

Three-level supersaturated designs

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Abstract

When experimentation is expensive and the number of factors is large, supersaturated designs can be helpful. They are essentially fractional factorial designs in which the number of factors is greater than the number of experimental runs. Previous studies have focused on two-level supersaturated designs. This paper presents a new class of three-level supersaturated designs with an equal occurrence property. It is shown that designs generated by such a universal construction method result in a low dependency among all columns. © 1999 Elsevier Science B.V. All rights reserved

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1. Introduction

When experimentation is expensive and the number of factors is large, supersaturated designs can be helpful. They are essentially fractional factorial designs in which the number of factors is greater than the number of experimental runs. In practice, the data collected by supersaturated designs are analyzed under the assumption of effect sparsity, i.e., a few dominant factors actually affect the response. Examples of supersaturated design applications can be found in Lin (1993, 1995).

All previous studies have focused on two-level supersaturated designs. Satterthwaite (1959) introduced the supersaturated design as a random balance design. Booth and Cox (1962) obtained seven supersaturated designs via computer search. A general construction method was not available until the appearance of Lin (1993). Recent work in this area includes the following. Lin (1993) described a construction method via half-fractions of Plackett and Burman (1946) designs. Wu (1993) and Iida (1994) described supersaturated designs created by adding the interaction columns in a Plackett and Burman design. Deng et al. (1994) showed some deficiencies of the $E(s^2)$ criterion and proposed a new criterion called resolution-rank. Lin (1995) examined the maximum number of columns that can be accommodated when the degree of the

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maximum dependency between columns is pre-specified. Nguyen (1996) described a method of constructing supersaturated designs from balanced incomplete block designs. Tang and Wu (1997) obtained a construction method for supersaturated designs with consideration of $E(s^2)$ -optimality. Yamada and Lin (1997) obtained supersaturated designs including an orthogonal base with consideration of the maximum dependency. Li and Wu (1997) developed columnwise-pairwise algorithms to construct supersaturated designs. Cheng (1997) provided more insight into the $E(s^2)$ criterion and presented a general form of supersaturated design.

This paper presents a new class of three-level supersaturated designs with the equal occurrence property. Specifically, each factor level occurs an equal number of times. A criterion to measure dependency of three-level supersaturated designs is defined. A construction method is given for generating designs with low dependency (see the definition below). Furthermore, some useful designs are generated and examined.

2. Design criteria for three-level supersaturated designs

Let N be a multiple of three and \mathcal{D}^N be the set of N -dimensional three-level equal occurrence vectors. A three-level supersaturated design, D , can be described as a selection of vectors d_1, \dots, d_K ($K > N$) from the set \mathcal{D}^N by a reasonable rule such that $D = [d_1, d_2, \dots, d_K]$. The equal occurrence property is desirable for most supersaturated design applications and thus will be used here.

In two-level supersaturated designs, the dependency between two equal occurrence vectors is measured by their inner product since the dependency between the two estimates of effects of the assigned factors can be represented by a function of the inner product. The inner product can be used to evaluate the dependency when the factors are both qualitative and quantitative. The dependency of the estimates is essentially invariant to the assignments of actual factor levels to the codes.

The inner product is meaningless for three-level qualitative factors. A direct application of the inner product as a measure of dependency would be acceptable for quantitative factors only. The χ^2 statistic is utilized to measure the dependency between two qualitative variables such as in a two-way contingency table. Thus, χ^2 is an appropriate measure to evaluate the dependency between two columns since it is applicable both to quantitative and qualitative factors.

Let $n^{ab}(d_i, d_j)$ be the number rows whose values are $[a, b]$ in the $N \times 2$ matrix $[d_i, d_j]$, then

$$\sum_{a,b=1,2,3} n^{ab}(d_i, d_j) = N.$$

The χ^2 statistic defined as

$$\chi^2(d_i, d_j) = \sum_{a,b=1,2,3} \frac{(n^{ab}(d_i, d_j) - N/9)^2}{N/9} \quad (1)$$

is used to evaluate the dependency between two columns d_i and d_j . The χ^2 value is equal to $2N$ and 0 when two columns are completely dependent and independent, respectively. It can be used for designs with any number of levels. For two-level designs, however, this is equivalent to the popular $E(s^2)$ criterion given by Booth and Cox (1962). To see this, let c_i and c_j be N -dimensional equal occurrence vectors consisting of -1 's and 1 's. Equal occurrence implies

$$n^{1-1}(c_i, c_j) = N/2 - n^{11}(c_i, c_j),$$

$$n^{-1-1}(c_i, c_j) = N/2 - n^{11}(c_i, c_j),$$

$$n^{-1-1}(c_i, c_j) = n^{11}(c_i, c_j).$$

Thus the squared inner product is

$$\begin{aligned} (c_i^T c_j)^2 &= (n^{-1-1}(c_i, c_j) + n^{11}(c_i, c_j) - n^{-11}(c_i, c_j) - n^{1-1}(c_i, c_j))^2 \\ &= (4n^{11}(c_i, c_j) - N)^2. \end{aligned}$$

On the other hand,

$$\begin{aligned} \chi^2(c_i, c_j) &= \sum_{a,b=-1,1} \frac{(n^{ab}(c_i, c_j) - N/4)^2}{N/4} \\ &= (4n^{11}(c_i, c_j) - N)^2/N = (c_i^T c_j)^2/N. \end{aligned} \tag{2}$$

Eq. (2) implies that χ^2 is essentially the same measure as the squared inner product for two-level vectors.

The average of the squared inner product of all combinations of paired columns is commonly used for evaluating the dependency in two-level supersaturated design, notably the $E(s^2)$ criterion. Likewise, for higher-level designs, we can use the following two criteria to evaluate the dependency of columns.

$$\begin{aligned} \max \chi^2 &= \max\{\chi^2(d_i, d_j) \mid 1 \leq i < j \leq K\}, \\ \text{ave } \chi^2 &= \sum_{1 \leq i < j \leq K} \chi^2(d_i, d_j)/(K(K-1)/2). \end{aligned}$$

3. A construction method for three-level supersaturated designs

Let c and \mathcal{C}^n be an n -dimensional two-level vector consisting of equal numbers of -1 's and 1 's and the set of c , respectively. We will develop a construction method for three-level supersaturated designs from any two-level designs. Let $C = [c_1, \dots, c_k]$ ($c_i \in \mathcal{C}^n$) be any two-level design whose maximum squared inner product over all paired columns is equal to p^2 , i.e., $\max\{(c_i^T c_j)^2 \mid 1 \leq i < j \leq k\} = p^2$.

Consider a matrix with $N = 3n$ rows and $K = 4k$ columns constructed by

$$\begin{aligned} D &= [d_{11}, \dots, d_{1k}, d_{21}, \dots, d_{2k}, \dots, d_{41}, \dots, d_{4k}] \\ &= \begin{bmatrix} \phi^{12}(C) & \phi^{12}(C) & \phi^{13}(C) & \phi^{23}(C) \\ \phi^{23}(C) & \phi^{13}(C) & \phi^{23}(C) & \phi^{12}(C) \\ \phi^{31}(C) & \phi^{23}(C) & \phi^{12}(C) & \phi^{13}(C) \end{bmatrix}, \end{aligned} \tag{3}$$

where $\phi^{ab}(\cdot)$ is an operator which transforms the elements from -1 to a and from 1 to b on the matrix/vector in (\cdot) . Clearly, design D is a three-level supersaturated design for $K > N$.

Theorem 1. For the design D in Eq. (3), we have

$$\max \chi^2 = \max \left\{ \frac{(N + 9p)^2}{8N}, \frac{N}{2} \right\}.$$

Proof. To prove the theorem, it is sufficient to show that

$$\max_{m,i,j} \{\chi^2(d_{mi}, d_{mj})\} = \max_{i,j} \left\{ \frac{(N + 9p_{ij})^2}{8N} \right\} = \frac{(N + 9p)^2}{8N}, \tag{4}$$

$$\max_{m,m^*,i} \{\chi^2(d_{mi}, d_{m^*i})\} = \frac{N}{2}, \tag{5}$$

$$\max_{m,m^*,i} \{\chi^2(d_{mi}, d_{m^*j})\} = \max_{i,j} \left\{ \frac{(N - 3p_{ij})^2 + 36p_{ij}^2}{8N} \right\} = \frac{(N + 3p)^2 + 36p^2}{8N}, \tag{6}$$

where $p_{ij} = c_i^T c_j$, $\max\{(c_i^T c_j)^2 | 1 \leq i < j \leq k\} = p^2$ and $m \neq m^*$ and $i \neq j$. The proofs for Eqs. (4)–(6) are given in the Appendix.

Theorem 1 generates three-level supersaturated designs from two-level supersaturated designs where the maximum dependency of the constructed design is ensured. For example, a three-level supersaturated design with $N = 24$ rows and $K = 140$ columns is generated from the two-level supersaturated design with $n = 8$ runs and $k = 35$ columns shown in Table 1. Some properties of the constructed designs are discussed in the next section.

For the case where the number of factors is smaller than the number of columns in the full design, a sub-design can be used. Define

$$D_1 = \begin{bmatrix} \phi^{12}(C) \\ \phi^{23}(C) \\ \phi^{31}(C) \end{bmatrix}, \quad D_2 = \begin{bmatrix} \phi^{12}(C) \\ \phi^{13}(C) \\ \phi^{23}(C) \end{bmatrix}, \quad D_3 = \begin{bmatrix} \phi^{13}(C) \\ \phi^{23}(C) \\ \phi^{12}(C) \end{bmatrix} \quad \text{and} \quad D_4 = \begin{bmatrix} \phi^{23}(C) \\ \phi^{12}(C) \\ \phi^{13}(C) \end{bmatrix}.$$

For example, from the full design of $(N, K) = (24, 140)$, a sub-design of $[D_1, D_2]$ has $35 \times 2 = 70$ columns. Eq. (4) shows that the frequency of the χ^2 values between two columns on a subdesign D_m is invariant to $m (1 \leq m \leq 4)$. Furthermore, Eqs (5) and (6) imply that the frequency of χ^2 values between a column from D_m and a column from D_{m^*} does not depend on m and m^* ($1 \leq m < m^* \leq 4$). In another words, the maximum and average χ^2 values are invariant to the selection of m and m^* .

Table 1
Two-level design used for constructing a three-level supersaturated design ($n = 8, k = 35$)

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
1	1	1	1	1	1	1	1	1	1	1	1	1	-1	-1	-1	-1	
1	1	-1	-1	1	-1	-1	1	1	-1	-1	-1	-1	-1	-1	1	1	
1	-1	1	-1	-1	1	-1	-1	-1	1	1	-1	-1	1	1	-1	-1	
1	-1	-1	1	-1	-1	1	-1	-1	-1	-1	1	1	1	1	1	1	
-1	1	1	1	-1	-1	-1	1	1	1	1	1	1	1	1	1	1	
-1	1	-1	-1	-1	1	1	-1	-1	1	-1	1	-1	-1	-1	1	-1	
-1	-1	1	-1	1	-1	1	1	-1	-1	-1	-1	1	1	-1	-1	-1	
-1	-1	-1	1	1	1	-1	-1	1	-1	1	-1	-1	-1	1	-1	1	
18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
-1	-1	1	1	1	1	1	1	1	1	1	1	1	1	-1	-1	-1	-1
1	1	1	1	1	1	1	1	1	1	-1	-1	-1	-1	1	1	1	1
1	1	1	1	1	1	-1	-1	-1	-1	1	1	1	1	1	1	1	1
-1	-1	-1	-1	-1	-1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	-1	-1	-1	1	-1	-1	-1	1	-1	-1	-1	1	-1	-1	-1	1
1	-1	-1	-1	1	-1	-1	-1	1	-1	-1	-1	1	-1	-1	-1	1	-1
-1	1	-1	1	-1	-1	-1	1	-1	-1	-1	1	-1	-1	-1	1	-1	-1
-1	-1	1	-1	-1	-1	1	-1	-1	-1	1	-1	-1	-1	1	-1	-1	-1

Table 2
Maximum, average and frequencies of χ^2 on the three-level supersaturated designs
(a) $N = 24$

K	Frequency (χ^2 values)						$\max \chi^2$	ave χ^2	Lower bound	χ^2 -eff.
	0.75	3.00	3.75	9.75	12.00	18.75				
28	0	336	0	0	42	0	12.00	4.00	2.55	0.64
140	408	5040	2136	1224	210	712	18.75	5.27	3.86	0.73

(b) $N = 36$

K	Frequency (χ^2 values)						$\max \chi^2$	ave χ^2	Lower bound	χ^2 -eff.
	0.00	4.00	4.50	10.00	18.00					
44	0	880	0	0	66		18.00	5.44	2.54	0.47
264	2640	9900	10560	7920	3696		18.00	6.71	3.86	0.57

(c) $N = 48$

K	Frequency (χ^2 values)						$\max \chi^2$	ave χ^2	Lower bound	χ^2 -eff.
	1.50	6.00	7.50	19.50	24.00	37.50				
60	0	1680	0	0	90	0	24.00	6.92	2.53	0.36
288	816	30800	4272	2448	426	1424	37.50	8.20	3.76	0.46

4. Examples

This section shows an application of the construction method based on Theorem 1 for $N = 24, 36$ and 48 . Extension of these results for larger N is straightforward. We apply Theorem 1 to both two-level orthogonal designs and two-level supersaturated designs.

4.1. Designs generated from two-level orthogonal designs

Let C be an n -run Plackett and Burman design. Theorem 1 can be used to generate three-level supersaturated designs with $N = 3n$ rows and $K = 4k = 4(n - 1)$ columns from the Hadamard matrix of order n . Table 2 shows the frequency of the χ^2 values from the generated designs. For example, when $N = 24$ and $K = 28$, the χ^2 values of all ${}_K C_2 = 378$ pairs are examined. The values of the design criteria ($\max \chi^2$ and ave χ^2) from the generated designs are also shown in the table. The maximum dependency $\max \chi^2$ is 12 from Theorem 1. In fact, the designs takes two χ^2 values, 3.00 and $N/2 = 12.00$. Furthermore, most pairs result in a χ^2 value of 3.00, meaning a low dependency. A similar result can be found in $(N, K) = (36, 44)$ and $(48, 60)$.

4.2. Designs generated from two-level supersaturated designs

For $N = 24$, Tang and Wu (1997) and Yamada and Lin (1997) obtained two-level supersaturated designs with $n = 8$ rows and $k = 35$ columns such that $p^2 = \max\{(c_i^T c_j)^2 \mid 1 \leq i < j \leq k\} = 4^2$. These two designs are in fact equivalent, as given in Table 1. Theorem 1 generates a three-level supersaturated design with $N = 24$ rows and $K = 140$ columns by substituting the two-level supersaturated design shown in Table 1 as C into Eq. (3). In addition, $\max \chi^2$ is 18.75 by Theorem 1.

A three-level supersaturated design with $N = 36$ rows can be generated from a two-level supersaturated design with $n = 12$ rows. Wu (1993) showed a two-level supersaturated design by adapting a Plackett and

Burman (1946) design. He produced additional columns by the interaction columns in the original design and obtained a two-level supersaturated design with $n = 12$ rows and $k = 66$ columns where $p^2 = 4^2$. A three-level supersaturated design with $N = 36$ rows and $K = 264$ columns can be generated from the two-level supersaturated design where $\max \chi^2 = 18.00$.

For $N = 48$, Tang and Wu (1997) obtained a two-level supersaturated design with 16 rows that minimizes $E(s^2)$. Yamada and Lin (1997) obtained a two-level supersaturated design that minimizes the maximum squared inner product. From Theorem 1, a two-level supersaturated design with small maximum squared inner product is desirable to minimize $\max \chi^2$ on the constructed three-level supersaturated design. Thus the two-level supersaturated design obtained by Yamada and Lin (1997) is preferable here. Specifically, let C_0 be the two-level supersaturated design with $n = 8$ rows and $k = 35$ columns shown in Table 1 such that $p^2 = 4^2$. A two-level supersaturated design C with $n = 16$ rows and $k = 71$ columns is constructed by

$$C = \begin{bmatrix} u & C_0 & C_0 \\ -u & C_0 & -C_0 \end{bmatrix},$$

where u is a vector of length eight consisting of 1's and $p^2 = 8^2$. A three-level supersaturated design with $N=48$ and $K=4k=284$ thus can be generated by substituting the matrix C into Eq. (3), where $\max \chi^2 = 37.50$.

Table 2 also shows the frequency of χ^2 values and the values of $\max \chi^2$ and $\text{ave } \chi^2$ from the three-level supersaturated designs generated from two-level supersaturated designs.

In all generated designs, most χ^2 values occur at a relatively low dependency level. For example, 78% of the χ^2 values are ≤ 3.75 for $(N, K) = (24, 140)$; 67% of the χ^2 values are ≤ 4.5 for $(N, K) = (36, 264)$. In all cases, the average of χ^2 value, $\text{ave } \chi^2$ is relatively small compared to $2N$, the completely dependent case.

4.3. Design evaluation

For supersaturated designs with any number of levels, Yamada and Matsui (1997) derived a lower bound on $\text{ave } \chi^2$. The lower bound includes the lower bound of $E(s^2)$ for two-level supersaturated design as a special case, where the bound of $E(s^2)$ was obtained by Nguyen (1996) and Tang and Wu (1997) independently. For three-level supersaturated designs, the lower bound of $\text{ave } \chi^2$ is given by

$$L_{\chi^2} = \frac{2N(2K - N + 1)}{(N - 1)(K - 1)}. \quad (7)$$

Using this lower bound, χ^2 -efficiency is defined as

$$\frac{L_{\chi^2}}{\text{ave } \chi^2}. \quad (8)$$

A design is χ^2 -optimal when χ^2 -efficiency is equal to 1.00. For example, Eq. (7) gives a lower bound of 3.86 for a three-level design with $N = 24$ rows and $K = 140$ columns. Since $\text{ave } \chi^2 = 5.27$ for the constructed design with $N = 24$ rows and $K = 140$, the χ^2 -efficiency of the design is 0.73. Table 2 also shows the values of χ^2 -efficiency for the constructed designs.

The lower bound and χ^2 -efficiency are also applicable for two-level supersaturated designs. Table 3 shows the χ^2 -efficiency values of the early two-level supersaturated designs by Satterthwaite (1959), and Booth and Cox (1962). The values are around 0.2–0.6, not close to 1. Table 3 also shows the values of χ^2 -efficiency for some designs constructed by Lin (1993) and Wu (1993). While some of those more recent designs are optimum, some are still far from optimum.

For the constructed designs in this paper, the values of χ^2 -efficiency are 0.36–0.73, comparing favorably to the early works listed in Table 3. This fact implies that the constructed three-level designs should be acceptable as initial work on three-level supersaturated designs.

Table 3

The values of χ^2 -efficiency on the early works of two-level supersaturated designs

Author(s)	n	k	χ^2 -efficiency
Satterthwaite (1959)	12	22	0.52
Satterthwaite (1959)	18	30	0.45
Satterthwaite (1959)	24	30	0.24
Booth and Cox (1962)	12	18	0.56
Booth and Cox (1962)	18	30	0.56
Booth and Cox (1962)	24	30	0.50
Lin (1993)	12	22	1.00
Lin (1993)	24	30	0.52
Wu (1993)	12	16	0.73
Wu (1993)	12	66	1.00

5. Concluding remarks

This paper shows a new class of supersaturated designs, those with three-level. The designs can be used for qualitative factors as well as quantitative factors. The χ^2 statistic of a two-way contingency table is used to measure the dependency between design columns. Furthermore, we construct some three-level supersaturated designs using a method which assures minimization of dependency. The three-level supersaturated designs are evaluated in terms of the average χ^2 value and should be acceptable as initial work on this new class of designs.

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Appendix

Proof of Eq. (4). Consider the two vectors,

$$d_{1i} = \begin{bmatrix} \phi^{12}(c_i) \\ \phi^{23}(c_i) \\ \phi^{31}(c_i) \end{bmatrix} \quad \text{and} \quad d_{1j} = \begin{bmatrix} \phi^{12}(c_j) \\ \phi^{23}(c_j) \\ \phi^{31}(c_j) \end{bmatrix}.$$

The first n rows of d_{1i} and d_{1j} are $\phi^{12}(c_i)$ and $\phi^{12}(c_j)$, respectively, and their correspondence is

$$\begin{bmatrix} n^{11}(\phi^{12}(c_i), \phi^{12}(c_j)) & n^{12}(\phi^{12}(c_i), \phi^{12}(c_j)) \\ n^{21}(\phi^{12}(c_i), \phi^{12}(c_j)) & n^{22}(\phi^{12}(c_i), \phi^{12}(c_j)) \end{bmatrix} = \begin{bmatrix} N/12 + p_{ij}/4 & N/12 - p_{ij}/4 \\ N/12 - p_{ij}/4 & N/12 + p_{ij}/4 \end{bmatrix}.$$

Similarly, the correspondence between d_{1i} and d_{1j} is

$$\begin{bmatrix} n^{11}(d_{1i}, d_{1j}) & n^{12}(d_{1i}, d_{1j}) & n^{13}(d_{1i}, d_{1j}) \\ n^{21}(d_{1i}, d_{1j}) & n^{22}(d_{1i}, d_{1j}) & n^{23}(d_{1i}, d_{1j}) \\ n^{31}(d_{1i}, d_{1j}) & n^{32}(d_{1i}, d_{1j}) & n^{33}(d_{1i}, d_{1j}) \end{bmatrix} = \begin{bmatrix} N/6 + 2p_{ij}/4 & N/12 - p_{ij}/4 & N/12 - p_{ij}/4 \\ N/12 - p_{ij}/4 & N/6 + 2p_{ij}/4 & N/12 - p_{ij}/4 \\ N/12 - p_{ij}/4 & N/12 - p_{ij}/4 & N/6 + 2p_{ij}/4 \end{bmatrix}. \quad (\text{A.1})$$

Now, substituting Eq. (A.1) into Eq. (1) gives $\chi^2(d_{1i}, d_{1j}) = (N + 9p_{ij})^2/8N$, as desired. For the general case of $\chi^2(d_{mi}, d_{mj})$, we have $N/12 - p_{ij}$ and $N/6 + 2p_{ij}/4$ appear six and three times respectively in the correspondence matrix. Eq. (4) is proved by substitution into Eq. (1).

Proof of Eq. (5). Consider the two vectors,

$$d_{1i} = \begin{bmatrix} \phi^{12}(c_i) \\ \phi^{23}(c_i) \\ \phi^{31}(c_i) \end{bmatrix} \quad \text{and} \quad d_{2i} = \begin{bmatrix} \phi^{12}(c_i) \\ \phi^{13}(c_i) \\ \phi^{23}(c_i) \end{bmatrix}.$$

The correspondence between d_{1i} and d_{1j} is

$$\begin{aligned} & \begin{bmatrix} n^{11}(d_{1i}, d_{2i}) & n^{12}(d_{1i}, d_{2i}) & n^{13}(d_{1i}, d_{2i}) \\ n^{21}(d_{1i}, d_{2i}) & n^{22}(d_{1i}, d_{2i}) & n^{23}(d_{1i}, d_{2i}) \\ n^{31}(d_{1i}, d_{2i}) & n^{32}(d_{1i}, d_{2i}) & n^{33}(d_{1i}, d_{2i}) \end{bmatrix} \\ &= \begin{bmatrix} n^{11}(\phi^{12}(c_i), \phi^{12}(c_i)) & 0 & n^{13}(\phi^{31}(c_i), \phi^{23}(c_i)) \\ n^{21}(\phi^{23}(c_i), \phi^{13}(c_i)) & n^{22}(\phi^{12}(c_i), \phi^{12}(c_i)) & 0 \\ 0 & n^{32}(\phi^{31}(c_i), \phi^{23}(c_i)) & n^{33}(\phi^{23}(c_i), \phi^{13}(c_i)) \end{bmatrix} \\ &= \begin{bmatrix} N/6 & 0 & N/6 \\ N/6 & N/6 & 0 \\ 0 & N/6 & N/6 \end{bmatrix}. \end{aligned} \quad (\text{A.2})$$

Now, substituting Eq. (A.2) into Eq. (1) gives $\chi^2(d_{1i}, d_{2i}) = N/2$. For the general case of $\chi^2(d_{mi}, d_{m^*i})$, we have $N/6$ and 0 appear six and three times respectively in the correspondence matrix. Eq. (5) is proved by substitution this appearance into Eq. (1).

Proof of Eq. (6). For the two vectors,

$$d_{1i} = \begin{bmatrix} \phi^{12}(c_i) \\ \phi^{23}(c_i) \\ \phi^{31}(c_i) \end{bmatrix} \quad \text{and} \quad d_{2j} = \begin{bmatrix} \phi^{12}(c_j) \\ \phi^{13}(c_j) \\ \phi^{23}(c_j) \end{bmatrix},$$

we have

$$\begin{bmatrix} n^{11}(d_{1i}, d_{2j}) & n^{12}(d_{1i}, d_{2j}) & n^{13}(d_{1i}, d_{2j}) \\ n^{21}(d_{1i}, d_{2j}) & n^{22}(d_{1i}, d_{2j}) & n^{23}(d_{1i}, d_{2j}) \\ n^{31}(d_{1i}, d_{2j}) & n^{32}(d_{1i}, d_{2j}) & n^{33}(d_{1i}, d_{2j}) \end{bmatrix} = \begin{bmatrix} N/12 + p_{ij}/4 & N/6 - 2p_{ij}/4 & N/12 + p_{ij}/4 \\ N/6 & N/12 + p_{ij}/4 & N/12 - p_{ij}/4 \\ N/12 - p_{ij}/4 & N/12 + p_{ij}/4 & N/6 \end{bmatrix}. \quad (\text{A.3})$$

Again, substituting Eq. (A.3) into Eq. (1) gives $\chi^2(d_{1i}, d_{2j}) = ((N - 3p_{ij})^2 + 36p_{ij}^2)/8N$. For the general case of $\chi^2(d_{mi}, d_{m^*j})$, $N/12 + p_{ij}/4$, $N/12 - p_{ij}/4$, $N/6$ and $N/6 - 2p_{ij}/4$ appear four times, twice, twice and once respectively in the correspondence matrix. Eq. (6) is proved by substitution this into Eq. (1). \square

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