

NOTE ON DISTRIBUTION FREE TESTING FOR DISCRETE DISTRIBUTIONS

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The paper proposes one-to-one transformation of the vector of components $\{Y_{in}\}_{i=1}^m$ of K. Pearson's chi-square statistic,

$$Y_{in} = \frac{\nu_{in} - np_i}{\sqrt{np_i}}, \quad i = 1, \dots, m,$$

into another vector $\{Z_{in}\}_{i=1}^m$, which, therefore, contains the same "statistical information", but is asymptotically distribution free. Hence, any functional/test statistic based on $\{Z_{in}\}_{i=1}^m$ is also asymptotically distribution free. Natural examples of such test statistics are traditional goodness of fit statistics from partial sums $\sum_{I \leq k} Z_{in}$.

The supplement shows how the approach works in the problem of independent interest: the goodness of fit testing of power-law distribution with Zipf's law and Karlin - Rouault law as particular alternatives.

1. Introduction. The main driver for this work was the need for a class of distribution free tests for discrete distributions. The basic step, reported in §2 below, could have been made long ago, maybe even soon after the publication of the classical papers of K. Pearson (1900) and R. Fisher (1922, 1924). However, the tradition of using the chi-square goodness of fit statistic became so widely spread and the point of view that, for discrete distributions, other statistics "have to" have their asymptotic distributions dependent on the individual probabilities, became so predominant and "evident", that it required a strong impulse to examine the situation again. It came, in this case, in the form of a question from Prof. Ritei Shibata: "why is the theory of distribution free tests for discrete distributions so much more narrow than for continuous distributions?". If it is true that sometimes a question is half of the answer, then this is one such case.

We recall that for continuous distributions, the idea of the time transformation $t = F(x)$ of Kolmogorov (1933), along with subsequent papers of

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Smirnov (1936) and Wald and Wolfowitz (1939), was always associated with a *class* of goodness of fit statistics. The choice of statistics invariant under this time transformation, at least since the paper of Anderson and Darling (1952), became an accepted principle in goodness of fit theory for continuous distributions. For discrete distributions, however, everything is locked on a single statistic, the chi-square goodness of fit statistic. It certainly is true that in cases like the maximum likelihood statistic for multinomial distributions (see, e.g., Kendall and Stuart (1963)) or like the empirical likelihood (see, e.g., Einmahl and McKeague (1999) and Owen (2001)) the chi-square statistic appears as a natural asymptotic object. Yet most of the time the choice of this statistic comes as a deliberate choice of one particular asymptotically distribution free statistic. The idea of a *class* of asymptotically distribution free tests, to the best of our knowledge, was never considered in any serious and systematic way.

This is a pity, because unlike the transformation $t = F(x)$, which is basically a tool for one-dimensional time x , if we do not digress onto the transformation of Rosenblatt (1952) or spatial martingales of Khmaladze (1993), the idea behind K. Pearson's chi-square test is applicable to any measurable space. The potential of its generalization seems, therefore, worth investigation.

We will undertake one such investigation in this paper. Namely, we will obtain a transformation of the vector Y_n of components of K. Pearson's chi-square statistic (see below) into a vector Z_n , which will be shown to be asymptotically distribution free. Therefore, any functional based on Z_n can be used as a statistic of asymptotically distribution free test for the corresponding discrete distribution. Thus, the paper demonstrates, we hope, that the geometric insight behind the papers of K. Pearson (1900) or R. Fisher (1924) goes considerably further than one goodness of fit statistic.

In the remaining part of this introduction we present a typical result of this paper. General results and other, may be more convenient, forms of the transformation are given in the appropriate sections later on.

Let p_1, \dots, p_m be a discrete probability distribution; all $p_i > 0$ and $\sum_{i=1}^m p_i = 1$. Denote $\nu_{1n}, \dots, \nu_{mn}$ the corresponding frequencies in a sample of size n and consider the vector Y_n of components of the chi-square statistic

$$Y_{in} = \frac{\nu_{in} - np_i}{\sqrt{np_i}}, \quad i = 1, \dots, m.$$

Let $X = (X_1, \dots, X_m)^T$ denote a vector of m independent $N(0, 1)$ random variables. As $n \rightarrow \infty$ the vector Y_n has a limit distribution of the zero-mean Gaussian vector $Y = (Y_1, \dots, Y_m)^T$ such that

$$(1) \quad Y = X - \langle X, \sqrt{p} \rangle \sqrt{p},$$

where \sqrt{p} denotes the vector $\sqrt{p} = (\sqrt{p_1}, \dots, \sqrt{p_m})^T$. Here and below we use notation $\langle a, b \rangle$ for inner product of vectors a and b in \mathbb{R}^m : $\langle a, b \rangle = \sum_{i=1}^m a_i b_i$.

According to (1) the vector Y is an orthogonal projection of X parallel to \sqrt{p} . Of course its distribution depends on \sqrt{p} – it is only the sum of squares

$$\langle Y, Y \rangle$$

which is chi-square distributed and hence has a distribution free from \sqrt{p} . It is for this reason that we do not have any other asymptotically distribution free goodness of fit test for discrete distributions except the chi-square statistic

$$\langle Y_n, Y_n \rangle = \sum_{i=1}^m \frac{(\nu_{in} - np_i)^2}{np_i}.$$

In particular, the asymptotic distribution of partial sums based on Y_{in} , like

$$\sum_{i=1}^k \frac{\nu_{in} - np_i}{\sqrt{np_i}} \quad \text{or} \quad \sum_{i=1}^k \frac{\nu_{in} - np_i}{\sqrt{n}}, \quad k = 1, 2, \dots, m,$$

which would be discrete time analogues of the empirical process, will certainly depend on \sqrt{p} , as will the asymptotic distribution of statistics based on them. Here we would like to refer to paper of Henze(2008), which advances the point of view that goodness of fit tests for discrete distributions should be thought of as based on on empirical processes in discrete time, i.e., on the partial sums on the right. In the same vein, the paper Choulakian *at al.* (1994) considered quadratic functionals based on these partial sums, as direct analogues of (weighted) omega-square statistics. We refer also to Goldstein *et al.* (2004), where tables for some quantiles of Kolmogorov – Smirnov statistics from the partial sums are calculated in the parametric problem, described in the supplement. These papers illustrate the dependence on the hypothetical distribution p very clearly.

We do not know many attempts to construct distribution free tests for discrete distributions, but one such, suggested in Greenwood and Nikulin (1996), stands out for its simplicity and clarity: any discrete distribution

function F_0 can be replaced by a piece-wise linear distribution function \tilde{F}_0 with the same values as F_0 at the (nowhere dense) jump points of the latter; this opens up possibility to use time transformation $t = \tilde{F}_0(x)$ and thus obtain distribution free tests. However, without inquiring what are the consequences of implied additional randomization between the jump points, this approach remains a one-dimensional tool.

In this paper we introduce a vector $Z_n = \{Z_{in}\}_{i=1}^m$ as follows: let r be the unit length “diagonal” vector with all coordinates $1/\sqrt{m}$, and put

$$(2) \quad Z_n = Y_n - \langle Y_n, r \rangle \frac{1}{1 - \langle \sqrt{p}, r \rangle} (r - \sqrt{p}).$$

More explicitly,

$$Z_{in} = \frac{\nu_{in} - np_i}{\sqrt{np_i}} - \frac{1}{\sqrt{m}} \sum_{j=1}^m \frac{\nu_{jn} - np_j}{\sqrt{np_j}} \frac{1}{1 - \sum_{j=1}^m \sqrt{p_j/m}} \left(\frac{1}{\sqrt{m}} - \sqrt{p_i} \right).$$

We will see that the following statement for Z_n is true:

PROPOSITION. *Let $\mathbb{I} = (1, \dots, 1)^T$ denote the vector with all m coordinates equal 1. The asymptotic distribution of Z_n is that of another, “standard”, orthogonal projection*

$$Z \stackrel{d}{=} X - \langle X, r \rangle r = X - \frac{1}{m} \langle X, \mathbb{I} \rangle \mathbb{I},$$

and therefore any statistic based on Z_n is asymptotically distribution free. The transformation of Y_n to Z_n is one-to-one.

Thus the problem of testing p is translated into the problem of testing uniform discrete distribution of the same dimension m .

In particular, partial sums

$$\sum_{i=1}^k Z_{in}, \quad k = 1, 2, \dots, m,$$

will asymptotically behave as a discrete time analog of the standard Brownian bridge. On the other hand, since the transformation from Y_n to Z_n is one-to-one, Z_n carries the same amount of “statistical information” as Y_n .

For the proof of proposition see Theorem 1 below. We will see that this is not an isolated result but one of several possible, and follows from one particular point of view, which is explained in the next section. We carry it on to the parametric case in section 3.

2. Pertinent unitary transformation. The idea behind the transformation (2) can be explained as follows: the problem with the vector Y is that it projects a standard vector X parallel to a specific vector, the vector \sqrt{p} . This vector changes and with it changes the distribution of Y . However, using an appropriate unitary operator, which incorporates \sqrt{p} , one can “turn” Y so that the result will be an orthogonal projection parallel to a standard vector. One such standard vector can be the vector $(1/\sqrt{m})\mathbb{I}$ above.

Slightly more generally, let q and r be two vectors of unit length in m -dimensional space \mathbb{R}^m . Apart from obvious particular choice of $r = (1/\sqrt{m})\mathbb{I}$ and $q = \sqrt{p} = (\sqrt{p_1}, \dots, \sqrt{p_m})^T$, we will consider other choices later on as well. Denote by $\mathcal{L} = \mathcal{L}(q, r)$ the 2-dimensional subspace of \mathbb{R}^m , generated by the vectors q and r , and by \mathcal{L}^* its orthogonal complement in \mathbb{R}^m . In the lemma below we write $q_{\perp r}$ for the part of q orthogonal to r , and $r_{\perp q}$ for the part of r orthogonal to q :

$$q_{\perp r} = q - \langle q, r \rangle r, \quad r_{\perp q} = r - \langle q, r \rangle q,$$

and let $\mu = \|q_{\perp r}\| = \|r_{\perp q}\|$. Obviously, vectors r and $q_{\perp r}/\mu$ form an orthonormal basis of \mathcal{L} and vectors q and $r_{\perp q}/\mu$ form another orthonormal basis. Consider

$$U = rc^T + q_{\perp r}d^T/\mu,$$

with some $c, d \in \mathcal{L}$, as a linear operator in \mathcal{L} .

LEMMA 1. (i) *The operator U is unitary if and only if the vectors c and d are orthonormal:*

$$\|c\| = \|d\| = 1, \quad \langle c, d \rangle = 0.$$

(ii) *The unitary operator U maps q to r ,*

$$Uq = r,$$

if and only if $c = q$ and $d = \pm r_{\perp q}/\mu$.

Altogether

$$U = rq^T \pm \frac{1}{\mu^2} q_{\perp r} r_{\perp q}^T$$

is the unitary operator in \mathcal{L} , which maps vector q to vector r . It also maps vector $r_{\perp q}$ to vector $\pm q_{\perp r}$.

Remark. In what follows in this section we will choose the sign +.

It is clear that if vector x is orthogonal to q and r then $Ux = 0$. In other words, U annihilates \mathcal{L}^* . Denote $I_{\mathcal{L}^*}$ the projection operator parallel to \mathcal{L} , so that it is the identity operator on \mathcal{L}^* and annihilates the subspace \mathcal{L} . Then the operator $I_{\mathcal{L}^*} + U$ is a unitary operator on \mathbb{R}^m . We use it to obtain our first result.

Suppose vector Y is projection of X , parallel to the vector q ,

$$Y = X - \langle X, q \rangle q.$$

THEOREM 1. (i) *The vector*

$$(3) \quad X' = (I_{\mathcal{L}^*} + U)X = X - \langle X, q \rangle (q - r) - \langle X, r_{\perp q} \rangle \frac{1}{1 - \langle q, r \rangle} (r - q)$$

is also a vector with independent $N(0, 1)$ coordinates.

(ii) *The vector*

$$(4) \quad Z = (I_{\mathcal{L}^*} + U)Y = Y - \langle Y, r \rangle \frac{1}{1 - \langle q, r \rangle} (r - q)$$

is projection of X' parallel to r :

$$Z = X' - \langle X', r \rangle r.$$

Proof. (i) By its definition vector Y is the orthogonal projection of X , parallel to q . Therefore, if we project it further as

$$R = Y - \langle Y, r_{\perp q} \rangle \frac{1}{\mu^2} r_{\perp q} = X - \langle X, q \rangle q - \langle X, r_{\perp q} \rangle \frac{1}{\mu^2} r_{\perp q},$$

we will obtain the vector R orthogonal to both q and r , that is, a vector in \mathcal{L}^* . If we apply operator $I_{\mathcal{L}^*}$ to R it will not change, while U will annihilate it, and thus

$$\begin{aligned} (I_{\mathcal{L}^*} + U)X &= R + U(\langle X, q \rangle q + \langle X, r_{\perp q} \rangle \frac{1}{\mu^2} r_{\perp q}) \\ &= R + \langle X, q \rangle r + \langle X, r_{\perp q} \rangle \frac{1}{\mu^2} q_{\perp r} \\ &= X - \langle X, q \rangle (q - r) - \langle X, r_{\perp q} \rangle \frac{1}{\mu^2} (r_{\perp q} - q_{\perp r}). \end{aligned}$$

Noting that

$$r_{\perp q} - q_{\perp r} = (r - q)(1 + \langle q, r \rangle) \quad \text{and} \quad \mu^2 = 1 - \langle q, r \rangle^2,$$

we obtain the right hand side of (3). Coordinates of X' are independent $N(0, 1)$ random variables if the covariance matrix $EX'X'^T$ is the identity matrix on \mathbb{R}^m . We have

$$\begin{aligned} EX'X'^T &= (I_{\mathcal{L}^*} + U)EXX^T(I_{\mathcal{L}^*} + U)^T = (I_{\mathcal{L}^*} + U)(I_{\mathcal{L}^*} + U^T) \\ &= I_{\mathcal{L}^*} + UU^T = I_{\mathcal{L}^*} + rr^T + \frac{1}{\mu^2}q_{\perp r}q_{\perp r}^T = I. \end{aligned}$$

(ii) Note that the orthogonality property of Y , $\langle Y, q \rangle = 0$, implies that $\langle X, r_{\perp q} \rangle = \langle Y, r \rangle$, and re-write (3) as

$$X' = (I_{\mathcal{L}^*} + U)X = Y - \langle Y, r \rangle \frac{1}{1 - \langle q, r \rangle} (r - q) + \langle X, q \rangle r.$$

Also note that

$$\langle X', r \rangle = \langle (I_{\mathcal{L}^*} + U)X, r \rangle = \langle X, (I_{\mathcal{L}^*} + U)^T r \rangle = \langle X, q \rangle,$$

so that Z is indeed the projection of X' we need:

$$Z = X' - \langle X', r \rangle r = Y - \langle Y, r \rangle \frac{1}{1 - \langle q, r \rangle} (r - q). \quad \square$$

The second statement of this theorem, together with the classical statement $Y_n \xrightarrow{d} Y$, and the choice of $r = (1, \dots, 1)/\sqrt{m}$ and $q = \sqrt{p}$, proves the proposition of the introduction.

The nature of the transformation and the proof given above does not depend on a particular choice of the vector r and is correct for any r of unit length. For example, we can choose $r = (1, 0, \dots, 0)^T$. Then the transformed vector Z_n will have coordinates

$$(5) \quad Z_{in} = \frac{\nu_{in} - np_i}{\sqrt{np_i}} - \frac{\nu_{1n} - np_1}{\sqrt{np_1}} \frac{1}{1 - \sqrt{p_1}} (\delta_{1i} - \sqrt{p_i}),$$

or

$$Z_{1n} = 0, \quad Z_{in} = \frac{\nu_{in} - np_i}{\sqrt{np_i}} - \frac{\nu_{1n} - np_1}{\sqrt{np_1}} \frac{1}{1 - \sqrt{p_1}} \sqrt{p_i}, \quad i = 2, \dots, m.$$

As a corollary of the previous theorem we obtain a vector with very simple asymptotic behavior.

COROLLARY 2. *If $Y_n \xrightarrow{d} Y = X - \langle X, \sqrt{p} \rangle \sqrt{p}$ then for the vector Z_n defined in (5) we have*

$$Z_n \xrightarrow{d} (0, X_2, \dots, X_m)^T.$$

To find the asymptotic distribution of statistics based on this choice of Z_n may be more convenient than in the previous case. Yet, the relationship between the two is one-to-one.

It is often the case that the probabilities p_1, \dots, p_m depend on a parameter, which has to be estimated from observed frequencies. This case needs additional consideration which we defer to the next section. However, there are also cases when the hypothetical probabilities are fixed, or the value of the parameter is estimated from previous samples, and therefore needs to be treated as a given. In these cases Theorem 1 is directly applicable.

One important case of this type is the two-sample problem. Namely, let events, labeled by $i = 1, 2, \dots, m$, be basically as above, and let $\nu'_{1n'}, \dots, \nu'_{mn'}$ and $\nu''_{1n''}, \dots, \nu''_{mn''}$ be frequencies of these events in two independent samples of size n' and n'' respectively. Let μ_1, \dots, μ_m denote the frequencies in the pooled sample of size $n = n' + n''$. Then the normalized differences

$$Y'_{in} = \frac{\nu'_{in'} - n'\mu_i/n}{\sqrt{n'\mu_i/n}}, \quad i = 1, \dots, m,$$

are the components of the two sample chi-square statistic: the sum of their squares is the statistic. Conditions which guarantee convergence of the vector Y'_n of these differences in distribution to the vector Y are well known (see, e.g., Rao (2002), or Einmahl, Khmaladze (2001) and references therein). Then it follows from Theorem 1, that under these conditions the vector Z'_n with coordinates

$$\begin{aligned} Z'_{in} &= \frac{\nu'_{in'} - n'\mu_i/n}{\sqrt{n'\mu_i/n}} - \frac{1}{\sqrt{m}} \sum_{j=1}^m \frac{\nu'_{jn} - n'\mu_j/n}{\sqrt{n'\mu_j/n}} \times \\ &\quad \times \frac{1}{1 + \sum_{j=1}^m \sqrt{\mu_j/nm}} \left(\frac{1}{\sqrt{m}} + \sqrt{\frac{\mu_i}{n}} \right) \end{aligned}$$

converges in distribution to vector $X - \langle X, \mathbb{I} \rangle \mathbb{I}/m$ and, hence, is asymptotically distribution free. To show this result one needs only to choose as q

the vector $(\sqrt{\mu_1/n}, \dots, \sqrt{\mu_m/n})^T$ in Theorem 1 above. Corollary 2 suggests another choice of the transformed vector with coordinates

$$Z_{in} = \frac{\nu'_{in'} - n'\mu_i/n}{\sqrt{n'\mu_i/n}} - \frac{\nu'_{1n} - n'\mu_1/n}{\sqrt{n'\mu_1/n}} \frac{1}{1 + \sqrt{\mu_1/n}} \sqrt{\frac{\mu_i}{n}}, \quad i = 2, \dots, m,$$

with also simple asymptotic behavior.

3. The case of estimated parameters. We will now see that the pivotal property of Y_n to behave as asymptotically orthogonal projection of X remains true for components of chi-square statistic with estimated parameter.

Indeed, if the hypothetical probabilities depend on a κ -dimensional parameter, $p_i = p_i(\theta)$, which is estimated via maximum likelihood or minimum chi-square, then the statistic

$$\sum_{i=1}^m \frac{(\nu_{in} - np_i(\hat{\theta}_n))^2}{np_i(\hat{\theta}_n)}$$

has chi-square distribution with $m - 1 - k$ degrees of freedom (see extensive review of this matter in Stigler (1999), Ch. 19). Notwithstanding great convenience of this result, note, however, that the asymptotic distribution of the vector \hat{Y}_n itself, with

$$(6) \quad \hat{Y}_{in} = \frac{\nu_{in} - np_i(\hat{\theta}_n)}{\sqrt{np_i(\hat{\theta}_n)}},$$

depends, under hypothesis, not only on the probabilities $p_i(\theta)$ at the true value of θ , but also on their derivatives in θ . Therefore, the limit distribution of statistics from \hat{Y}_n in general will depend on the hypothetical parametric family and on the value of the parameter.

At the same time, it is well known since long ago (see, e.g., Cramér (1946), Ch. 20; a modern treatment can be found in van der Vaart (1998)) that under mild assumptions the maximum likelihood (and minimum chi-square) estimator possesses asymptotic expansion of the form

$$\sqrt{n}(\hat{\theta}_n - \theta) = \Gamma^{-1} \sum_{i=1}^m Y_{in} \frac{\dot{p}_i(\theta)}{\sqrt{p_i(\theta)}} + o_P(1),$$

where $\dot{p}_i(\theta)$ denotes the κ -dimensional vector of derivatives of $p_i(\theta)$ in θ and

$$\Gamma = \sum_{i=1}^m \frac{\dot{p}_i(\theta)\dot{p}_i(\theta)^T}{p_i(\theta)}$$

denotes the $\kappa \times \kappa$ Fisher information matrix. At the same time, the expansion

$$\hat{Y}_{in} = Y_{in} - \frac{\dot{p}_i(\theta)^T}{\sqrt{p_i(\theta)}} \sqrt{n}(\hat{\theta}_n - \theta) + o_P(1)$$

is also true. Combining these two expansions one obtains:

$$(7) \quad \hat{Y}_{in} = Y_{in} - \frac{\dot{p}_i(\theta)^T}{\sqrt{p_i(\theta)}} \Gamma^{-1} \sum_{i=1}^m Y_{in} \frac{\dot{p}_i(\theta)}{\sqrt{p_i(\theta)}} + o_P(1).$$

Use notation

$$\hat{q}_i = \Gamma^{-1/2} \frac{\dot{p}_i(\theta)}{\sqrt{p_i(\theta)}}, \quad i = 1, \dots, m,$$

and remember that

$$\sum_{i=1}^m \sqrt{p_i(\theta)} \frac{\dot{p}_i(\theta)^T}{\sqrt{p_i(\theta)}} = 0,$$

i.e., that the vectors in i , which form \dot{p}/\sqrt{p} , are orthogonal to the vector \sqrt{p} . Therefore all κ coordinates of q_i form, in i , vectors, which are orthonormal and orthogonal to the vector $\sqrt{p(\theta)}$. Together with (1) this implies the convergence in distribution of \hat{Y}_n to Gaussian vector

$$(8) \quad \hat{Y} = X - \langle X, \sqrt{p} \rangle \sqrt{p} - \langle X, \hat{q} \rangle \hat{q}.$$

It is easily seen that expression (8) describes \hat{Y} as orthogonal projection of X parallel to vectors \sqrt{p} and \dot{p}/\sqrt{p} (see Khmaladze (1979) for analogous description of empirical processes). Using this description, we can extend the method of §2 to the present situation.

Indeed, let us assume from now on that $\kappa = 1$, which will make the presentation more transparent. Having two vectors, $q = \sqrt{p(\theta)}$ and \hat{q} , which determine the asymptotics of \hat{Y}_n , let us choose now a standard vector r of unit length and another vector, \hat{r} , also of unit length and orthogonal to r . Heuristically, one may think of it as a normalized “score function” for some “standard” family around r . For example, choose $r = (1/\sqrt{m})\mathbb{I}$ and choose

any unit vector, such that $\sum_{i=1}^m \hat{r}_i = 0$. Two such choices, we think, will be particularly useful: for m even

$$\frac{1}{\sqrt{m}}(1, \dots, 1, -1, \dots, -1)^T,$$

or

$$\frac{1}{\sqrt{m}}(1, \dots, 1, -1, \dots, -1, 1, \dots, 1)^T$$

with the “plateau” of -1 s taken $m/2$ -long, and for m odd put, say, the last coordinate equal 0.

Whatever the choice of \hat{r} , suppose we chose and fixed it. It is obvious that the vector

$$(9) \quad \hat{Z} = X - \langle X, r \rangle r - \langle X, \hat{r} \rangle \hat{r}$$

has a distribution totally unconnected, and, hence, free from the parametric family $p(\theta)$. Consider now the subspace $\hat{\mathcal{L}} = \mathcal{L}(q, \hat{q}, r, \hat{r})$. We do not need to insist that it is a 4-dimensional subspace, but typically it is, at least, as far as we have freedom in \hat{r} . Let $\hat{\mathcal{L}}^*$ denote the orthogonal complement of $\hat{\mathcal{L}}$ to \mathbb{R}^m . Two bases of the space $\hat{\mathcal{L}}$ will be useful: one is formed by r, \hat{r}, b_3, b_4 where b_3 and b_4 are re-arrangements of q and \hat{q} , which are orthonormal and orthogonal to r and \hat{r} ; the other is formed by q, \hat{q}, a_3, a_4 where a_3 and a_4 are re-arrangements of r and \hat{r} , which are orthonormal and orthogonal to q and \hat{q} . We will consider particular forms of these vectors later on.

LEMMA 2. *The operator*

$$\hat{U} = r q^T + \hat{r} \hat{q}^T + b_3 a_3^T + b_4 a_4^T$$

is a unitary operator on $\hat{\mathcal{L}}$ and such that

$$\hat{U} q = r, \quad \hat{U} \hat{q} = \hat{r}.$$

THEOREM 3. *Under convergence in distribution of the vector \hat{Y}_n with coordinates (6) to the Gaussian vector \hat{Y} given by (8), the vector*

$$(10) \quad \hat{Z}_n = \hat{Y}_n - \langle \hat{Y}_n, a_3 \rangle (a_3 - b_3) - \langle \hat{Y}_n, a_4 \rangle (a_4 - b_4)$$

converges in distribution to the Gaussian vector \hat{Z} given by (9). Therefore, any statistic based on Z_n is asymptotically distribution free.

Proof. Let $\hat{\mathcal{L}}^*$ be orthogonal complement of the subspace $\hat{\mathcal{L}}$ in \mathbb{R}^m and let \hat{I} be projector on the $\hat{\mathcal{L}}^*$. We need to verify two things: (a) that the vector \hat{Z} can be obtained as

$$\hat{Z} = (\hat{I} + \hat{U})\hat{Y}$$

and (b) that its explicit form is as given in the theorem. We show (a) slightly differently from what was done in Theorem 1. Namely, recall that the covariance operator of \hat{Y} is the projector $E\hat{Y}\hat{Y}^T = I - qq^T - \hat{q}\hat{q}^T$, where I stands for an identity operator on \mathbb{R}^m , and consider the covariance operator of $(\hat{I} + \hat{U})\hat{Y}$:

$$E(\hat{I} + \hat{U})\hat{Y}\hat{Y}^T(\hat{I} + \hat{U})^T = (\hat{I} + \hat{U})(I - qq^T - \hat{q}\hat{q}^T)(\hat{I} + \hat{U})^T.$$

However, $(\hat{I} + \hat{U})I(\hat{I} + \hat{U})^T = I$ while $(\hat{I} + \hat{U})q = r$ and $(\hat{I} + \hat{U})\hat{q} = \hat{r}$. This implies that

$$(\hat{I} + \hat{U})(I - qq^T - \hat{q}\hat{q}^T)(\hat{I} + \hat{U})^T = I - rr^T - \hat{r}\hat{r}^T,$$

which is the covariance operator of \hat{Z} .

To show (b) use the basis q, \hat{q}, a_3, a_4 and the orthogonality of \hat{Y} to q and \hat{q} to find that the projection of \hat{Y} on $\hat{\mathcal{L}}$ can be written as

$$\langle \hat{Y}, a_3 \rangle a_3 + \langle \hat{Y}, a_4 \rangle a_4$$

and therefore the difference $\hat{Y} - \langle \hat{Y}, a_3 \rangle a_3 - \langle \hat{Y}, a_4 \rangle a_4$ will remain unchanged by the operator \hat{I} . At the same time $\hat{U}a_3 = b_3$ and $\hat{U}a_4 = b_4$. This leads to the following form of our transformed vector \hat{Z} :

$$(\hat{I} + \hat{U})\hat{Y} = \hat{Y} - \langle \hat{Y}, a_3 \rangle (a_3 - b_3) - \langle \hat{Y}, a_4 \rangle (a_4 - b_4).$$

□

With regard to practical applications, there are several natural choices of vectors a_3, a_4 . For example, denote $r_{\perp q\hat{q}}$ the part of r orthogonal to both q and \hat{q} and choose

$$a_3 = \frac{1}{\|r_{\perp q\hat{q}}\|} r_{\perp q\hat{q}} = \frac{1}{\|r_{\perp q\hat{q}}\|} (r - \langle r, q \rangle q - \langle r, \hat{q} \rangle \hat{q})$$

and, similarly, choose a_4 as

$$a_4 = \frac{1}{\|\hat{r}_{\perp r q\hat{q}}\|} \hat{r}_{\perp r q\hat{q}} = \frac{1}{\|\hat{r}_{\perp r q\hat{q}}\|} (\hat{r} - \langle \hat{r}, q \rangle q - \langle \hat{r}, \hat{q} \rangle \hat{q} - \langle \hat{r}, a_3 \rangle a_3).$$

In dual way, we can choose specific b_3 and b_4 as

$$b_3 = \frac{1}{\|q_{\perp r\hat{r}}\|} q_{\perp r\hat{r}} = \frac{1}{\|q_{\perp r\hat{r}}\|} (q - \langle q, r \rangle r - \langle q, \hat{r} \rangle \hat{r})$$

and

$$b_4 = \frac{1}{\|\hat{q}_{\perp qr\hat{r}}\|} \hat{q}_{\perp qr\hat{r}} = \frac{1}{\|q_{\perp qr\hat{r}}\|} (\hat{q} - \langle \hat{q}, r \rangle r - \langle \hat{q}, \hat{r} \rangle \hat{r} - \langle \hat{q}, b_3 \rangle b_3).$$

A more symmetric choice would be

$$a_3 = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1+\rho}} \left(\frac{1}{\|r_{\perp q\hat{q}}\|} r_{\perp q\hat{q}} + \frac{1}{\|\hat{r}_{\perp q\hat{q}}\|} \hat{r}_{\perp q\hat{q}} \right)$$

and

$$a_4 = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1-\rho}} \left(\frac{1}{\|r_{\perp q\hat{q}}\|} r_{\perp q\hat{q}} - \frac{1}{\|\hat{r}_{\perp q\hat{q}}\|} \hat{r}_{\perp q\hat{q}} \right),$$

where ρ is correlation coefficient between $r_{\perp q\hat{q}}$ and $\hat{r}_{\perp q\hat{q}}$. Note that in both cases the inner products $\langle \hat{Y}, a_3 \rangle$ and $\langle \hat{Y}, a_4 \rangle$ become linear combinations of just $\langle \hat{Y}, r \rangle$ and $\langle \hat{Y}, \hat{r} \rangle$. For the last, symmetric choice, for example, they are

$$\frac{1}{\sqrt{2}} \left(\frac{1}{\|r_{\perp q\hat{q}}\|} \langle \hat{Y}, r \rangle \pm \frac{1}{\|\hat{r}_{\perp q\hat{q}}\|} \langle \hat{Y}, \hat{r} \rangle \right)$$

respectively.

Although the choice of $r = (1/\sqrt{m})\mathbb{1}$ is a natural one, the different choice of the vectors r and \hat{r} leads to simpler form of the transformed vector with convenient and simple asymptotic distribution. Namely, let $r = (1, 0, \dots, 0)^T$ and $\hat{r} = (0, 1, 0, \dots, 0)^T$. Then $\langle \hat{Y}, r \rangle$ and $\langle \hat{Y}, \hat{r} \rangle$ become

$$\frac{1}{\sqrt{2}} \frac{1}{\sqrt{1 \pm \rho}} \left(\frac{1}{\sqrt{1 - q_1^2 - \hat{q}_1^2}} \hat{Y}_1 \pm \frac{1}{\sqrt{1 - q_2^2 - \hat{q}_2^2}} \hat{Y}_2 \right)$$

respectively, with

$$\rho = \frac{-q_1 q_2 - \hat{q}_1 \hat{q}_2}{\sqrt{1 - q_1^2 - \hat{q}_1^2} \sqrt{1 - q_2^2 - \hat{q}_2^2}}.$$

The form of vectors a_3, a_4, b_3 and b_4 also becomes simpler. And similar to Corollary 2, we have

COROLLARY 4. *If $r = (1, 0, \dots, 0)^T$ and $\hat{r} = (0, 1, 0, \dots, 0)^T$ and if $\hat{Y}_n \xrightarrow{d} \hat{Y}$ with \hat{Y} described in (8), then for the vector \hat{Z}_n described in the Theorem 3, we have*

$$\hat{Z}_n \xrightarrow{d} \hat{Z} = (0, 0, X_3, \dots, X_m)^T$$

where X_3, \dots, X_m are independent and $N(0, 1)$ -distributed.

Remark. Although explicit coordinate representation through vectors a_3, a_4, b_3, b_4 is useful in several ways, another representation may be simpler, especially when more than one parameter is present. Let us start with notation

$$U_{q,r} = I - \frac{2}{\|r - q\|^2} (r - q)(r - q)^T.$$

This is a unitary operator in \mathbb{R}^m , which maps q into r and r into q , while any vector orthogonal to r and q is mapped into itself. Note that $\|r - q\|$ is Hellinger distance between distributions given by probabilities (r_1^2, \dots, r_m^2) and (q_1^2, \dots, q_m^2) and that

$$\|r - q\|^2 = 2(1 - \langle q, r \rangle).$$

We thus see that $U_{q,r}$ is simply a shorter notation for the operator $I_{\mathcal{L}^*} + U$ of Section 2. Now consider an image $\tilde{q} = U_{q,r}\hat{q}$ of \hat{q} . This vector is orthogonal to r . Consider another operator $U_{\tilde{q},\hat{r}}$. Since both \tilde{q} and \hat{r} are orthogonal to r , this operator will leave r unchanged, while mapping \tilde{q} to \hat{r} . The product $U_{\tilde{q},\hat{r}}U_{q,r}$ will be another form of the operator $\hat{I} + \hat{U}$ and (10) can be written as

$$\hat{Z}_n = U_{\tilde{q},\hat{r}}U_{q,r}\hat{Y}_n.$$

This recursive representation can obviously be extended for any $\kappa > 1$.

4. On numerical illustrations. One would hope that numerical verification of the whole approach will be attempted in the future. This will require substantial amount of time and more room than the present paper could allow. We also stress that this paper does not advocate any particular test – its aim is to provide a satisfactory foundation on which various goodness of fit tests can be based. However, in the supplement Khmaladze (2013) we tried the approach on a testing problem of independent interest: goodness of fit testing of the power-law distributions with Zipf’s law and Karlin - Rouault law as alternatives. We show some illustrations of how particular test statistics based on partial sums of Y_{in} and partial sums of Z_{in} perform in this problem.

In this section we restrict ourselves with one numerical illustration of how quickly the asymptotic distribution freeness of vector \hat{Z}_n of (10) start manifesting itself for finite n . For this we considered three different choices of p_1, \dots, p_m of the same $m = 10$. As the first choice we picked these probabilities at random: 9 uniform random variables have been generated once and the resulting uniform spacings were used as these probabilities; as the

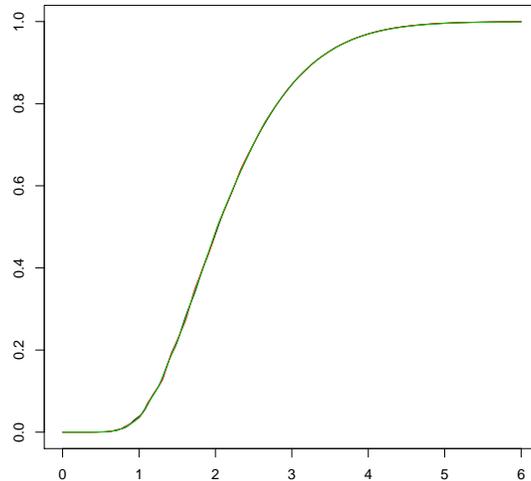


FIG 1. *Distribution functions of the statistic d_{mn}^Z for three different discrete distributions, as described in the text. 10,000 simulations of samples of size $n = 200$ have been used. The dimension of the discrete distributions (number of different events) was $m = 10$.*

second and third choice we used increments $\Delta F(i/10)$, $i = 1, \dots, 10$, of beta distribution function with a bell shaped density, with parameters 3 and 3, and then with J -shaped density, with parameters 0.8 and 1.5.

From each of these distributions we generated 10 000 samples of size $n = 200$, and for each sample calculated a discrete version of Kolmogorov - Smirnov statistic

$$d_{mn}^Z = \max_{1 \leq k \leq m} \left| \sum_{j \leq k} Z_{in} \right|$$

Figure 1 shows three graphs of the resulting empirical distribution functions.

In our choice of n we tried to achieve what is typically required for an application of K. Pearson's chi-square statistics – that all np_i will be at least 10. Otherwise we tried to choose n not large. For $n = 200$ the requirement $np_i \geq 10$ was not strictly satisfied, and in the last two cases we had about three cells with np_i about 5. This could have somewhat spoiled the asymptotic result, but has not. If the three graphs are not very distinct, that is because for all three cases they are very close. Our statistic d_{mn}^Z indeed looks distribution free.

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