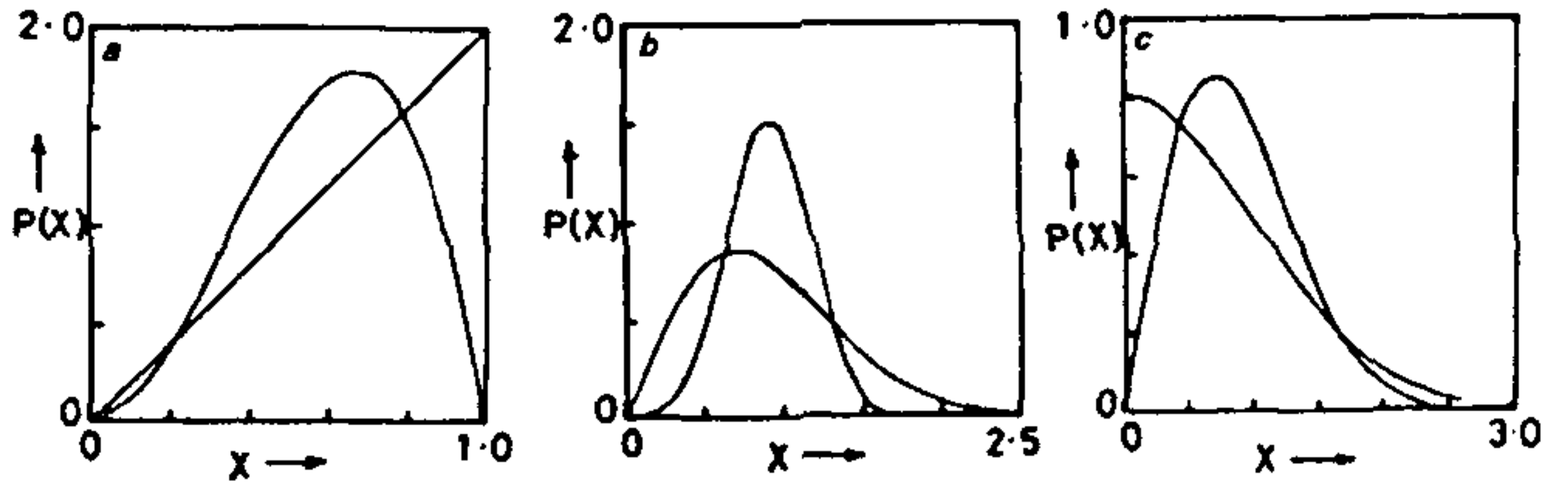

Figure 1. The graphs of the PDFs used to specify H_0 and H_1 for three cases. Curves (1 *a*), (1 *b*) and (1 *c*) are for the three cases considered in Table 1.

Table 1. Description of the three hypothetical cases used to test NPTEST

Case	PDFs used in hypotheses testing		Domain of definition of the PDFs	Ref. fig.	The PDF used to generate the sample
	$f_0(x)$	$f_1(x)$			
1	$2x$	$12x^2(1-x)$	$0 \leq x \leq 1$	1 *a*	$f_0(x)$
2	$2x\exp(-x^2)$	$4x^3\exp(-x^4)$	$x \geq 0$	1 *b*	$f_0(x)$
3	$\sqrt{2/\pi}\exp(-x^2/2.0)$	$2x\exp(-x^2)$	$x \geq 0$	1 *c*	$f_1(x)$

Note: (i) For case 1, $f_0(x)$ is the PDF of the beta distribution[5] with parameters $m = 2$ and $n = 1$ and $f_1(x)$ is the PDF of the beta distribution with parameters $m = 3$ and $n = 2$
(ii) For case 2, $f_0(x)$ is the PDF of the Weibull distribution[5] with parameters $n = 2$ and $\sigma = 1$ and $f_1(x)$ is the PDF of the Weibull distribution with parameters $n = 4$ and $\sigma = 1$
(iii) For case 3, $f_0(x)$ and $f_1(x)$ are the PDFs of the normalized structure factor magnitude for the centric and acentric Wilson distributions[6,7] which occur in the field of X-ray crystallography.

Table 2. Results obtained from NPTEST for the 3 cases described in Table 1

Case	Critical region	Observed value of the test statistic	Decision obtained regarding the PDF of the sample	PDF used to generate the sample
1	$[-0.149$	0.126	$f_0(x)$	$f_0(x)$
2	$[-0.587$	0.583	$f_0(x)$	$f_0(x)$
3	$[-0.148$	−0.225	$f_1(x)$	$f_1(x)$

Note: $\alpha = 0.05$. '$[x_0$' stands for the interval $0 \le x \le x_0$.

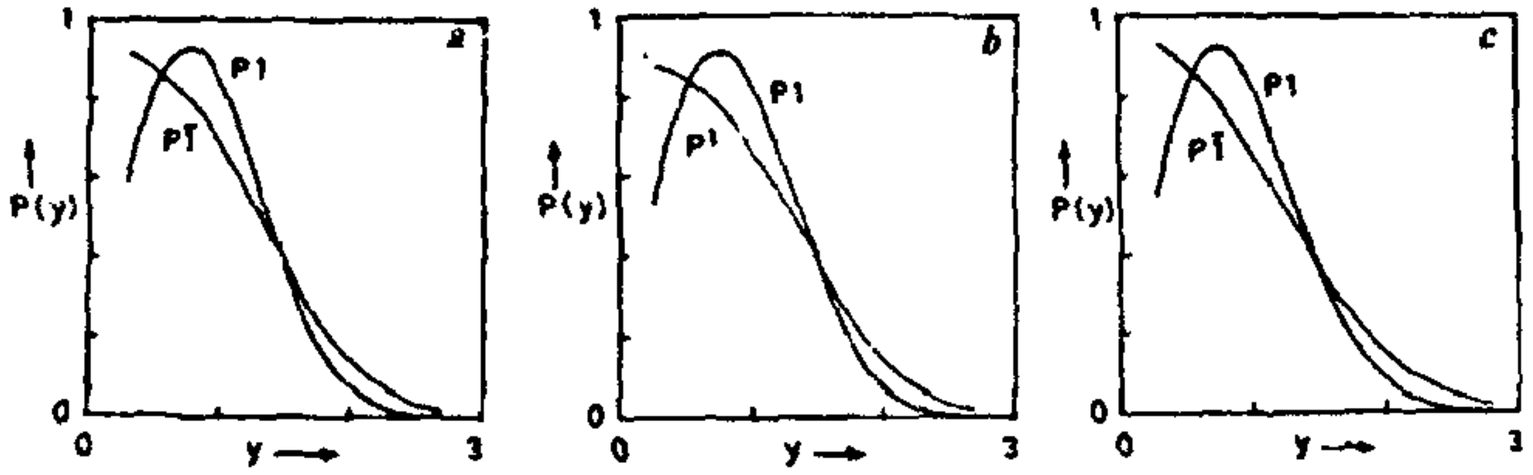

Figure 2. The graphs of the PDFs of y for three crystallographic situations. Curves (2 *a*), (2 *b*) and (2 *c*) are for the crystals 1, 2 and 3 of Table 3.

PDFs $f_0(x)$ and $f_1(x)$ for the first case are defined on the finite interval $0 \le x \le 1$, those for the second and the third are defined on the interval $0 \le x < \infty$. For the latter two cases the theoretical truncated distributions valid for the interval $0 \le x < b$ were used in the test. The values of b for the second and third cases were determined such that the probability $\Pr(0 \le x \le b)$, calculated using that PDF which tends to zero less slowly, is greater than or equal to 0.999. The sample data which lies in the interval $0 \le x \le b$ was used in the test for the cases 2 and 3. The results obtained from the tests conducted using NPTEST for these three cases are given in Table 2 which shows that correct decisions are obtained in all the cases.

The algorithm was also tested for three situations met with in X-ray crystallography. The PDF of the normalized structure factor magnitude y for a triclinic crystal containing 2 heavy atoms per unit cell besides a large number of light atoms is given by[7]

$$P(y) = (1/\sigma_2)(2/\pi)^{3/2} \exp(-y_N^2/2{\sigma_2}^2) \left[\int_0^{\pi/2} \exp[-{\sigma_1}^2 \sin^2\psi/{\sigma_2}^2] \times \cos h[\sqrt{2}\,\sigma_1 y_N \sin\psi/{\sigma_2}^2]\, d\psi \right], \quad (12)$$

if the space group of the crystal is $P\bar{1}$ and by

$$P(y) = (4y_N/\pi{\sigma_2}^2) \exp(-{y_N}^2/{\sigma_2}^2) \left[\int_0^{\pi/2} \exp[-(2{\sigma_1}^2 \sin^2\psi/{\sigma_2}^2) \times I_0[2\sqrt{2}\,\sigma_1 y_N \sin\psi/{\sigma_2}^2]\, d\psi \right], \quad (13)$$

if the space group of the crystal is $P1$. The parameter σ_1^2 is a measure of the contribution of the heavy atoms to the local average intensity relative to that from all the atoms in the unit cell of the crystal and $\sigma_2^2 = 1 - \sigma_1^2$. A crystallographer meets with the problem of deciding whether the space group of the crystal under investigation is $P1$ or $P\bar{1}$ from the normalized structure amplitude data (called, y-values) which could be obtained from the intensities of X-ray reflections. This problem can be solved by testing whether the observed y-data fits better either (12) or (13). Since σ_1^2 is a slowly varying function of the $(\sin\theta/\lambda)$ where 2θ is the angle of scattering and λ is the wavelength of X-rays, an average value of σ_1^2 is to be determined for the reflections used in the test and this average value is to be used to compute the table of values of the PDFs of y corresponding to the null and alternative hypotheses. The tests were conducted by using the truncated PDFs, the limits a and b being determined from an analysis of y-values. Relevant details of the three crystals used in the tests are given in Table 3 and the theoretical PDFs of y corresponding to the hypothesis H_0 (i.e., space

Table 3. Details of the three crystals[8–10] used to test NPTEST

Crystal	Asymmetric unit	Space group	a	b	σ_1^2
1	$C_5H_{12}NO_3Cl$	$P\bar{1}$	0.314	2.700	0.53
2	$C_{39}H_{52}N_3O_{12}Br$	$P\bar{1}$	0.286	2.700	0.56
3	$C_{16}H_{22}NOCl$	$P\bar{1}$	0.287	2.800	0.44

Table 4. Results obtained from NPTEST for the three crystals described in Table 3

Crystal	Critical region	Observed value of the test statistic	Decision obtained regarding the space group of the crystal	Actual space group of the crystal
1	$[-0.020$	0.038	$P\bar{1}$	$P\bar{1}$
2	$[-0.021$	0.032	$P\bar{1}$	$P\bar{1}$
3	$[-0.023$	0.047	$P\bar{1}$	$P\bar{1}$

Note: $\alpha = 0.05$. '$[x_0$' stands for the interval $0 \leq x \leq x_0$.

group of the crystal is $P1$) and H_1 (i.e., space group of the crystal is $P\bar{1}$) are shown in Figure 2. The results obtained from the tests are given in Table 4. It is seen that correct results are obtained in all the three cases.

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Self-diffusion coefficient of 86-Rb in mica-rich soils

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The self-diffusion coefficient of 86-Rb in four surface soils derived from mica-rich parent materials was determined at field capacity. Its values ranged from 0.54×10^{-10} to 1.674×10^{-10} cm^2 sec^{-1} at zero level K and from 1.788×10^{-10} to 7.02×10^{-10} cm^2 sec^{-1} at 50 ppm level K. These values were found much lower than the values reported elsewhere earlier. Enrichment of these soils with 50 ppm carrier-K resulted in a tremendous increase in the Da–Rb values.

THE movement of K through diffusion is important in soils[1]. Potassium does not have any suitable isotope to use in labelling soil. The ^{42}K and ^{43}K have half-lives only in hours, while enrichment of natural isotope, ^{40}K and the stable isotope ^{41}K is very expensive. The rubidium was tested as a tracer of K in soil studies[2]. The process of Rb uptake from soil by plant roots is similar to that of K uptake[3,4]. The self-diffusion of ^{86}Rb was found linearly correlated positively with soil moisture[5]. In view of this, an experiment was conducted to study the self-diffusion coefficient of ^{86}Rb in soils derived from mica-rich parent materials. Such information particularly for the soils of India is meagre.

Surface soils of four representative pedons of Giridih and Munger districts of Bihar were collected. Half-cell technique as outlined by Sen and Deb[6] was used to study the Rb-diffusion, at two K-levels i.e. 0 and 50 ppm K. The tagging of soils with 86-Rb was performed taking 1 μCi/g of soil. A calculated amount of water corresponding to water content at 0.3 bar (field capacity) was added. Activity of tagged and untagged soil portions was measured using a G. M. counter. All the determinations were made in duplicate. The apparent self-diffusion coefficient of ^{86}Rb was then calculated by using the integrated form of the equation derived by Phillips and Brown[7] and presented in Table 1.

The self-diffusion coefficient ^{86}Rb in all four soils at zero level K ranged from 0.54×10^{-10} to 1.674×10^{-10} cm^2 s^{-1}. The enrichment of these soils with 50 ppm carrier-K before determining the Da Rb, however, resulted in a tremendous increase in the Da Rb values at field capacity. This increase in Da Rb appears to be possibly due to an increase in soil solution concentration of K. The values for Da Rb in these mica-rich soils were observed to be generally lower than the values reported earlier[7,8]. Such low values of Da Rb might have been due to the fact that the soil clays were rich in