Identifiability and Estimation of Probabilities from Multiple Databases with Incomplete Data and Sampling Selection

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Abstract. For an application problem, there may be multiple databases, and each database may not contain complete variables or attributes, that is, some variables are observed but some others are missing. Further, data of a database may be collected conditionally on some designed variables. In this paper, we discuss problems related to data mining from such multiple databases. We propose an approach for detecting identifiability of a joint distribution from multiple databases. For an identifiable joint distribution, we further present the expectation-maximization (EM) algorithm for calculating the maximum likelihood estimates (MLEs) of the joint distribution.

1 Introduction

With development and popularity of computers, various databases have been built, which contain different variables or attributes, and whose data are collected in different conditions. For example, in medical research, some researchers collect data of these variables, but other researchers may collect data of other variables; On the other hand, some data are from follow-up studies, but other data may be from case-control studies. Distributions of diseases and associations among variables should be evaluated by combining all databases from different researches. There are several statistical approaches for combining multiple databases, such as file-matching for large databases and split questionnaire survey sampling [5, 6]. Multiple databases are depicted as a hypergraph in [1, 4]. In these approaches, a database involving a subset of variables is treated as a sample from a marginal distribution of these variables. In this paper, we consider that a database involving a subset of variables may be a sample drawn conditionally on some other variables, called designed variables.

Identifiability and estimation of a joint distribution of variables are two important problems for data mining from multiple databases. In this paper, we show conditions for identifiability of a joint distribution from marginal and conditional distributions of observed variables, and we propose an approach for detecting identifiability. For an identifiable joint distribution, we present the expectation-maximization (EM) algorithm for calculating the maximum likelihood estimates (MLEs) of the joint distribution [3, 4]. In the partial imputation EM algorithm [4], there must be a database containing all variables and other databases are

drawn from marginal distributions. In this paper, we show that the database containing all variables may be unnecessary for identifying the joint distribution of all variables, and our algorithm for finding MLEs also deals with databases drawn from conditional distributions.

Section 2 gives notation and definitions. In Section 3, we show conditions for identifiability of a joint distribution from multiple databases. In Section 4, we apply the EM algorithm to calculate MLEs of the joint distribution. Section 5 gives a numerical example to illustrate our approach. Finally, Section 6 presents a simulation to evaluate the estimates.

2 Notation and Definitions

Let $V = \{x_1, \dots, x_p\}$ denote the set of all variables included in an interested system, and assume that all variables in V are discrete. Let $p(V = v)$ denote the distribution of variables in V . Suppose that there are K databases, $D_1, \dots, D_K$. For the database D_k , let A_k denote the set of designed variables which is used to stratify the population into subpopulations with different values of A_k , let B_k denote the set of observed variables, and let $V_k = A_k \cup B_k$ represent the set of variables involved in the database D_k . Denote the database D_k as $[B_k|A_k]$, which means that variables in B_k are observed conditionally on variables in A_k . For the database D_k , let $n_k(b_k|a_k)$ denote the frequency of observed individuals with value $B_k = b_k$ in the subpopulation of $A_k = a_k$. Below we first give a general definition of identifiability [2].

Definition 1. Consider a vector Y of random variables having a distribution $F(y; \theta)$ that depends on an unknown parameter vector θ . θ is identifiable by observation of Y if distinct values for θ yield distinct distributions of Y , that is, $\theta_1 \neq \theta_2 \Rightarrow F(y; \theta_1) \neq F(y; \theta_2)$.

Informally, identifiability means that these databases contain sufficient information such that the joint distribution can be uniquely determined. In the case of multiple databases, we say that the joint distribution $P(V)$ is identifiable by databases $[B_1|A_1], \dots, [B_K|A_K]$ if distinct values for $P(V)$ yield distinct values for vector $(P(B_1|A_1), P(B_2|A_1), \dots, P(B_K|A_K))$.

3 Conditions for Identifiability from Multiple Databases

In this section, we show a condition for identifiability of the joint distribution of V from multiple databases $[B_1|A_1], \dots, [B_K|A_K]$. We first show several lemmas which are used to prove the condition for identifiability.

Lemma 1. Suppose that there are only two databases $D_1 = [B|A]$ and $D_2 = [A|B]$ where $A \cup B = V$. Then the joint distribution $P(V)$ of variables in V is identifiable.

Proof. Since $P(B|A)/P(A|B) = P(B)/P(A)$, we have $\sum_B [P(B|A)/P(A|B)] = \sum_B [P(B)/P(A)] = 1/P(A)$. Thus we can find $P(A, B) = P(B|A)P(A) =$

$P(B|A)/[\sum_B P(B|A)/P(A|B)]$. Since $P(A, B)$ is a function of $P(A|B)$ and $P(B|A)$ and since they are identifiable by the databases $[A|B]$ and $[B|A]$ respectively. So we get that $P(A, B)$ is identifiable by the databases $[B|A]$ and $[A|B]$.

Lemma 2. *Suppose that there are only two databases $D_1 = [B_1|A_1]$ and $D_2 = [B_2|A_2]$ and that $A_i \cup B_i = V$ for $i = 1$ and 2 . Define $A = A_1 \cap A_2$ and $B = V \setminus A$. Then the conditional probability $P(B|A)$ is identifiable by the databases, where the conditional probability $P(B|\emptyset)$ is defined as the marginal probability $P(B)$.*

Proof. If $A = \emptyset$, then the result can be obtained immediately from Lemma 1. Below we consider the case of $A \neq \emptyset$. Define $C_1 = A_1 \setminus A$ and $C_2 = A_2 \setminus A$. Then $A_1 = C_1 \cup A$, $A_2 = C_2 \cup A$, $C_1 \cap C_2 = \emptyset$ and $C_i \cap A = \emptyset$ for $i = 1, 2$. We have

$$\frac{P(B_1|A_1)}{P(B_2|A_2)} = \frac{P(A_2)}{P(A_1)} = \frac{P(C_2, A)}{P(C_1, A)}.$$

Thus,

$$\sum_{C_2} \frac{P(B_1|A_1)}{P(B_2|A_2)} = \sum_{C_2} \frac{P(C_2, A)}{P(C_1, A)} = \frac{P(A)}{P(C_1, A)} = \frac{1}{P(C_1|A)}.$$

Further, we have

$$P(B_1|A_1)P(C_1|A) = P(B_1|C_1, A)P(C_1|A) = P(B_1, C_1|A) = P(B|A).$$

We get that $P(B|A)$ is a function of $P(B_1|A_1)$ and $P(A_1|B_1)$ and thus $P(B|A)$ is identifiable by $[B_1|A_1]$ and $[B_2|A_2]$.

Lemma 3. *Suppose that there are K databases, $[B_1|A_1], \dots, [B_K|A_K]$, and $A_k \cup B_k = V$ for all k . The joint distribution $P(V)$ is identifiable if $\bigcap_{i=1}^n A_i = \emptyset$.*

Proof. This result can be obtained immediately by applying Lemma 2 repeatedly to each pair of databases.

Now we propose an algorithm for detecting identifiability of the joint distribution $P(V)$ from K databases, $[B_1|A_1], \dots, [B_K|A_K]$, where $A_k \cup B_k \subseteq V$.

Algorithm: Detect identifiability of $P(V)$ from the K databases.

1. Initialize $t = 0$, $[B_k^{(0)}|A_k^{(0)}] = [B_k|A_k]$ for all k , and $V^{(0)} = V$. Below we repeatedly check whether $P(V^{(t)})$ is identifiable by databases $[B_k^{(t)}|A_k^{(t)}]$ for all k .
2. Find a database $[B_i^{(t)}|A_i^{(t)}]$ such that $B_i^{(t)} \cup A_i^{(t)} = V^{(t)}$. If there is no such a database, then $P(V)$ is not identifiable and stop the algorithm.
3. Let $V^{(t+1)} = A_i^{(t)}$, $[B_k^{(t+1)}|A_k^{(t+1)}] = [B_k^{(t)} \setminus B_i^{(t)}|A_k^{(t)} \setminus B_i^{(t)}]$ for all k , and $t = t + 1$.
4. Repeat Steps 2 and 3 until $V^{(t)} = \emptyset$.

If the algorithm returns an empty set $V^{(t)}$, then the probability $P(V)$ is identifiable. Below we first give an example to illustrate the algorithm, and then we show the correctness of the algorithm.

Example 1. Consider that there are seven variables $V = \{1, 2, 3, 4, 5, 6, 7\}$ and five databases $[456|1237]$, $[147|23]$, $[45|6]$, $[2|1347]$, $[3|45]$. We apply the above algorithm to the databases to detect identifiability of $P(V)$.

For the first iteration, at Step 2, we find $[B_1|A_1] = [456|1237]$ with $A_1 \cup B_1 = V$. At Step 3, we reset the set to be identified as $V^{(1)} = A_1 = [1237]$, remove variables 4, 5 and 6 in B_1 from all databases and obtain databases for the next iteration as $[17|23]$, $[2|137]$ and $[3]$. For the second iteration, at Step 2, we find $A_1^{(1)} \cup B_1^{(1)} = V^{(1)} = [1237]$. At Step 3, set $V^{(2)} = A_1^{(1)} = [23]$, remove variables 1 and 7 in $B_1^{(1)}$ and obtain databases $[2|3]$, $[3]$. For the third iteration, we get $V^{(3)} = [3]$ and database $[3]$. For the fourth iteration, we get $V^{(4)} = \emptyset$ and thus we say that $P(V)$ is identifiable.

Lemma 4. *Suppose that there are two databases $[B_1|A_1]$ and $[B_2|A_2]$. Define $V_i = A_i \cup B_i$ for $i = 1$ and 2 , $V_0 = V_1 \cap V_2$ and $A = A_1 \cap A_2$. Then $P(V_0 \setminus A|A)$ is identifiable by the two databases if $V_1 \setminus V_2 \subseteq B_1$ and $V_2 \setminus V_1 \subseteq B_2$.*

Proof. From $[B_1|A_1]$ we can get $P(B_1|A_1)$, and in turn we can obtain $P(B_1 \setminus (V_1 \setminus V_2)|A_1)$. Similarly we can obtain $P(B_2 \setminus (V_2 \setminus V_1)|A_2)$. From the conditions $V_1 \setminus V_2 \subseteq B_1$ and $V_2 \setminus V_1 \subseteq B_2$, we have $A_1 \subseteq V_2$ and $A_2 \subseteq V_1$ respectively. Thus we get $B_1 \setminus (V_1 \setminus V_2) \cup A_1 = V_1 \cap V_2$ and $B_2 \setminus (V_2 \setminus V_1) \cup A_2 = V_1 \cap V_2$. By Lemma 2, we know that $P(V_0 \setminus A|A)$ can be obtained.

Corollary 1. *Suppose that $V_2 \subseteq V_1$ and A_1 can be partitioned into two sets A and B (that is, $A_1 = A \cup B$ and $A \cap B = \emptyset$) such that $A \subseteq A_2$ and $B \subseteq B_2$. Then $P(B|A)$ is identifiable and thus $P(V_1 \setminus A|A)$ is identified.*

Proof. Since $A_1 = A \cup B$, we get $V_2 = A_2 \cup B_2 \supseteq A \cup B = A_1$. Thus we have $V_1 \setminus V_2 \subseteq B_1$. From supposition we have $V_2 \setminus V_1 = \emptyset \subseteq B_2$. From Lemma 4, we obtain that $P(B|A)$ is identifiable. We have

$$P(B_1|A_1) \times P(B|A) = \frac{P(V_1)}{P(A_1)} \times \frac{P(A_1)}{P(A)} = P(V_1 \setminus A|A).$$

Thus we showed that $P(V_1 \setminus A|A)$ is identifiable.

Example 2. Suppose that $V = \{1, 2, 3, 4, 5, 6, 7\} = V_1$ and $V_2 = \{1, 2, 4, 5, 7\}$ and that we have two databases $[B_1|A_1] = [1236|457]$ and $[B_2|A_2] = [24|157]$. Partition A_1 as $A = \{5, 7\}$ and $B = \{4\}$. Since $A \subseteq A_2$ and $B \subseteq B_2$, we get from Corollary 1 that $P(4|57)$ and $P(1, 2, 3, 4, 6|57)$ are identifiable.

Theorem 1. *The probability $P(V)$ is identifiable by databases $[B_1|A_1]$, $\dots$, $[B_K|A_K]$ if the algorithm returns an empty set $V^{(t)}$.*

Proof. We first show the result following the iterations of the algorithm. At the first iteration, we have immediately that $P(B_i^{(0)}|A_i^{(0)})$ is identifiable by the database $[B_i^{(0)}|A_i^{(0)}]$ where $A_i^{(0)} \cup B_i^{(0)} = V$. At the second iteration, we partition $V^{(1)} = A_i^{(1)} \cup B_i^{(1)}$ into two sets $A_i^{(1)}$ and $B_i^{(1)}$, which must be contained by A_k and B_k of some original database $[B_k|A_k]$ respectively. By Corollary 1, we have that $P(V \setminus A_i^{(1)}|A_i^{(1)})$ is identifiable. Following the iterations, we can obtain that $P(V \setminus A_i^{(t)}|A_i^{(t)})$ is identifiable. If $A_i^{(t)} = \emptyset$ is obtained at the t -th iteration, then $P(V)$ is identifiable.

4 Maximization Likelihood Estimation of Probabilities

For a joint probability $P(V)$ which is identifiable, we propose the EM algorithm for calculating MLEs from databases $[B_1|A_1], \dots, [B_K|A_K]$. Data in each database, say $D_k = [B_k|A_k]$, may be incomplete (i.e. A_k is a pure subset of V), and they may be obtained conditionally on designed variables B_k . For simplicity, we show only a simple case of two variables $V = \{X, Y\}$ and two databases $[X|Y]$ and $[Y|X]$. The algorithm can be easily extended to a general case.

Let $n_1(x|y)$ denote the observed frequency of individuals with $X = x$ conditional on $Y = y$ in the first database for $x = 1, \dots, I$; and let $n_2(y|x)$ denote that with $Y = y$ conditional on $X = x$ in the second database for $y = 1, \dots, J$. Below we present the EM algorithm for calculating MLEs $\{\hat{p}_{xy}\}$ of the joint probabilities $P(X = x, Y = y)$ for all x and y . We treat the frequencies $\{n_1(x|y), \forall x\}$ as the y -th column of an $I \times J$ contingency table $\{n_1^{(y)}(i, j), \forall i, j\}$. Similarly, $\{n_2(y|x), \forall y\}$ as the x -th row of an $I \times J$ contingency table $\{n_2^{(x)}(i, j), \forall i, j\}$. Assume that the total frequency $n_k^{(m)} = \sum_{i,j} n_k^{(m)}(i, j)$ follows a Poisson distribution with parameter $\lambda_k(m)$ and that $\{n_k^{(m)}(i, j), \forall i, j\}$ follows a multinomial distribution with parameters $\{p_{ij}\}$ given a total frequency $n_k^{(m)}$.

At the E-step of the EM algorithm, we find the expected frequencies of $\{n_1^{(y)}(i, j), \forall i, j\}$ and $\{n_2^{(x)}(i, j), \forall i, j\}$. At the M-step, we find the MLEs $\{\hat{p}_{ij}, \forall i, j\}$ and $\{\lambda_k(m), \forall k, m\}$. The EM algorithm for calculating MLEs is given below.

1. E-step:

$$\begin{aligned}\hat{n}_k^{(m)}(i, j) &= E[n_k^{(m)}(i, j) | \{n_1(x|y)\}, \{n_2(y|x)\}, \{\lambda_k^{(t)}(m)\}, \{p_{ij}^{(t)}\}] \\ &= \lambda_k^{(t)}(m) \times p_{ij}^{(t)},\end{aligned}$$

for i, j, k and m .

2. M-step:

$$\begin{aligned}\hat{\lambda}_k^{(t+1)}(m) &= \sum_{i,j} \hat{n}_k^{(m)}(i, j), \\ \hat{p}_{ij}^{(t+1)} &= \frac{1}{N} \sum_{k,m} \hat{n}_k^{(m)}(i, j),\end{aligned}$$

where the total frequency N equals $\sum_{k,m,i,j} \hat{n}_k^{(m)}(i, j)$.

3. Repeat the E-step and M-step until some convergence criterion is achieved.

5 A Numerical Example

In this section, we use an artificial data to illustrate our approach. Suppose that we have a case-control study and a follow-up study on association between smoking and lung cancer, as shown in Tab. 1. In the case-control study with databases $[X|Y]$, we have 709 cases and 709 controls, and then ask their smoking history. In the follow-up study with databases $[Y|X]$, we have a smoker group of 2000 individuals and a non-smoker group of 2000 individuals, and follow their states for years. Combining these databases, we can identify the joint distribution of X and Y and the marginal distributions of X and Y (see Tab. 1), any of which is not identifiable by using only one of $[X|Y]$ and $[Y|X]$. Especially, the MLE of the relative risk, $\hat{P}(Y = 1|X = 1)/\hat{P}(Y = 1|X = 0) = 3.1160$, can be found by combining all data in these databases. It is more efficient than the MLE of the relative risk $(8/2000)/(2/2000) = 4$ obtained by using data only from the follow-up study since there are a few of cancer cases in the follow-up study.

Table 1. A case-control study and a follow-up study on smoking and lung cancer

	Case-control study			Follow-up study		MLEs of probabilities	
	Smoker	Non-smoker	Total	Smoker	Non-smoker	Smoker	Non-smoker
	$X = 1$	$X = 0$		$X = 1$	$X = 0$	$X = 1$	$X = 0$
Cancer ($Y = 1$)	688	21	709	8	2	0.0067	0.0002
Control ($Y = 0$)	650	59	709	1992	1998	0.9082	0.0849
Total				2000	2000		

6 Simulation

Consider two binary variables $V = \{X_1, X_2\}$ with values 0 and 1. Suppose that there are two databases $[X_1|X_2]$ and $[X_2|X_1]$. From the results in Section 3, we know that the joint probabilities of X_1 and X_2 are identifiable from these databases. Below we give a numerical simulation to illustrate estimation of the joint probability $P(x_1, x_2)$. From the true distribution given in Tab. 2,

Table 2. True probabilities and their estimates

	True value	Estimates	
		Mean	Standard error
p_{00}	0.1000	0.0993	0.0230
p_{01}	0.2000	0.2004	0.0372
p_{10}	0.3000	0.3007	0.0499
p_{11}	0.4000	0.3994	0.0507

we generate each of databases $[X_1 = i|X_2 = j]$ and $[X_2 = j|X_1 = i]$ for all i and j from a binomial distribution with sample size 50. Then we apply the EM algorithm to calculate MLEs $\hat{p}_{ij}$ with the initial values $(p_{00}, p_{01}, p_{10}, p_{11}) = (0.25, 0.25, 0.25, 0.25)$ and $\lambda = 100$. The desired convergence accuracy is 10^{-6} . We repeat the simulation 1000 times. The results of means and standard errors are given in Tab. 2. It can be seen that estimates are very close to their true probabilities.

Acknowledgements

We would like to thank the two referees for their valuable comments and suggestions that improved the presentation of this paper. This research was supported by NSFC 10431010, NBRP 2005CB523301 and MSAR.

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