

**CORRELATION ESTIMATOR FOR UNBALANCED DATA**

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**KEY WORDS:** Intra -cluster correlation, Categorical data, Estimation, Variance, Testing.

**1. INTRODUCTION**

In this paper, we present the correlations for inter- and intra-levels and for intra-cluster, and show its closed forms of variance derived by Delta method. In Section 2, we define a population and three types of correlation. Section 4 introduces sample estimate of these correlations and its variance. In Section 4, asymptotic distributions are discussed. Finally in Section 5, we present a drug test example.

**2. POPULATION**

The population U of interest is decomposed into A clusters  $U = (U_1, \dots, U_i, \dots, U_A)$ . The cluster  $U_i$  consists of  $B_i$  final units as  $U_i = (U_{i1}, \dots, U_{ij}, \dots, U_{iB_i})$ . Within the final unit,  $U_{ij}$ , the generic measurement level will be denoted by h, with a total of r levels or cells, and the cells are mutually exclusive and exhaustive. Total number of population units is  $N = \sum_{i \in A} B_i$ .

Let the random variable  $y_{hij}$  be the realization of the unit  $U_{ij}$ , continuous or discrete, and define a model for  $y_{hij}$  as

$$y_{hij} = \pi_h + \beta_{hi} + e_{hij}$$

for  $h = 1, \dots, r, i = 1, \dots, A,$  and  $j = 1, \dots, B_i$ .

We assume the random variables  $\beta_{hi}$ 's and  $e_{hij}$ 's are uncorrelated and the existence of the first two moments of  $y_{hij}$ 's. The expectation and variance are expressed as  $E(y_{hij}) = \pi_h$  and  $var(y_{hij}) = \sigma_{bhh}^2 + \sigma_{ehh}^2$ .

**2.1. DEFINITION OF CORRELATION**

We assume that the clusters are independent. But any two units in the same cluster are correlated by the common intra cluster correlation matrix R with  $\rho_{hh}$  on the diagonal for  $h = h'$  and  $\rho_{hh'}$  on the off-diagonal for  $h \neq h'$ :

$$\rho_{hh'} = \frac{\frac{\sigma_{\beta hh}^2}{\sigma_{\beta hh}^2 + \sigma_{ehh}^2} \sigma_{\beta hh'}^2}{\sqrt{(\sigma_{\beta hh}^2 + \sigma_{ehh}^2) \times (\sigma_{\beta h'h'}^2 + \sigma_{eh'h'}^2)}}$$

The correlation over all cells is defined:

$$\rho = \frac{\sum_h \sigma_{\beta hh}^2}{\sum_h (\sigma_{\beta hh}^2 + \sigma_{ehh}^2)}$$

The sum of the trace in nonsingular matrix is the same as the sum of its eigenvalues, that is the sum of diagonal elements. Thus, the sum of diagonal elements is used for the estimation of overall correlation. This definition provides only positive correlation, which arises in most practical situations. Negative correlation sometimes occurs in actual data and we might set  $\rho = 0$  for conservative inferences.

**2.2. CATEGORICAL VARIABLE**

Let the random variable  $y_{hij} = 1$  if the  $U_{ij}$ -th unit falls into the h-th cell, and = 0 otherwise.

$$Let y_h = \sum_{i=1, A} \sum_{j=1, B_i} Y_{hij}$$

be the population counts in the h-th cell, and the cells are mutually exclusive and exhaustive and

$N = \sum_{h=1, r} Y_h$  be the entire units in the population. Denote the vector of population cell frequencies by  $Y^T = (Y_1, \dots, Y_h, \dots, Y_r)$  and the corresponding proportions by vector  $\Pi^T = (\Pi_1, \dots, \Pi_h, \dots, \Pi_r)$ . We impose some restrictions on these proportions:  $\Pi_h = Y_h/N$ ,  $\Pi_h > 0$  for all  $h$ , and  $\sum_h \Pi_h = 1$ .

Define pairwise probability for the members in a same cluster as

$$p(Y_{hi j} = Y_{h' i' j'} = 1) = \delta_{hh'} \text{ if } i=i' \text{ } j \neq j' \text{ } h \neq h',$$

$$p(Y_{hi j} = Y_{h' i' j'} = 1) = \delta_{hh} \text{ if } i=i' \text{ } j \neq j' \text{ } h=h',$$

where  $\delta_{hh'}$  is the probability that one member of pair falls in the cell  $h$  while the other in the cell  $h'$ .  $\delta_{hh}$  is the probability that both members fall into the same cell  $h$ .

Note that the sum over all cells,  $\sum_{hh'} \delta_{hh'} = 1$ . If both members of pair fall in the same cell or they are completely dependent, the off-diagonal elements are zero and the sum of the diagonal elements is one.

For categorical variables, we may define the intra-level and inter-level correlation by

$$\rho_{hh'} = \frac{\frac{\delta_{hh} - \Pi_h^2}{\Pi_h (1 - \Pi_h)}}{\frac{\delta_{hh'} - \Pi_h \Pi_{h'}}{\sqrt{\Pi_h (1 - \Pi_h) \Pi_{h'} (1 - \Pi_{h'})}}}$$

and the overall correlation by

$$\rho = \frac{\sum_{h=1, r} (\delta_{hh} - \Pi_h^2)}{\sum_{h=1, r} \Pi_h (1 - \Pi_h)}.$$

These two definitions involve only the parameters,  $\Pi_h$ 's,  $\delta_{hh}$ , and  $\delta_{hh'}$  while the definitions of continuous variables involve  $\sigma_{chh}^2$  and  $\sigma_{ehh}^2$ .

### 3. SAMPLE

We now assume that a probability sample  $S$  is taken from the population  $U$  described above. The estimations are to be made on the basis of a sample  $S = \{(i, j) : i \in S^*; j \in S_i\}$ , where  $S^*$  is a sample of "a" clusters out of  $A$  clusters, and  $S_i$  is a sample of  $b_i$  units from the  $B_i$  units in the  $i$ th cluster.

We also assume that the sample fractions are ignorable under the model we use. In fact the sampling design is not important under the model assumption. We do not specify the sampling design in both stages except that it is a probability measure on the set of all possible samples.

The sample clusters are indexed by  $i$ ;  $S^* = (S_1, \dots, S_i, \dots, S_a)$ , and the final sample units in the  $i$ -th cluster are indexed by  $j$ ;  $S_i = (u_{i1}, \dots, u_{ij}, \dots, u_{ibi})$ . Note that the indexes  $i$  and  $j$  for the population unit  $U_{ij}$  are not the same as those used for the sample unit  $u_{ij}$ . The cluster sizes are assumed known, but of different size, and the total number of sample units is  $n = \sum_i b_i$ .

The lower case  $y_{hi j}$  is the realization of observation on the sample unit  $u_{ij}$ .

#### 3.1. ESTIMATION

There are three types of correlations to estimate. The first case  $\rho_{hh}$  arises when any two members in a same cluster fall in the same category  $h$ . The second case  $\rho_{hh'}$  arises when one member falls into one cell  $h$  while remaining member into a different cell  $h'$ . The third case  $\rho$  is the correlation for intra-cluster or overall levels.

Landis and Koch (1977) obtained the estimator of  $\rho$  in terms of ANOVA mean squares. We express the correlation  $\rho$  in terms of

$$d_{hi j} = (y_{hi j} - \bar{y}_h)$$

for the level  $h$  to simplify the notation.

There would be four combinations

of  $d_{hij}$  for units and cells as ( $h=h'$  and  $j=j'$ ), ( $h=h'$  and  $j \neq j'$ ), ( $h \neq h'$  and  $j=j'$ ), and ( $h \neq h'$  and  $j \neq j'$ ) for each cluster. These four situations are described below and involved in the variance estimation shown in Section 3.3.

Since the clusters are independent, we find the variance and covariance of each cluster and sum them all for total.

(1) The variance of  $y_{hij}$  for  $h=h'$  and  $j=j'$  in cluster  $i$  is estimated as

$$s_{hhi} = \frac{\sum_j d_{hij}^2}{b_i}$$

The mean  $ms_{hh}$  of  $s_{hhi}$  is the sum of all  $s_{hhi}$ 's divided by "a", and the variance of the variance  $s_{hhi}$  is estimated by

$$\hat{V}ar(s_{hhi}) = \frac{1}{(a-1)} \sum_i (s_{hhi} - ms_{hh})^2$$

(2) Similarly the covariance between  $y_{hij}$  and  $y_{h'ij'}$  for  $h = h'$  and  $j \neq j'$  is estimated by

$$t_{hhi} = \frac{\sum_{j \neq j'} d_{hij} d_{h'ij'}}{b_i (b_i - 1)}$$

The mean  $mt_{hh}$  of  $t_{hhi}$  is the sum of all  $t_{hhi}$ 's divided by "a". The variance of the covariances of  $t_{hhi}$ 's is estimated by

$$\hat{V}ar(t_{hhi}) = \frac{\sum_i (t_{hhi} - mt_{hh})^2}{a-1}$$

(3) The covariance of  $y_{hij}$  and  $y_{h'ij'}$  for  $h \neq h'$  and  $j = j'$  is estimated as

$$s_{hh'i} = \frac{\sum_j d_{hij} d_{h'ij'}}{b_i}$$

The mean  $ms_{hh'}$  is the sum of all  $s_{hh'i}$ 's

divided by "a". The variance of the covariance of  $s_{hh'i}$ 's is estimated by

$$\hat{V}ar(s_{hh'i}) = \frac{\sum_i (s_{hh'i} - ms_{hh'})^2}{a-1}$$

(4) The covariance of  $y_{hij}$  and  $y_{h'ij'}$  or cross product of  $d_{hij}$  and  $d_{h'ij'}$  for  $j \neq j'$  and  $h \neq h'$  is

$$t_{hh'i} = \frac{\sum_{j \neq j'} d_{hij} d_{h'ij'}}{b_i (b_i - 1)}$$

The mean  $mt_{hh'}$  of  $t_{hh'i}$  is the sum of all  $t_{hh'i}$ 's divided by "a". The variance of the covariance is estimated by

$$\hat{V}ar(t_{hh'i}) = \frac{\sum_i (t_{hh'i} - mt_{hh'})^2}{a-1}$$

The covariance between  $s_{hhi}$  and  $t_{hhi}$  is estimated by

$$\hat{C}(s_{hhi} t_{hhi}) = \frac{\sum_i (s_{hhi} - ms_{hh}) (t_{hhi} - mt_{hh})}{a-1}$$

Other covariances can be obtained similarly.

Define design constants for the  $i$ -th first stage unit to be

$$g_i = (n - 1) / [(a - 1)b_i],$$

$$c_i = [g_i b_i - d] / b_i \text{ and}$$

$$d = (n^2 - \sum_{i=1, a} b_i^2) / (n(a-1)).$$

$d$  is the average number of second stage units within each first stage unit and  $n = \sum_{i=1, a} b_i$ .

Express an estimator of correlation of  $\rho_{hh'}$  by

$$\hat{\rho}_{hh'} = \frac{U_{hh'}}{\sqrt{D_{hh'} D_{h'h'}}$$

$$U_{hh'} = (1/a) \sum_{i=1, a} [(g_i - 1)s_{hh'i} + g_i t_{hh'i}],$$

$$D_{hh} = (1/a) \sum_{i=1, a} [(c_i + d - 1)s_{hhi} + c_i t_{hhi}],$$

$$D_{h'h} = (1/a) \sum_i [(c_i + d - 1)s_{h'h'i} + c_i t_{h'h'i}].$$

It is easy to see that  $E(U_{hh}) = \sigma_{chh}^2$  and

$$E(D_{hh}) = (\sigma_{chh}^2 + \sigma_{ehh}^2) \text{ for } h = h'.$$

For the balanced data of  $b_i = b$ , above constants are reduced to  $d = b$ ,  $n = ab$ ,  $g_i = (n-1)/(n-b)$ , and  $c_i = (b-1)/(n-b)$ .

However, the estimator  $\hat{\rho}_{hh}$  is biased due to the dependency of numerator and denominator. But the bias is in the order of  $a^{-1/2}$  because the bias is less than or equal to  $CV(D_{hh}) \times SE(\hat{\rho}_{hh})$ , the coefficient of variation of  $D_{hh}$  is bounded and the standard error of  $\hat{\rho}_{hh}$  is in the order of  $a^{-1/2}$ .

It is not difficult to show directly the bias is in the order  $1/a$ , so the bias becomes small for a large "a".

The estimator of overall correlation coefficient  $\rho$  is given by

$$\hat{\rho} = \frac{\sum_{h=1, r} U_{hh}}{\sum_{h=1, r} D_{hh}}$$

The bias of overall correlation also becomes small for a large "a".

### 3.2 CATEGORICAL VARIABLE

The correlation of categorical variables, defined in Section 2.2, can be estimated as following.

The two parameters  $\pi_h$  and  $\delta_{hh}$  are unbiasedly estimated by

$$\hat{\pi}_h = \frac{\sum_{i=1, a} \sum_{j=1, b_i} Y_{ijh}}{n}$$

$$\hat{\delta}_{hh} = \frac{\sum_{i=1, a} (Y_{i+h}^2 - \sum_{j=1, b_i} Y_{ijh}^2)}{H}$$

where  $H = \sum_{i=1, a} b_i(b_i - 1)$ .

It can be shown that sample estimator of  $\rho_{hh}$  for  $h = h'$  for the categorical variables is

$$\check{\rho}_{hh} = \frac{\hat{\delta}_{hh} - \hat{\pi}_h^2 + \frac{(\hat{\pi}_h - \hat{\delta}_{hh})}{n}}{\hat{\pi}_h(1 - \hat{\pi}_h) - \frac{H(\hat{\pi}_h - \hat{\delta}_{hh})}{n^2}}$$

We can similarly estimate the inter-class estimator for  $h \neq h'$  for categorical variables. The overall correlation is estimated by

$$\check{\rho} = \frac{\sum_h (\hat{\delta}_{hh} - \hat{\pi}_h^2) + \frac{(1 - \sum_h \hat{\delta}_{hh})}{n}}{(1 - \sum_h \hat{\pi}_h^2) - \frac{H(1 - \sum_h \hat{\delta}_{hh})}{n^2}}.$$

The second terms in the numerator and denominator becomes small for a large "n". Although the numerator and denominator are unbiased, the correlation is biased estimator due to the correlation between the numerator and denominator, but the bias is in the order of  $1/n$ , and becomes small for large n.

The asymptotic variance of the correlations for categorical variables are shown in another study (Choi, 1987).

These correlation estimators are consistent since the estimates of a parameter function is consistent as the same function of consistent estimators of the parameters as seen in maximum likelihood estimation.

Although two sets of formulas are developed for different variables, one for continuous and another for categorical variables, both give almost same results when applied to categorical variables, as seen from the previous study (Choi, 1987). The first set may be used when total sum of squares is available, while the second set is easier to use when we have information on  $\pi_h$  and  $\delta_{hh}$ .

### 3.3. VARIANCE ESTIMATION

we attempt to find the variances

of these correlations by Delta method. The variance of  $\hat{\rho}_{hh}$ ,  $\hat{\rho}_{hh'}$ , and  $\hat{\rho}$  is presented below:

### Variance of $\hat{\rho}_{hh}$

Denote the partial derivatives of  $\hat{\rho}_{hh}$  with respect to  $(s_{hhi}, t_{hhi})$ , evaluated at  $(s_{hhi}, t_{hhi}) = (S_{hhi}, T_{hhi})$  by  $d_{shhi} = (1/D_{hh}^2) [(g_i - 1)D_{hh} - (c_i + d - 1)U_{hh}]$  and  $d_{thhi} = (1/D_{hh}^2) [g_i D_{hh} - c_i U_{hh}]$ .

$$\begin{aligned} \text{Var}(\hat{\rho}_{hh}) = & \frac{1}{A} \sum_i [(d_{shhi}^2 \text{Var}(s_{hhi}) \\ & + d_{thhi}^2 \text{Var}(t_{hhi}) \\ & + 2d_{shhi} d_{thhi} \text{Cov}(s_{hhi} t_{hhi})] \end{aligned}$$

### Variance of $\hat{\rho}_{hh'}$

$\hat{\rho}_{hh'}$  involves six variables:

(1)  $t_{hhi}$ , (2)  $t_{h'h'i}$ , (3)  $t_{hh'i}$ , (4)  $s_{hhi}$ , (5)  $s_{h'h'i}$ , and (6)  $s_{hh'i}$ . Let the variance of these six variables expressed by  $V_{11i}$ ,  $V_{22i}$ ,  $V_{33i}$ ,  $V_{44i}$ ,  $V_{55i}$ , and  $V_{66i}$ , where the subscripted number corresponds to the variable numbers (1) to (6), and the covariances between these six variables by  $V_{12i}$ ,  $V_{13i}$ ,  $V_{14i}$ ,  $V_{15i}$ ,  $V_{16i}$ ,  $V_{23i}$ ,  $V_{24i}$ ,  $V_{25i}$ ,  $V_{26i}$ ,  $V_{34i}$ ,  $V_{35i}$ ,  $V_{36i}$ ,  $V_{45i}$ ,  $V_{46i}$ , and  $V_{56i}$ .

Also denote the partial derivative of  $\hat{\rho}_{hh'}$  with respect to each of these six variables by  $d_{1i}$ ,  $d_{2i}$ ,  $d_{3i}$ ,  $d_{4i}$ ,  $d_{5i}$ , and  $d_{6i}$  for  $\partial \rho_{h'h} / \partial t_{hhi} = -c_i U_{hh'} / [2 (D_{h'h'})^{1/2} (D_{hhi})^{3/2}]$   
 $\partial \rho_{h'h} / \partial t_{h'h'i} = -c_i U_{hh'} / [2 (D_{hh})^{1/2} (D_{h'h'i})^{3/2}]$   
 $\partial \rho_{h'h} / \partial t_{hh'i} = g_i / (D_{hh} D_{h'h'})^{1/2}$   
 $\partial \rho_{h'h} / \partial s_{hhi} = -(c_i + d - 1) U_{hh'} / [2 D_{hhi}^{3/2} (D_{h'h'})^{1/2}]$   
 $\partial \rho_{h'h} / \partial s_{h'h'i} = -(c_i + d - 1) U_{hh'} / [2 (D_{h'h'i})^{3/2} D_{hh}^{1/2}]$   
 $\partial \rho_{h'h} / \partial s_{hh'i} = (g_i - 1) / (D_{hh} D_{h'h'})^{1/2}$

$$\begin{aligned} \text{Var}(\hat{\rho}_{hh'}) = & \frac{1}{A} \sum_i [\sum_{k=1}^6 d_{ki}^2 V_{kki} \\ & + \sum_{k \neq k'}^6 d_{ki} d_{k'i} V_{kk'i}] \end{aligned}$$

The  $\text{Var}(\hat{\rho}_{hh'})$  reduces to  $\text{Var}(\hat{\rho}_{hh})$  when we replace the estimates with

subscripts  $hh'$  and  $h'h'$  by those of  $hh$ .

### Variance of $\hat{\rho}$

For  $\text{Var}(\hat{\rho})$ , we need the partial derivatives of overall correlation with respect to  $s_{hhi}$  and  $t_{hhi}$ , evaluated at  $(s_{hhi}, t_{hhi}) = (S_{hhi}, T_{hhi})$ . Denote them by  $d_{rshhi}$ , and  $d_{rthhi}$  for  $\partial \hat{\rho} / \partial s_{hhi} = (1/D^2) [(g_i - 1)D - U(c_i + d - 1)]$ ,  $\partial \hat{\rho} / \partial t_{hhi} = (1/D^2) [g_i D - U c_i]$ .

$$\begin{aligned} \text{Var}(\hat{\rho}) = & \frac{1}{A} \sum_i \left\{ \sum_h [d_{rshhi}^2 \text{Var}(s_{hhi}) \right. \\ & + d_{rthhi}^2 \text{Var}(t_{hhi}) \\ & + 2d_{rshhi} d_{rthhi} \text{Cov}(s_{hhi} t_{hhi})] \\ & + \sum_{h \neq h'} [d_{rshhi} d_{rsh'h'i} \text{Cov}(s_{hhi} s_{h'h'i}) \\ & + d_{rshhi} d_{rth'h'i} \text{Cov}(s_{hhi} t_{h'h'i}) \\ & + d_{rsh'h'i} d_{rthhi} \text{Cov}(s_{h'h'i} t_{hhi}) \\ & \left. + d_{rthhi} d_{rth'h'i} \text{Cov}(t_{hhi} t_{h'h'i}) \right\} \end{aligned}$$

The estimator of above variances also can be obtained by replacing each component with its respective sample estimate based on the "a" sample clusters.

Unless we need a closed form of variance to investigate which parts do major roles in variance, we may use a resampling method. If randomly executed, resampling methods produce similar results as current method does.

We assumed that partial derivatives were possible and that non-linear terms could be negligible for delta method used in this section.

### 4. ASYMPTOTIC DISTRIBUTION

The asymptotic test  $z_{hh}$  shown below is based mainly on the three components:  $E(\hat{\rho}_{hh}) = \rho_{hh} + o_p(a^{-1})$ , variance, and null hypothesis

$$\rho_{hh} = \rho_{0hh} :$$

$$z_{hh} = \frac{\hat{\rho}_{hh} - \rho_{0hh}}{\sqrt{\text{var}(\hat{\rho}_{hh})}} \rightarrow N(0, 1)$$

for a large "a". Note that  $\sqrt{a}(\hat{\rho}_{hh} - \rho_{hh}) \rightarrow N(0, D^TVD)$  as  $a \rightarrow \infty$

where V is  $\text{Var}(\hat{\Psi}_{hh})$ , and D is the derivative matrix of  $\hat{\rho}_{hh}$  with respect to  $\hat{\Psi}_{hh}$ , evaluated at  $\Psi_{hh}^T = (S_{hh}, T_{hh})$ . This is the direct result of the linear expansion of  $\hat{\rho}_{hh} = \rho_{hh} + \frac{\partial \rho_{hh}}{\partial \Psi} (\hat{\Psi} - \Psi) + o(a^{-1})$ .

Similarly, the test statistic for  $H_0: \rho = \rho_0$  is

$$z = \frac{\hat{\rho} - \rho_0}{\sqrt{\text{Var}(\hat{\rho})}} \rightarrow N(0, 1)$$

where  $\text{Var}(\hat{\rho})$  is shown previously.

The asymptotic test statistics for categorical variables can be similarly formulated as those of above.

## 5. DRUG TEST

Miller and Landis (1991) studied a clinical data to see if individual is improved by treatment. 107 persons are treated by drug, and 102 by placebo, and classified them as (1) worse or no change, (2) slight improvement, or (3) more improvement or cured. Nine investigators examined the patients, considered as nine clusters. Patients treated by an investor are considered as the units in cluster.

The Intra-cluster Correlation of Treatment group is 0.223 with standard deviation of 0.178 and  $z = 1.253$ , while that of Placebo Group is 0.109 with standard deviation of 0.130 and  $z = 0.838$ .

Individual correlations are not

significant at  $\alpha = 0.05$  under the null hypothesis of no correlations.

The over-all correlations, 0.223 and 0.109, are useful to estimate the design effect for correlated members in cluster. For example, the design effect for the treatment group is  $[1 + 0.223(12-1)] = 3.453$ , and that of placebo group is  $[1 + 0.109(11.3-1)] = 2.123$ . The number 12 and 11.3 are the average number of cluster members for treatment and placebo groups, respectively.

Although above individual correlations, 0.223 and 0.109, are not significant, the design effects, 3.453 and 2.123, arising from the correlation are quite big, and should not be ignored.

If normal test or t-test statistic were calculated as if data were based on a simple random sample, it should be adjusted by dividing it with the square root of design effect.

For example, the difference between two proportions for two levels, level 1 and level 3, in the treatment group is 44/107 (=24/107 - 68/107). Normal test score is  $z = 0.0624$  under the simple random sample assumption. Being adjusted by the design effect for intra-cluster correlation, corrected score is  $z' = 0.0336 = z/(3.453)^{1/2}$  under the null hypothesis of equal proportion.

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