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Comparison of Three Binomial-related Models in the Estimation of Correlations[1]

Myung-Sang Moon[2]

Abstract

It has been generally recognized that conventional binomial or Poisson model provides poor fits to the actual correlated binary data due to the extra-binomial variation. A number of generalized statistical models have been proposed to account for this additional variation. Among them, beta-binomial, correlated-binomial, and modified-binomial models are binomial-related models which are frequently used in modeling the sum of n correlated binary data. In many situations, it is reasonable to assume that n correlated binary data are exchangeable, which is a special case of correlated binary data. The sum of n exchangeable correlated binary data is modeled relatively well when the above three binomial-related models are applied. But the estimation results of correlation coefficient turn to be quite different. Hence, it is important to identify which model provides better estimates of model parameters(success probability, correlation coefficient). For this purpose, a small-scale simulation study is performed to compare the behavior of above three models.

Keywords : Beta-Binomial Model, Binomial-related Models, Correlated-Binomial Model, Exchangeable, Modified-Binomial Model

1. Introduction

The binary data are elemental to many discrete models including the conventional binomial model. Three assumptions underlie that model. Given a sequence of n Bernoulli trials, they are;

① each Bernoulli trial is classified as 1 under "success", and 0 under "failure",
② the probability of "success" is constant,
③ the Bernoulli trials are independent.

Recently, researchers(Altham 1978, Madsen 1993, Paul 1985 & 1987) have moved to

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1) This Research was supported by the 2002-2004 Yonsei Maeji Research Fund.
2) Associate Professor, Department of Information and Statistics, Yonsei University, Wonju, Kangwon-Do 222-701, Korea,
E-mail : statmoon@dragon.yonsei.ac.kr

generalize the conventional binomial model by exploring the implications of the violation of two conventional assumptions ② and/or ③. The more difficult one to handle is to allow the dependence among n binary data(violation of assumption ③). The binary data obtained from certain toxicological experiment in which the outcome of interest is the occurrence of dead or malformed fetuses in a litter is a typical example. It results in the correlated binary data and in most cases, it additionally introduces the violation of assumption ②. Beta-binomial model(Williams 1975; BBM), correlated-binomial model(Kupper and Haseman 1978; CBM), and modified-binomial model(Ng 1989; MBM) are well-known models obtained with the violation of conventional binomial model assumption ③.

Since the dependence is allowed among n binary data, they are correlated each other. And, in many situations, it is reasonable to assume that correlated n binary data are exchangeable. In other words, the order in which we label the trials does not play any role. Assuming exchangeability, Ng calculates the estimates of success probabilities and correlation coefficients of three distinct real data sets given in Haseman and Soares(1976) by applying the above three models. For all three data sets, it turns out that the estimates of success probabilities are almost the same for three models, but those of correlation coefficients are markedly different. Since the true correlation coefficients of three data sets are not known, there is no way to compare the three models based on their estimates of correlation coefficients. That fact warrants a simulation study to compare these three models based on the estimates of correlation coefficients. In this work, a small-scale simulation study is performed to compare the behavior of three models assuming exchangeability.

This work is composed of four sections. In section 2, three binomial-related models(BBM, CBM, MBM) are briefly introduced, and their (log) likelihood functions or probability mass functions(p.m.f.) used in finding maximum likelihood estimates(MLE) are given as functions of success probabilities and correlation coefficients. Section 3 is devoted to simulation study. Exchangeable n correlated binary data are simulated, and MLE's of three models are found using numerical method. Comparison of three models is made by calculating mean squared error(MSE). Some concluding remarks are provided in the final section.

2. Three binomial-related models

In this section, three binomial-related models and their (log) likelihood functions or p.m.f.'s are introduced. They are used in finding MLE's of success probability ($=p$) and correlation coefficient ($=\rho$) of three models in simulation study. Let $X_i = \sum_{j=1}^{n_i} X_{ij},\ i=1,2,\cdots,N;$ $j=1,2,\cdots,n_i$, where the Bernoulli random variable X_{ij} takes value 1 with success probability p, and 0 with failure probability $q=1-p$.

(1) Beta-binomial model

The BBM can be derived from the assumption that, conditioned on the success probability, X_i follows the conventional binomial model. Under this assumption, correlation coefficient between X_{ij} and X_{ik} given the success probability is 0 for every $j \neq k$. To introduce intraclass correlation between X_{ij} and X_{ik}, it is usually assumed that the success probability varies according to some probability law, and a common choice is beta distribution(Williams 1975) with parameters α and δ. This assumption introduces extra variation to the conventional binomial model, and as a result, X_{ij}'s are unconditionally dependent with positive correlation. Then, the unconditional model of X_i is beta-binomial whose p.m.f. is given by;

$$P(X_i = x_i) = \binom{n_i}{x_i} \frac{B(\alpha + x_i, n_i + \delta - x_i)}{B(\alpha, \delta)}, \quad x_i = 0, 1, 2, \cdots, n_i. \tag{2.1}$$

Under (2.1),

$$E(X_i) = n_i \left(\frac{\alpha}{\alpha + \delta} \right) = n_i p \quad \text{and} \quad Corr(X_{ij}, X_{ik}) = (\alpha + \delta + 1)^{-1} = \rho,$$

where p and ρ represent the success probability and intraclass correlation coefficient between X_{ij} and X_{ik}, $j \neq k$, respectively. It is assumed that the correlation coefficient between X_{ij} and X_{ik} is equal for every pairwise combination of X_{ij}'s. The log-likelihood function(Kupper et. al. 1986, p.87) of the data can be derived from (2.1), and it takes the form

$$\sum_{i=1}^{N} \left\{ \sum_{j=0}^{x_i - 1} \ln \left[p + \frac{j\rho}{(1-\rho)} \right] + \sum_{j=0}^{n_i - x_i - 1} \ln \left[(1-p) + \frac{j\rho}{(1-\rho)} \right] - \sum_{j=0}^{n_i - 1} \ln \left[1 + \frac{j\rho}{(1-\rho)} \right] \right\}, \tag{2.2}$$

where terms not involving the parameters p and ρ have been ignored.

(2) Correlated-binomial model

Under the conventional binomial model assumption, the p.m.f. of X_i is given as;

$$P_{(1)}(x_i) = \binom{n_i}{x_i} p^{x_i} (1-p)^{n_i - x_i}. \tag{2.3}$$

However, when the assumption of conventional binomial model is questionable, Bahadur(1961) has suggested the following most general expression of $P(x_i)$.

$$P(x_i) = P_{(1)}(x_i) \cdot f(x_{i1}, x_{i2}, \cdots, x_{in_i}),$$

where $f(x_{i1}, x_{i2}, \cdots, x_{in_i})$ is the "correction factor" multiplied in order to correct for the lack of mutual independence among the X_{ij}'s. According to his results, "correction factor" is a function of the pairwise correlations among the X_{ij}'s, the 3rd order correlations, etc., up to

n_i-th order correlation. Since $P(x_i)$ is too complex to use, an approximation is necessary. A second-order approximation, $P_{(2)}(x_i)$, which neglect all correlations higher than order two is frequently used since it performs quite adequately. It is defined as follows(Kupper & Haseman 1978, p.72), and is used in the simulation of this work.

$$P_{(2)}(x_i) = \binom{n_i}{x_i} p^{x_i}(1-p)^{n_i - x_i} \cdot \left\{1 + \frac{\rho}{2p(1-p)} \left[(x_i - n_i p)^2 + x_i(2p-1) - n_i p^2\right]\right\}. \quad (2.4)$$

Bahadur has also shown that it is a valid model iff

$$-\frac{2}{n_i(n_i-1)} \cdot \min\left(\frac{p}{1-p}, \frac{1-p}{p}\right) \le \rho \le \frac{2p(1-p)}{(n_i-1)p(1-p) + (1/4) - \gamma_0}, \quad (2.5)$$

where $\gamma_0 = \min_{x_i}\{[x_i - (n_i - 1)p - (1/2)]^2\}$.

(3) Modified-binomial model

The MBM is derived by modifying the conventional binomial model sequentially through $n_i - 1$ steps. It is a mixture of conventional binomial models similar to Altham's additive model, and it becomes more spread out(positive correlation) or more peaked(negative correlation) than the conventional binomial model depending on the parameter values. The detailed modification scheme is given by Ng(1989, p.3480-3481) for $n_i = 4$. The general p.m.f. of MBM is defined as;

$$MB_{n_i}(x_i) = \sum_{j=1}^{n_i} [qB_{n_i - j}(x_i) + pB_{n_i - j}(x_i - j)]\,\theta_{j-1}(1-\theta_j)\cdots(1-\theta_{n_i - 1}),$$
$$x_i = 0, 1, 2, \cdots, n_i, \quad (2.6)$$

where $\theta_0 = 1$ and other θ_j's are subject to the constraints that $MB_{n_i}(x_i) \ge 0$ for all x_i. In the above, $B_{n_i}(x_i)$ denotes the p.m.f. of the conventional binomial model with parameters n_i and p as (2.3). The MBM is a proper model as long as all the θ_j's are between 0 and 1, inclusively. However, in general, the parameter space of θ_j's depends on n_i and p, and is not of a simple form. In the simulation study performed in this work, it is assumed that $\theta_j = \theta$ for all $j = 1, 2, \cdots, n_i$. Even then, no general closed form solution of the parameter space of θ can be found. Only numerical solution is available. As mentioned earlier, the exchangeable X_{ij}'s are assumed in this paper, and in this case, if $X_i = \sum_{j=1}^{n_i} X_{ij}$ follows the MBM, the joint p.m.f. of X_{ij}'s can be completely specified. Using this joint p.m.f., the correlation coefficient between X_{ij} and X_{ik} is found as;

$$\rho = \sum_{j=2}^{n_i} \frac{j(j-1)}{n_i(n_i-1)} \theta_{j-1}(1-\theta_j)\cdots(1-\theta_{n_i-1}). \tag{2.7}$$

In the simulation study of next section, MLE of θ is calculated first using the MBM likelihood function obtained from (2.6), and is inserted in (2.7) to obtain the MLE of ρ afterwards.

3. Simulation Study

The main purpose of this work is a simulation study to compare the behavior of three binomial-related models in the estimation of success probability and correlation coefficient of correlated binary data. Exchangeable correlated binary data are assumed for all models, and the simulation is proceeded as follows:

Step 1; Simulate $N(=500)$ sets of n_i exchangeable correlated binary data X_{ij} ($i=1,2,\cdots,N$; $j=1,2,\cdots,n_i$) with success probability p_i and correlation coefficient ρ_i. It can be done according to the procedure given at Lunn and Davis(1998, p.487-488). Let Y_{ij} and Z_i be independent random variables distributed as Bernoulli(p_i). Define $X_{ij} = (1-U_{ij})Y_{ij} + U_{ij}Z_i$, where U_{ij} is also an independent random variable distributed as Bernoulli($\sqrt{\rho_i}$). Then, it can be easily shown that $Corr(X_{ij}, X_{ik}) = \rho_i, \ \forall j \neq k$. Hence, it is necessary to simulate $2n_i+1$ independent Bernoulli random variables to obtain n_i exchangeable correlated binary data with correlation coefficient ρ_i.

Step 2; Construct the (log) likelihood functions for BBM, CBM, and MBM using the equations (2.2), (2.4), and (2.6), respectively.

Step 3; Find the MLE of parameters(success probability and correlation coefficient) using the simulated data in Step 1 and (log) likelihood functions given in Step 2. Since all the (log) likelihood functions are messy, numerical method should be used to find MLE of each parameter. It is done using FORTRAN program.

Step 4; Calculate the mean, variance, and MSE for each combination of parameter values. Make a comparison and decide which model gives the best estimation results.

In this simulation, the number of exchangeable correlated binary data, the success probability, and the correlation coefficient are set to equal for all $N=500$ sets. That is, $n_i = n$, $p_i = p$, and $\rho_i = \rho$ for $i=1,2,\cdots,N$. The followings are a list of combinations of parameter values used in simulation.

(a) Number of exchangeable correlated binary data($=n$) ; (5, 10, 15, 20),

(b) Success probability($=p$) ; (0.10, 0.30, 0.50),

(c) Correlation coefficient($=\rho$) ; (0.05, 0.10, 0.15, 0.20, 0.25).

For each combination of parameter values, $N=500$ data sets are simulated and MLE's(= $\hat{p}, r$) of p, ρ are calculated. This procedure is replicated 50 times, and 50 MLE's are obtained. From them, MSE of each model parameter is calculated and properties of BBM, CBM and MBM are compared.

Simulation results are given in [Table 1] ~ [Table 3] of Appendix. The ratio of MSE for CBM and/or MBM relative to that for BBM is given in [Table 1] and [Table 2]. Only the results of BBM and MBM are listed in [Table 1], since the correlation coefficient of each parameter value combination in that table is not included in the permissible range (2.5) of CBM. In [Table 2], simulation results for three models are provided. The detailed values of mean, variance and MSE for some combination of parameter values are included in [Table 3] as an example. The smallest MSE for each combination of parameter values is typed with bold-face, so the model with bold-faced MSE is the best one for that combination.

From [Table 1], it is clear that BBM outperforms MBM in the estimation of p and ρ. In almost all cases(except only three cases), MSE's of BBM are much smaller than those of MBM, especially for ρ. As can be seen in [Table 3](although not all the cases are included), the estimation results of p using BBM are pretty much satisfactory for all cases but those of ρ are not, even though much better than MBM. That is, the bias of BBM in the estimation of ρ is relatively large in many cases although it gets better as p approaches 0.5 for each fixed n and ρ. It seems that BBM underestimates ρ, whereas MBM overestimates.

The same conclusions mentioned in the above paragraph can be made in the comparison of BBM and MBM for each combination of parameter values in [Table 2]. Also it can be seen that BBM outperforms CBM in most cases of estimating ρ, except when $p=0.5$. In that case, BBM and CBM show almost the same properties. As is shown in [Table 3], the biases of BBM and CBM in estimating ρ are fairly large when p is small, but they get better as p approaches 0.5. It turns out that BBM and CBM underestimate ρ, whereas MBM overestimates. But the bias of BBM is much smaller than those of CBM and MBM, and as a result, BBM is the best in estimating ρ. The estimation results of p are fairly good and almost the same for three models.

4. Conclusions

Assuming exchangeability, the properties of the three binomial-related models(BBM, CBM, MBM) are compared using simulation study for various combinations of parameter values. The estimation results of success probability are turned out to be fairly good for all models.

For those of correlation coefficient, BBM shows the best result in almost all cases although the results of all models are unsatisfactory. It is also found that the behavior of BBM and CBM in estimating the correlation coefficient improves as the success probability approaches 0.50.

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Appendix : Simulation results

[Table 1]: Simulation results for BBM and MBM; MBM/BBM = MSE(MBM)/MSE(BBM

n	p	ρ		MBM/BBM
10	0.1	.20	$\hat{p}$	1.532
			r	5.699
		.25	$\hat{p}$	1.024
			r	2.667
	0.3	.20	$\hat{p}$	1.375
			r	6.560
		.25	$\hat{p}$	1.345
			r	3.773
	0.5	.20	$\hat{p}$	1.583
			r	7.759
		.25	$\hat{p}$	2.204
			r	5.074
15	0.1	.15	$\hat{p}$	1.320
			r	4.845
		.20	$\hat{p}$	1.034
			r	2.172
		.25	$\hat{p}$	1.295
			r	0.993
	0.3	.15	$\hat{p}$	1.517
			r	8.035
		.20	$\hat{p}$	3.899
			r	7.782
		.25	$\hat{p}$	6.006
			r	3.607
	0.5	.15	$\hat{p}$	2.040
			r	11.243
		.20	$\hat{p}$	3.406
			r	14.677
		.25	$\hat{p}$	4.391
			r	9.242

n	p	ρ		MBM/BBM
20	0.1	.10	$\hat{p}$	1.638
			r	11.757
		.15	$\hat{p}$	1.770
			r	2.679
		.20	$\hat{p}$	2.304
			r	0.818
		.25	$\hat{p}$	3.489
			r	0.340
	0.3	.10	$\hat{p}$	2.114
			r	12.792
		.15	$\hat{p}$	8.660
			r	13.256
		.20	$\hat{p}$	17.161
			r	4.651
		.25	$\hat{p}$	26.591
			r	1.403
	0.5	.10	$\hat{p}$	1.850
			r	26.350
		.15	$\hat{p}$	4.484
			r	31.813
		.20	$\hat{p}$	14.545
			r	23.774
		.25	$\hat{p}$	22.500
			r	10.588

[Table 2]: Simulation results for three binomial-related models;
CBM/BBM = MSE(CBM)/MSE(BBM), MBM/BBM = MSE(MBM)/MSE(BBM)

n	p	ρ		CBM/BBM	MBM/BBM
5	0.1	.05	$\hat{p}$	1.015	1.083
			r	0.886	1.926
		.10	$\hat{p}$	1.120	1.377
			r	1.671	3.637
		.15	$\hat{p}$	1.264	1.363
			r	3.558	3.513
		.20	$\hat{p}$	1.746	1.406
			r	5.724	3.838
		.25	$\hat{p}$	2.828	1.512
			r	7.528	2.967
	0.3	.05	$\hat{p}$	0.973	0.984
			r	0.835	1.481
		.10	$\hat{p}$	1.078	1.018
			r	0.973	1.476
		.15	$\hat{p}$	1.277	1.339
			r	1.396	1.392
		.20	$\hat{p}$	2.226	1.302
			r	2.097	1.542
		.25	$\hat{p}$	3.378	1.744
			r	3.325	1.306
	0.5	.05	$\hat{p}$	1.059	0.967
			r	0.969	1.154
		.10	$\hat{p}$	0.999	0.972
			r	0.928	1.267
		.15	$\hat{p}$	0.912	1.211
			r	0.736	1.279
		.20	$\hat{p}$	0.900	0.987
			r	1.067	1.169
		.25	$\hat{p}$	0.917	1.023
			r	1.572	1.200

n	p	ρ		CBM/BBM	MBM/BBM
10	0.1	.05	$\hat{p}$	1.215	2.312
			r	1.939	10.680
		.10	$\hat{p}$	3.135	3.347
			r	4.675	19.496
		.15	$\hat{p}$	9.918	2.397
			r	4.415	7.355
	0.3	.05	$\hat{p}$	1.182	1.465
			r	0.794	1.819
		.10	$\hat{p}$	2.998	1.631
			r	1.876	4.015
		.15	$\hat{p}$	5.789	1.609
			r	3.734	5.313
	0.5	.05	$\hat{p}$	0.990	0.941
			r	0.846	3.317
15	0.1	.05	$\hat{p}$	1.766	3.761
			r	3.552	30.017
		.10	$\hat{p}$	8.424	2.671
			r	3.758	14.671
	0.3	.05	$\hat{p}$	1.440	1.472
			r	1.501	2.669
		.10	$\hat{p}$	12.559	1.609
			r	3.553	7.625
	0.5	.05	$\hat{p}$	0.986	1.181
			r	0.956	4.116
20	0.1	.05	$\hat{p}$	4.290	4.193
			r	3.804	36.645
	0.3	.05	$\hat{p}$	2.835	1.252
			r	2.539	5.481
	0.5	.05	$\hat{p}$	1.072	0.965
			r	1.642	3.342

[Table 3]: Detailed simulation results for some parameter combinations

n	p	ρ		BBM			CBM			MBM		
				Ave.	Var.	MSE	Ave.	Var.	MSE	Ave.	Var.	MSE
10	0.1	.05	$\hat{p}$	0.0999	1.78	**1.78**	0.1010	2.05	2.16	0.1043	2.26	4.11
			r	0.0427	12.57	**17.93**	0.0330	5.87	34.76	0.0829	83.59	191.50
		.10	$\hat{p}$	0.1016	3.95	**4.21**	0.1081	6.69	13.19	0.1095	5.02	14.08
			r	0.0862	19.24	**38.33**	0.0589	9.97	179.20	0.1819	75.82	747.30
		.15	$\hat{p}$	0.1007	3.59	**3.64**	0.1156	11.71	36.11	0.1065	4.45	8.73
			r	0.1194	25.84	**119.60**	0.0787	19.77	528.00	0.2403	63.90	879.60
	0.3	.05	$\hat{p}$	0.2995	5.54	**5.56**	0.3016	6.32	6.57	0.3036	6.88	8.14
			r	0.0510	9.47	9.58	0.0482	7.28	**7.60**	0.0501	17.43	17.43
		.10	$\hat{p}$	0.3025	8.56	**9.20**	0.3131	10.36	27.57	0.3075	9.44	15.00
			r	0.0979	11.29	**11.74**	0.0877	6.86	22.03	0.1159	21.97	47.14
		.15	$\hat{p}$	0.3010	12.05	**12.14**	0.3240	12.69	70.28	0.3054	16.61	19.53
			r	0.1415	19.12	**26.35**	0.1201	9.00	98.40	0.1822	36.63	140.00
	0.5	.05	$\hat{p}$	0.4984	7.02	7.27	0.4981	6.84	7.20	0.4987	6.67	**6.84**
			r	0.0509	7.81	7.90	0.0494	6.64	**6.68**	0.0381	11.99	26.20
15	0.1	.05	$\hat{p}$	0.1004	1.93	**1.95**	0.1032	2.44	3.44	0.1068	2.75	7.32
			r	0.0410	3.75	**11.78**	0.0300	2.02	41.84	0.1068	31.10	353.60
		.10	$\hat{p}$	0.1019	3.81	**4.17**	0.1155	11.19	35.16	0.1072	5.91	11.15
			r	0.0777	11.71	**61.44**	0.0530	9.61	230.90	0.1918	58.98	901.40
	0.3	.05	$\hat{p}$	0.3008	4.75	**4.82**	0.3044	4.98	6.94	0.3033	5.99	7.09
			r	0.0470	4.58	**5.47**	0.0425	2.51	8.21	0.0483	14.31	14.60
		.10	$\hat{p}$	0.3010	4.93	**5.02**	0.3229	10.81	63.06	0.3023	7.57	8.08
			r	0.0927	7.54	**12.84**	0.0797	4.40	45.62	0.1272	23.99	97.90
	0.5	.05	$\hat{p}$	0.5003	4.70	4.71	0.5007	4.60	**4.64**	0.4996	5.55	5.56
			r	0.0505	4.25	4.27	0.0476	3.53	**4.08**	0.0415	10.32	17.57
20	0.1	.05	$\hat{p}$	0.1018	1.50	**1.83**	0.1071	2.82	7.86	0.1075	2.03	7.68
			r	0.0409	4.31	**12.52**	0.0286	1.87	47.63	0.1149	37.91	458.80
	0.3	.05	$\hat{p}$	0.3000	4.28	**4.28**	0.3079	5.92	12.13	0.3021	4.93	5.36
			r	0.0475	2.37	**3.00**	0.0423	1.75	7.63	0.0570	11.55	16.46
	0.5	.05	$\hat{p}$	0.5011	4.41	4.53	0.5010	4.76	4.85	0.5012	4.23	**4.37**
			r	0.0491	2.96	**3.04**	0.0447	2.23	5.00	0.0473	9.43	10.17

[Note]: Var. and MSE values are obtained by multiplying 10^5 to the original values.