

Palindromic Bernoulli distributions

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Abstract: We introduce and study a subclass of joint Bernoulli distributions which has the palindromic property. For such distributions the vector of joint probabilities is unchanged when the order of the elements is reversed. We prove for binary variables that the palindromic property is equivalent to zero constraints on all odd-order interaction parameters, be it in parameterizations which are log-linear, linear or multivariate logistic. In particular, we derive the one-to-one parametric transformations for these three types of model specifications and give simple closed forms of maximum likelihood estimates. Several special cases are discussed and a case study is described.

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1. Introduction

A sequence of characters, such as QR*-TS, becomes a palindromic sequence when the order of the characters is reversed and appended, here to give QR*-TSST-*RQ. The notion is used in somewhat modified forms, among others, in musicology, biology and linguistics. An example of a palindromic sentence which respects the spacings between words is ‘step on no pets’.

Here, we adapt the term to Bernoulli distributions. For a single binary variable, the distribution is palindromic if it is uniform, that is if both levels occur with probability 1/2. For a Bernoulli distribution of d binary variables A_1, \dots, A_d , having a probability mass function $p(a)$ with a in the set of all binary d -vectors, the distribution is palindromic if $p(a) = p(\sim a)$ for all a , where $\sim a$ is the complement of a ; for instance, $\sim a = (0, 1, 0)$ for $a = (1, 0, 1)$.

With $\alpha, \beta, \gamma, \delta$ denoting probabilities, bivariate and trivariate palindromic Bernoulli distributions can be written, as in the following tables:

| | | | | | | | | |
|-------|-----------|----------|-----|-----------|------------------|-------------------|-------------------|------------------|
| A_1 | A_2 : 0 | 1 | sum | A_3 : 0 | 0 | 1 | 1 | sum |
| 0 | α | β | 1/2 | A_1 | A_2 : 0 | 1 | 0 | 1 |
| 1 | β | α | 1/2 | 0 | α | γ | δ | β |
| sum | 1/2 | 1/2 | 1 | 1 | β | δ | γ | α |
| | | | | sum | $\alpha + \beta$ | $\gamma + \delta$ | $\gamma + \delta$ | $\alpha + \beta$ |
| | | | | | | | | 1 |

Continuous distributions may also be palindromic. This concept extends the discussion of the diverse forms of multivariate symmetry by Serfling (2006) since it operationalizes his notion of central symmetry in an attractive way. Let the above binary vector a define for d mean-centred continuous variables their orthant probabilities. Such a distribution is palindromic if the probabilities of the $d(a)$ -orthant and the $d(\sim a)$ -orthant coincide for all a . Examples are for instance mean-centred Gaussian and spherical distributions.

For general discrete variables, the palindromic property differs from *complete symmetry* defined by Bhapkar & Darroch (1990). Complete symmetric tables satisfy the condition $p(a) = p(\sigma(a))$, for any a and for any permutation σ of the indices. Edwards (2000, app. C) median-dichotomized joint Gaussian distributions and proved that the resulting binary probabilities give a non-hierarchical log-linear model in which all odd-order interactions vanish, that is all terms involving an odd number of factors are zero.

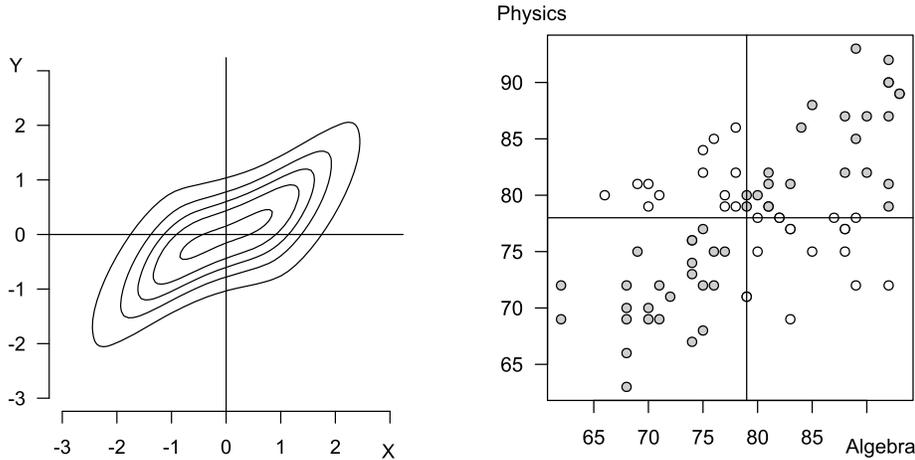


FIG 1. Contour levels of a centrally symmetric bivariate density (left) and a median dichotomized sample (right); these data are from the case study of Section 6.

In this paper, we study properties of palindromic Bernoulli distributions in general. In particular, we prove that the vanishing of all odd-order log-linear interactions is not only a necessary but also a sufficient condition. We show the same characterization for models linear-in-probabilities, Streitberg (1990), and for the multivariate logistic parametrization, Glonek & McCullagh (1995), and explain why palindromic Bernoulli distributions with Markov structure are in the regular exponential family.

2. Characterization in terms of interaction parameters

In this section we introduce three types of parameterization and we show that the palindromic Bernoulli distributions can be characterized by the vanishing of all odd-order interactions, no matter whether these are log-linear, linear or multivariate logistic terms.

2.1. Notation

Let $A = (A_1, \dots, A_d)$ be a random vector with a *multivariate Bernoulli* distribution. Thus, A takes values $a = (a_1, \dots, a_d)$ in the set $\mathcal{I} = \{0, 1\}^d$ with probabilities

$$p(a) = \Pr(A_1 = a_1, \dots, A_p = a_p), \quad \sum_{a \in \mathcal{I}} p(a) = 1.$$

For simplicity, we assume $p(a) > 0$ for all a . The probability distribution of A is determined by the $2^d \times 1$ vector π containing all the probabilities $p(a)$ and belonging to the $(2^d - 1)$ -dimensional simplex. We list vectors a in a lexicographic

order such that the first index in a runs fastest, then the second changes and the last index runs slowest. Cells of a corresponding contingency table are in vector $b \in \mathcal{I}$.

Given a subset $M \subseteq V$ of the variables, the marginal distribution of the variables A_v , for $v \in M$ has itself a joint Bernoulli distribution, in the same lexicographic order:

$$p_M(a_M) = \Pr(A_v = a_v, \text{ for all } v \in M).$$

We use three well-studied parameterizations for joint Bernoulli distributions, that is the log-linear, the linear and the multivariate logistic parameterizations and show how and why they differ even for palindromic Bernoulli distributions.

In general, a parameterization of A is a smooth one-to-one transformation, mapping π into a $2^p \times 1$ vector $\theta = G(\pi)$, say, whose entries θ_b , are called *interaction parameters*. To index interactions, it is useful to have a one-to-one mapping between the cells in b and subsets of $V = \{1, \dots, p\}$. For $p = 3$:

| | Lexicographic order | | | | | | | |
|-----------------|---------------------|------------|------------|---------------|------------|---------------|---------------|----------------|
| cells in b : | 000 | 100 | 010 | 110 | 001 | 101 | 011 | 111 |
| subset of V : | \emptyset | 1 | 2 | 12 | 3 | 13 | 23 | 123 |
| θ_b : | θ_\emptyset | θ_1 | θ_2 | θ_{12} | θ_3 | θ_{13} | θ_{23} | θ_{123} |

The cardinality of the set b , denoted by $|b| = \sum_v b_v$, gives the number of ones in vector b . Depending on $|b|$ being odd or even, an interaction parameter θ_b is said to be of odd or even order. For instance, the even-order θ_{13} is a two-factor interaction of A_1 and A_3 .

2.2. Log-linear parameters

Log-linear parameters are contrasts of log probabilities, that is linear combinations of $\log p(a)$, with weights adding to zero. The vector of the log-linear parameters is

$$\lambda = \mathcal{H}_d^{-1} \log \pi \tag{2.1}$$

where

$$\mathcal{H}_d = \underbrace{\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}}_d.$$

is a $2^d \times 2^d$ symmetric design matrix whose generic entry is $h_{ab} = (-1)^{a \cdot b}$ for $(a, b) \in \mathcal{I} \times \mathcal{I}$. Its inverse, the contrast matrix, is $\mathcal{H}_d^{-1} = 2^{-d} \mathcal{H}_d$. The special form of \mathcal{H}_d , chosen here, uses so-called *effect coding*; see for instance Wermuth & Cox (1992). The individual interactions can be written as

$$\lambda_b = 2^{-d} \sum_{a \in \mathcal{I}_V} (-1)^{a \cdot b} \log p(a), \tag{2.2}$$

where $a \cdot b = a_1 b_1 + \cdots + a_p b_p$ is the inner product of the two binary vectors a and b ; see Haberman (1973, p. 619). In equation (2.2), the symbol b is interpreted for λ_b as a subset of V and in the expression $(-1)^{a \cdot b}$ as binary vector.

The inverse mappings from λ to π may be explicitly computed as

$$\pi = \exp(\mathcal{H}_d \lambda), \quad p(a) = \exp \left[\sum_{b \in \mathcal{I}} (-1)^{a \cdot b} \lambda_b \right]. \tag{2.3}$$

Bernoulli distributions with positive cell probabilities belong to the so-called regular exponential family with the vector λ containing the canonical parameters.

2.3. Linear interactions or moment parameters

In contrast to log-linear models, the linear-in-probability models, discussed for instance by Cox & Wermuth (1992, app. 2), and their interactions are based on moments. The vector $\xi = \mathcal{H}_d \pi$ is a *moment parameter vector* and the mapping between ξ and λ is one-to-one and differentiable; see Barndorff-Nielsen (1978, p. 121).

The moment vector ξ is proportional to the expected value of the sufficient statistics for λ . With y denoting the vector of the frequencies and by the symmetry of \mathcal{H}_d of equation (2.1), this vector of sufficient statistics is $\mathcal{H}_d y$. The elements of ξ , called also *linear interactions*, are

$$\xi_b = \sum_{a \in \mathcal{I}} (-1)^{a \cdot b} p(a) \tag{2.4}$$

and gives as inverse transformations

$$\pi = 2^{-d} \mathcal{H}_d \xi, \quad p(a) = 2^{-d} \sum_{b \in \mathcal{I}} (-1)^{a \cdot b} \xi_b. \tag{2.5}$$

For instance, with $d = 2$ the two-factor linear interaction is $\xi_{11} = p_{00} - p_{01} - p_{10} + p_{11}$.

For the transformed random variables $D_v = (-1)^{A_v}$, which take value 1 if $A_v = 0$ and -1 if $A_v = 1$, the individual interactions are

$$\xi_b = E \left(\prod_{v \in V} D_v^{b_v} \right). \tag{2.6}$$

Because the element $(-1)^{a \cdot b}$ in equation (2.4) may be written with $d_v = (-1)^{a_v}$ as

$$(-1)^{a \cdot b} = (-1)^{a_1 b_1} \times \dots \times (-1)^{a_p b_p} = \prod_{v \in V} (d_v)^{b_v},$$

equation (2.4) gives the expected value of this product with respect to $p(a)$.

Equation (2.6) implies that each moment parameter, ξ_b , is a *marginal parameter*, defined in the marginal distribution of the random vector $(A_v)_{v \in b}$, while the log-linear parameter λ_b is defined in the joint distribution. Therefore there is, in general, no simple relation between the log-linear parameter λ_b^M , say, in the marginal distribution $p_M(a_M)$ and λ_b , the log-linear parameter in the joint distribution, but there are exceptions, see Example 4.2 and Section 5. By contrast, the moment vector ξ_b^M defined in $p_M(a_M)$ coincides with ξ_b .

According to an important result by Barndorff-Nielsen (1978, pp. 121–122) for regular exponential families, for an arbitrary partition of the parameter

vectors λ and ξ in two sub-vectors such that $\lambda = (\lambda_{\mathcal{A}}, \lambda_{\mathcal{B}})$ and $\xi = (\xi_{\mathcal{A}}, \xi_{\mathcal{B}})$, the distribution π is uniquely parameterized by the mixed vector $(\lambda_{\mathcal{A}}, \xi_{\mathcal{B}})$ or by $(\xi_{\mathcal{A}}, \lambda_{\mathcal{B}})$ and there is a diffeomorphism between this *mixed parameterization* and the log-linear parameter λ or the moment parameter ξ .

2.4. Multivariate logistic parameters

The *multivariate logistic parametrization*, introduced by Glonek & McCullagh (1995), is defined by the highest order log-linear parameters, considered here under effect coding, in each possible marginal distribution of A . The parameters are given by the vector $\eta = (\eta_b)_{b \subseteq V}$ where

$$\eta_b = \lambda_b^b, \quad b \subseteq V. \quad (2.7)$$

Kauermann (1997) showed that the mapping $T : \lambda \mapsto \eta$ from the log-linear to the multivariate logistic parameters is a diffeomorphism by proving that T is a composition of smooth transformations between the canonical, the moment and the mixed parameters. More details are given below in Subsection 2.5.

Let $\Lambda = \mathbb{R}^{2^p - 1}$ be the parameter space for the log-linear parameters λ . Then the parameter space $E = T(\Lambda)$ for η is the image of λ under the transformation T . Explicit forms for the inverse function $T^{-1} : E \rightarrow \Lambda$ are known for $p = 1$ or $p = 2$ and in special cases, such as in Example 4.2. An algorithm provided by Qaqish & Ivanova (2006) detects simultaneously whether the vector η is compatible with a proper probability vector π .

2.5. Properties of the palindromic Bernoulli distributions

We now study several properties of palindromic Bernoulli distributions and start by proving that these distributions are closed under marginalization.

Proposition 2.1. *If $p(a)$ is a palindromic Bernoulli distribution then, for any subset M of the variables, the marginal distribution $p_M(a_M)$ is palindromic.*

Proof. Partition $a = (a_N, a_M)$ and let $p_M(a_M) = \sum_{a_N \in \{0,1\}^{|N|}} p(a_N, a_M)$. Then if the distribution is palindromic, $p(a_N, a_M) = p(\sim a_N, \sim a_M)$ and

$$p_M(a_M) = \sum_{\sim a_N \in \{0,1\}^{|N|}} p(\sim a_N, \sim a_M) = p_M(\sim a_M). \square$$

Next, we characterise the distribution by zero constraints on interactions.

Proposition 2.2. *A Bernoulli distribution is palindromic if and only if, with $\theta_b = \xi_b$ or $\theta_b = \lambda_b$, all odd-order linear or log-linear interactions vanish, that is if and only if*

$$\theta_b = 0, \quad \text{for all } b \subseteq V \text{ with } |b| \text{ odd.}$$

Proof. 1) (If A is palindromic then all odd-order $\xi_b = 0$.) Any linear interaction can be written as

$$\xi_b = \sum_{a \in \mathcal{I}_1} (-1)^{a \cdot b} p(a) + \sum_{a \in \mathcal{I}_1} (-1)^{(\sim a) \cdot b} p(\sim a), \quad (2.8)$$

where \mathcal{I}_1 denotes the subset of cells having a one as first element. Thus \mathcal{I}_1 contains half of the cells. If the distribution is palindromic, $p(\sim a) = p(a)$ and $(-1)^{(\sim a) \cdot b} = (-1)^{|b|}(-1)^{a \cdot b}$. Thus,

$$\xi_b = \sum_{a \in \mathcal{I}_1} (-1)^{a \cdot b} p(a) + (-1)^{|b|} \sum_{a \in \mathcal{I}_1} (-1)^{a \cdot b} p(a). \tag{2.9}$$

When $|b|$ is odd then $(-1)^{|b|} = -1$ and $\xi_b = 0$; see also Edwards (2000, App. C).

2) (If all odd-order $\xi_b = 0$, then $p(\sim a) = p(a)$.) If all odd-order interactions vanish, then

$$p(a) = \frac{1}{2^d} \sum_{b \in \mathcal{I}_{\text{even}}} (-1)^{a \cdot b} \xi_b, \tag{2.10}$$

where $\mathcal{I}_{\text{even}}$ is the subset of the cells b such that $|b|$ is even. Thus,

$$p(\sim a) = \frac{1}{2^p} \sum_{b \in \mathcal{I}_{\text{even}}} (-1)^{(\sim a) \cdot b} \xi_b = \frac{1}{2^p} \sum_{b \in \mathcal{I}_{\text{even}}} (-1)^{|b|} (-1)^{a \cdot b} \xi_b = p(a), \tag{2.11}$$

because $|b|$ is even. So the distribution is palindromic.

3) The same arguments apply for the log-linear parameterization. The distribution is palindromic if and only if $\log p(a) = \log p(\sim a)$ for all a . Therefore, using equation (2.2), and the previous lines of reasoning, $\lambda_b = 0$ whenever $|b|$ is odd. Conversely, if all odd-order log-linear parameters λ_b vanish, then from

$$\log p(a) = \sum_{b \in \mathcal{I}} (-1)^{a \cdot b} \lambda_b$$

we get $\log p(a) = \log p(\sim a)$ and the distribution is palindromic. □

By equation (2.6) and Proposition 2.2, the joint distribution of A is palindromic if and only if all the odd-order moments of $D = (-1)^A$ are zero. Also, as the palindromic property is characterized by linear constraints on the canonical parameters λ , we have the following result.

Corollary 2.3. *Palindromic Bernoulli distributions are a regular exponential family.*

We show next a similar characterization for the multivariate logistic parameterization.

Proposition 2.4. *A Bernoulli distribution is palindromic if and only if all odd-order multivariate logistic parameters vanish, that is if and only if*

$$\eta_b = 0, \quad \text{for all } b \subseteq V \text{ with } |b| \text{ odd.}$$

The analogous result for the larger class of complete hierarchical marginal log-linear parameterizations, Bergsma & Rudas (2002), will be discussed elsewhere.

The proof uses a transformation $T: \lambda \mapsto \eta$ introduced by Kauermann (1997, p. 265). The composition of smooth one-to-one transformations T_M gives T , for each nonempty subset $M \subseteq V$. The functions T_M operate on parameter

TABLE 1
 The sequence of transformations required to obtain the multivariate logistic parameter η from the log-linear parameter λ .

| Transformation | Parameters | | | | | | | Intermediate result |
|------------------------|------------|----------|-------------|----------|-------------|-------------|--------------|---------------------|
| $T_{123}(\lambda)$ | ξ_1 | ξ_2 | ξ_{12} | ξ_3 | ξ_{13} | ξ_{23} | η_{123} | $\theta^{(1)}$ |
| $T_{23}(\theta^{(1)})$ | ξ_1 | ξ_2 | ξ_{12} | ξ_3 | ξ_{13} | η_{23} | η_{123} | $\theta^{(2)}$ |
| $T_{13}(\theta^{(2)})$ | ξ_1 | ξ_2 | ξ_{12} | ξ_3 | η_{13} | η_{23} | η_{123} | $\theta^{(3)}$ |
| $T_{12}(\theta^{(3)})$ | ξ_1 | ξ_2 | η_{12} | ξ_3 | η_{13} | η_{23} | η_{123} | $\theta^{(4)}$ |
| $T_3(\theta^{(4)})$ | ξ_1 | ξ_2 | η_{12} | η_3 | η_{13} | η_{23} | η_{123} | $\theta^{(5)}$ |
| $T_2(\theta^{(5)})$ | ξ_1 | η_2 | η_{12} | η_3 | η_{13} | η_{23} | η_{123} | $\theta^{(6)}$ |
| $T_1(\theta^{(6)})$ | η_1 | η_2 | η_{12} | η_3 | η_{13} | η_{23} | η_{123} | η |

transformations between the canonical and the moment parametrizations, as follows. If $M = V$,

$$T_M(\lambda_{\mathcal{P}(V)\setminus V}, \lambda_V) = (\xi_{\mathcal{P}(V)\setminus V}, \lambda_V).$$

If $M \subset V, |M| \neq 1$:

$$T_M(\dots, \xi_{\mathcal{P}(V)\setminus V}, \xi_M, \dots) = (\dots, \xi_{\mathcal{P}(M)\setminus M}, \eta_M, \dots)$$

and the remaining parameters, which are not listed, are left unchanged. Finally, if $|M| = 1$,

$$T_M(\xi_M, \dots) = (\eta_M, \dots).$$

For instance, to clarify, to get $\eta = T(\lambda)$ for three variables we define

$$T(\lambda) = T_1 \circ T_2 \circ T_3 \circ T_{12} \circ T_{13} \circ T_{23} \circ T_{123}(\lambda)$$

and Table 1 gives the details of the required transformations T_M .

Proof. Let $\text{odd} = \{b \in \{0, 1\}^{|V|} : |b| \text{ odd}\}$ be the subset of all odd-order interactions. Then, below we show that $\eta_{\text{odd}} = 0$ if and only if $\lambda_{\text{odd}} = 0$.

From Proposition 2.2 we know that a binary distribution is palindromic if and only if $\lambda_{\text{odd}} = 0$. If π is palindromic then all the marginal distributions $p_b(a_b), b \subseteq V$ are palindromic and thus in each of them, such that $|b|$ is odd, $\lambda_b^b = \eta_b = 0$. Thus, $\eta_{\text{odd}} = 0$. Let $\text{even} = \mathcal{P}(V) \setminus \text{odd}$. Then

$$T(\lambda_{\text{even}}, \lambda_{\text{odd}} = 0) = (\eta_{\text{even}}, \eta_{\text{odd}} = 0). \tag{2.12}$$

Conversely, if $\eta_{\text{odd}} = 0$, let η_{even} be arbitrarily chosen such as $(\eta_{\text{even}}, \eta_{\text{odd}}) = 0 \in E_0 \subset E$ (the parameter space of the η s). As E_0 is connected we can directly use equation (2.12) and the smoothness of the inverse transformation T^{-1} to get

$$T^{-1}(\eta_{\text{even}}, \eta_{\text{odd}} = 0) = (\lambda_{\text{even}}, \lambda_{\text{odd}} = 0),$$

and thus the distribution π is palindromic. □

TABLE 2
Illustration of the the different parameters with a 2³ table; constant terms omitted.

| | | | | | | | | |
|------------------|-------------|-----|-----|-------------|-----|---------------|-------------|-----|
| cells b : | 000 | 100 | 010 | 110 | 001 | 101 | 011 | 111 |
| 80 π : | 15 | 9 | 1 | 15 | 15 | 1 | 9 | 15 |
| subsets of V : | \emptyset | 1 | 2 | 12 | 3 | 13 | 23 | 123 |
| ξ : | – | 0 | 0 | 1/2 | 0 | –1/5 | 1/5 | 0 |
| λ : | – | 0 | 0 | $\log(5)/2$ | 0 | –1/5 | 1/5 | 0 |
| η : | – | 0 | 0 | $\log(3)/2$ | 0 | – $\log(3)/2$ | $\log(3)/2$ | 0 |

Table 2 illustrates the different parameters with a 2³ table.

Next, we state a result connected with binary probability distributions *generated by a linear triangular system*, as studied in Wermuth, Marchetti & Cox (2009). Their joint probabilities may be defined by the recursive factorization

$$\Pr(A_1 = a_1, \dots, A_d = a_d) = \Pr(A_1 = a_1) \times \prod_{s=2}^d \Pr(A_s = a_s \mid A_1 = a_1, \dots, A_{s-1} = a_{s-1})$$

with uniform margins. With β_{sj} denoting linear regression coefficients,

$$\Pr(A_s = a_s \mid A_1 = a_1, \dots, A_{s-1} = a_{s-1}) = \frac{1}{2} (1 + \sum_{j=1}^{s-1} \beta_{sj} (-1)^{a_s + a_j}). \tag{2.13}$$

The conditional expected values of A_s given variables $A_{[s-1]} = (A_1, \dots, A_{s-1})$ are linear regressions with only main effects and no constant term. For these distributions, all the even-order linear interactions are known functions of the marginal correlations; see Wermuth, Marchetti & Cox (2009, eq. (2.4)). Here, we prove in Appendix A the following result and get back to such systems later.

Proposition 2.5. *If a binary probability distribution is generated with a linear triangular system, then it is palindromic.*

3. Independences and dependences

Palindromic Bernoulli distributions share some but not all of the properties of joint Gaussian distributions. We elaborate here on properties of independences, of undirected dependences, also called associations, and of directed dependences, also called effects. Conditional independence of variables A, B given variable O , say, is written as $A \perp\!\!\!\perp B \mid O$, while the complement of it, called conditional dependence of A, B given O , is written as $A \pitchfork B \mid O$; see Wermuth & Sadeghi (2012).

Starting with properties of general Bernoulli distributions, several measures of dependence are equivalent with respect to independences and the sign of a dependence; see Xie, Ma & Geng (2008, thm. 1). The same happens for Gaussian distributions. In addition, for bivariate palindromic Bernoulli distributions, many measures of dependence are even in one-to-one correspondence; see e.g. Wermuth & Marchetti (2014). For the three variable table in Section 1, conditional measures of main interest for (A_1, A_2) at level 0 of A_3 are

$$\begin{aligned}
 & (\alpha\delta)/(\beta\gamma), \text{ the odds-ratio,} \\
 & \{\delta/(\gamma + \delta)\} - \{\beta/(\alpha + \beta)\}, \text{ the chance difference for success,} \\
 & \{\delta/(\gamma + \delta)\}/\{\beta/(\alpha + \beta)\}, \text{ the relative chance for success and} \\
 & \rho_{12|k=0} = (\alpha\delta - \beta\gamma)\{(\alpha + \beta)(\gamma + \delta)(\alpha + \gamma)(\beta + \delta)\}^{-\frac{1}{2}}, \text{ the conditional} \\
 & \text{correlation.}
 \end{aligned}$$

Thus, the chance difference for success and the conditional correlation $\rho_{12|k=0}$ are multiples of the cross-product difference, $\alpha\delta - \beta\gamma$, and coincide if and only if the probabilities for success are identical for A_1 and A_2 . Moreover, the odds-ratio is equal to the relative chance if and only if $A_1 \perp\!\!\!\perp A_2 | A_3$, that is if and only if $\alpha\delta = \beta\gamma$. A dependence is positive if $\rho_{12|k=0}$ (or the chance difference) is positive or the odds-ratio (or the relative chance) is > 1 .

It can be verified that $\rho_{12|k=0} = \rho_{12|k=1}$, and given the linear form of the conditional expectation $E(A_1, A_2 | A_3 = k) = \rho_{12|k}$, it follows from Baba Shibata & Sibuya (2004, thm. 1) that the constant conditional correlation $\rho_{12|k}$ equals the partial correlation

$$\rho_{12.3} = (\rho_{12} - \rho_{13}\rho_{23})/c \quad \text{where } c = \{(1 - r_{13}^2)(1 - r_{23}^2)\}^{1/2}.$$

Special one-to-one relations among the mentioned different measure of dependence are given in the following Proposition, proved in Appendix A.

Proposition 3.1. *In a trivariate palindromic distribution:*

- (i) $A_1 \perp\!\!\!\perp A_2 | A_3 \iff \lambda_{12} = 0 \iff \rho_{12|3} = 0 \iff \rho_{12.3} = 0,$
- (ii) $A_1 \pitchfork A_2 | A_2 > 0 \iff \lambda_{12} > 0 \iff \rho_{12|3} > 0 \iff \rho_{12.3} > 0,$
- (iii) $A_1 \pitchfork A_2 | A_3 < 0 \iff \lambda_{12} < 0 \iff \rho_{12|3} < 0 \iff \rho_{12.3} < 0.$

However, even if the chance difference is identical at all level combinations of the remaining variables, the relative chance for success may vary widely. This shows for the palindromic distribution in Example 3.1, where the relative chance at level combination (0, 0) of A_3, A_4 is more than 10 times higher than at (1, 1). This may become more extreme with equality just in sign.

Example 3.1 $\left[\begin{array}{cccccccc} \text{lev. of } A_1, A_2, A_3, A_4 : & 0000 & 1000 & 0100 & 1100 & 0010 & 1010 & 0110 & 1110 \\ & 9200 & \pi : 4095 & 91 & 91 & 47 & 91 & 47 & 47 & 91 \end{array} \right]$

The explanation is the presence of a four-factor log-linear interaction in the 2^4 table.

3.1. Induced dependences and effect reversal

Next, we give three examples of binary palindromic tables, which illustrate what have been called the weak and the strong versions of the Yule-Simpson paradox. In Examples 3.2 and 3.3, an independence gets destroyed by changing the conditioning sets and in Example 3.4 the sign of a dependence gets reversed after marginalizing. The three examples illustrate in addition, that in all palindromic Bernoulli distribution not only conditional parameters are relevant but also the marginal parameters and, in particular, also simple correlations, due to the

one-to-one relation between an odds-ratio and the correlation in their bivariate distributions. In the following examples the symbol λ' indicates the log-linear interactions in effect-coding obtained from the counts. They are identical to previous λ parameters except for the constant term, where $\lambda_\emptyset = \lambda'_\emptyset - \log n$.

Example 3.2 $\left[\begin{array}{l} \text{levels } ijk \text{ of } A, B, O : 000 \ 100 \ 010 \ 110 \ 001 \ 101 \ 011 \ 111 \\ A \perp\!\!\!\perp B|O \\ \& A \not\perp\!\!\!\perp B \end{array} \right. \left[\begin{array}{ccccccc} 100 \ \pi : & 32 & 8 & 8 & 2 & 2 & 8 & 8 & 32 \\ \text{log-lin. interaction } \lambda' : & 2.08 & 0 & 0 & 0 & 0 & 0.69 & 0.69 & 0 \end{array} \right]$

Example 3.3 $\left[\begin{array}{l} \text{levels } ijk \text{ of } A, B, O : 000 \ 100 \ 010 \ 110 \ 001 \ 101 \ 011 \ 111 \\ A \not\perp\!\!\!\perp B|O \\ \& A \perp\!\!\!\perp B \end{array} \right. \left[\begin{array}{ccccccc} 400 \ \pi : & 90 & 60 & 40 & 10 & 10 & 40 & 60 & 90 \\ \text{log-lin. interaction } \lambda' : & 3.65 & 0 & 0 & -0.25 & 0 & 0.45 & 0.65 & 0 \end{array} \right]$

Example 3.4 $\left[\begin{array}{l} \text{levels } ijk \text{ of } A, B, O : 000 \ 100 \ 010 \ 110 \ 001 \ 101 \ 011 \ 111 \\ A \not\perp\!\!\!\perp B|O \text{ pos.} \\ \& A \not\perp\!\!\!\perp B \text{ neg.} \end{array} \right. \left[\begin{array}{ccccccc} 400 \ \pi : & 100 & 50 & 40 & 10 & 10 & 40 & 50 & 100 \\ \text{log-lin. interaction } \lambda' : & 3.63 & 0 & 0 & -0.17 & 0 & 0.52 & 0.63 & 0 \end{array} \right]$

To understand the examples the following matrices with marginal and partial correlations are given for the three examples. The variables are (A, B, O) in this order. The matrices show correlations, ρ_{st} , for $(s, t) = (1, 2), (1, 3), (2, 3)$ in the lower triangle and partial correlations, $\rho_{st.v} = -\rho^{st} / \sqrt{\rho^{ss}\rho^{tt}}$, in the upper triangle; v denotes the remaining variable and ρ^{st} is a concentration, that is an element in the inverse covariance matrix.

| | | | | | | | | |
|------|------|------|------|-------|------|------|-------|------|
| 1 | 0 | 0.51 | 1 | -0.18 | 0.35 | 1 | -0.13 | 0.41 |
| 0.36 | 1 | 0.51 | 0 | 1 | 0.52 | 0.10 | 1 | 0.50 |
| 0.60 | 0.60 | 1 | 0.30 | 0.50 | 1 | 0.40 | 0.50 | 1 |

Note that in Example 3.1, we have $\rho_{12} = \rho_{13}\rho_{23}$ and in Example 3.2, $\rho_{12.3} = -\rho_{13.2}\rho_{23.1}$.

Though these situations may be surprising when one sees them for the first time, they have simple explanations. The strong version of the Simpson’s paradox in Example 3.4 results for pair (A, B) , say, when there are substantial dependences $A \not\perp\!\!\!\perp B|O$ and $A \not\perp\!\!\!\perp O|B$, and a strong dependence $B \not\perp\!\!\!\perp O$; see (Wermuth, 1987, sec. 6).

The weak versions are due to a dependence-inducing property. This property is shared by joint Gaussian distributions; see e.g. Wermuth & Cox (1998, lem. 2.1) and is known as *singleton transitivity* when it is used for graphs representing a large class of graphical Markov models; see Wermuth (2015, eqs. (10), (11)). The property has been studied for binary variables by Simpson (1951, sec. 11) and Birch (1963, discussion of eq. (5.1)), in the form

$$(A \perp\!\!\!\perp B \mid O \text{ and } A \perp\!\!\!\perp B) \text{ implies } (A \perp\!\!\!\perp O \text{ or } B \perp\!\!\!\perp O). \tag{3.1}$$

Equivalently, equation (3.1) is formulated as dependence-inducing with

$$(A \not\perp\!\!\!\perp O \text{ and } B \not\perp\!\!\!\perp O) \text{ implies } (A \perp\!\!\!\perp B|O \text{ or } A \perp\!\!\!\perp B) \text{ but not both,}$$

and it applies to triples of variables also when a common conditioning set is added to each statement. For variables A, B, O this shows as in Fig. 2 in graphs which are Vs:



FIG 2. Pairs of Vs for binary A, B, O with non-vanishing dependencies associated to each edge present; left: $A \perp\!\!\!\perp B|O$ and $A \pitchfork B$ is represented by a source \mathbb{V} and by its Markov-equivalent, concentration-graph \mathbb{V} ; right: $A \perp\!\!\!\perp B$ and $A \pitchfork B|O$ is represented by a sink \mathbb{V} and by its Markov-equivalent, covariance-graph \mathbb{V} .

In our examples for (A, B, O) , the log-linear interaction vector λ tells for Example 3.2 that the concentration graph is a \mathbb{V} since $\lambda_{12} = 0$; for Examples 3.3 and 3.4 that it is a complete graph since all two-factor terms are nonzero. On the other hand, the correlation matrices tell for Example 3.3 that the covariance graph is a \mathbb{V} since $\rho_{12} = 0$.

The two weak versions of the Yule-Simpson paradox show that a distribution may have more independences than those displayed in its graphical representation. This has also been called its lack of faithfulness to the graph; see Spirtes Glymour & Scheines (2000).

3.2. Combination of independences

For three binary variables, the combination of independences was first studied by Birch (1963, sec. 5): $(A \perp\!\!\!\perp B|O \text{ and } A \perp\!\!\!\perp O|B) \implies A \perp\!\!\!\perp BO$, but $(A \perp\!\!\!\perp B \text{ and } A \perp\!\!\!\perp O) \implies A \perp\!\!\!\perp BO$ holds only when the three-factor interaction is lacking.

More generally, if independences combine both downwards and upwards in a distribution as explained below, then the complete independence, $a \perp\!\!\!\perp bc$, has several equivalent decompositions. Let a, b, c be disjoint subsets of $\{1, 2, \dots, d\}$ for the random variables X_1, X_2, \dots, X_d , where each of a, b, c contains at least one element, then

$$\begin{aligned} a \perp\!\!\!\perp bc &\iff (a \perp\!\!\!\perp b|c \text{ and } b \perp\!\!\!\perp c) \\ &\iff (a \perp\!\!\!\perp b \text{ and } a \perp\!\!\!\perp c) \iff (a \perp\!\!\!\perp b|c \text{ and } a \perp\!\!\!\perp c|b). \end{aligned} \tag{3.2}$$

In all probability distribution, the first equivalence holds but the third and fourth statement are only implied by $a \perp\!\!\!\perp bc$. If the third statement implies $a \perp\!\!\!\perp bc$, the independences combine upwards and if the fourth statement implies $a \perp\!\!\!\perp bc$, they combine downward. Equation (3.2) is a known property of joint Gaussian distributions; see Lněnička & Matúš (2007, def. 1), and Marchetti & Wermuth (2009, app. 2), and of traceable regressions; see Wermuth (2012, cor. 1). In the context of graphical Markov models, the upward and downward combination of independences are called the composition and the intersection property, respectively. Both are also properties of all currently known probabilistic graphs; see Sadeghi & Lauritzen (2014).

A general sufficient condition for the downward combination in discrete distributions are strictly positive probabilities, which are assumed in this paper.

In contrast to Gaussian distributions, in palindromic Bernoulli distributions independences need not combine upwards. An extreme form of this is in Example 3.5, where the correlation matrix is the identity matrix, even though the four variables are dependent.

Example 3.5 $\left[\begin{array}{l} \text{lev. of } A_1, A_2, A_3, A_4 : 0000 \ 1000 \ 0100 \ 1100 \ 0010 \ 1010 \ 0110 \ 1110 \\ 880 \ \pi : \ 100 \ 10 \ 10 \ 100 \ 10 \ 100 \ 100 \ 10 \end{array} \right]$

Here, the independences do not combine upwards since, for instance, both $A_1A_2 \perp\!\!\!\perp A_3$ and $A_1A_2 \perp\!\!\!\perp A_4$ are satisfied, but $A_1A_2 \not\perp\!\!\!\perp A_3A_4$ holds instead of $A_1A_2 \perp\!\!\!\perp A_3A_4$. The reason is the reciprocal behaviour of the conditional odds-ratios which implies that the only nonzero log-linear interaction is the four-factor term and that the conditional correlations vary with the levels of the third variable and can therefore not coincide with a partial correlation.

Similarly, the equality of conditional correlations may get destroyed with special covariance structures even when there is essentially no log-linear four-factor interaction. In Example 3.6, this happens with a *funnel graph* which generalises the sink V to more than two uncoupled nodes pointing to a common response; see Lupparelli, Marchetti & Bergsma (2009) for estimation in such covariance graph models.

Example 3.6 $\left[\begin{array}{l} \text{lev. of } A_1, A_2, A_3, A_4 : 0000 \ 1000 \ 0100 \ 1100 \ 0010 \ 1010 \ 0110 \ 1110 \\ 888 \ \pi : \ 87 \ 24 \ 102 \ 9 \ 60 \ 51 \ 87 \ 24 \end{array} \right]$

The importance of this type of palindromic structure is that it models studies using a 2^k factorial design with equal allocation of the study subjects to all level combinations and special sampling so as to get equal chances of success and of failure for a binary response A_1 .

4. Some special cases

We discuss now palindromic distributions arising when a Gaussian distribution is median dichotomized. Further, some details concerning the specification and estimation of undirected graphical models are given.

4.1. Median dichotomization

Let (X_1, X_2) have a joint distribution function F_{12} with marginal distributions functions F_1 and F_2 . Let further $U_1 = F_1(X_1)$ and $U_2 = F_2(X_2)$ be the probability integral transforms of X_1 and X_2 , so that U_1 and U_2 are uniform. Also let \tilde{X}_j be the medians of X_j , $j = 1, 2$. Consider now the median dichotomized variables,

$$A_1 = \mathbb{I}[U_1 > \frac{1}{2}], \quad A_2 = \mathbb{I}[U_2 > \frac{1}{2}] \tag{4.1}$$

where $\mathbb{I}[\cdot]$ is the indicator function. Then, the joint distribution of A_1 and A_2 is a bivariate palindromic Bernoulli distribution, as given in Section 1, with $\alpha = P(U_1 > \frac{1}{2}, U_2 > \frac{1}{2})$.

The variables $D_1 = (-1)^{A_1}$ and $D_2 = (-1)^{A_2}$, taking values $1, -1$, have mean zero and unit variance, so that $\xi_{12} = E(D_1 D_2)$, the correlation coefficient between D_1 and D_2 , becomes the *cross-sum difference* of the joint probabilities

$$\xi_{12} = 2\alpha - 2\beta = 4\alpha - 1. \tag{4.2}$$

Thus the correlation between two binary variables, which is a multiple of the cross-product difference, coincides in a bivariate palindromic Bernoulli distribution with the cross-sum difference. This was not noted, when ξ_{12} was proposed as a measure of dependence between any two random variables X_1 and X_2 by Blomqvist (1950):

$$\begin{aligned} 4\alpha - 1 &= \Pr\{(X_1 - \tilde{X}_1)(X_2 - \tilde{X}_2) > 0\} - \Pr\{(X_1 - \tilde{X}_1)(X_2 - \tilde{X}_2) < 0\} \\ &= 2\Pr(U_1 \leq \frac{1}{2}, U_2 \leq \frac{1}{2}) + 2\Pr(U_1 > \frac{1}{2}, U_2 > \frac{1}{2}) - 1. \end{aligned}$$

Remark 4.1. The probability α may be interpreted as the copula $C(\frac{1}{2}, \frac{1}{2})$ of the random vector (X_1, X_2) , where the function $C(u, v) = \Pr(U_1 \leq u, U_2 \leq v)$, $0 \leq u \leq 1, 0 \leq v \leq 1$.

With the linear interaction expansion of equation (2.5), the distribution of D_1, D_2 is

$$P(D_1 = i, D_2 = j) = \frac{1}{4}(1 + \xi_{12}ij), \quad i, j = 1, -1. \tag{4.3}$$

After median-dichotomizing $d > 2$ continuous variables, the resulting binary variables $A_v, v = 1, \dots, d$ are still marginally uniform, but their joint distribution is palindromic only for centrally symmetric variables, that is when $X_v - \tilde{X}_v$ has the same distribution as $-(X_v - \tilde{X}_v)$ for each $X_v, v = 1, \dots, d$.

With $d = 3$, the joint distribution of the median-dichotomized variables is palindromic with parameters α, β, γ and δ , as given in Section 1. Their marginal correlations are

$$\xi_{12} = 4\alpha + 4\delta - 1, \quad \xi_{13} = 4\alpha + 4\gamma - 1, \quad \xi_{23} = 4\alpha + 4\beta - 1$$

and the joint probability distribution is, with $i, j, k = 1, -1$.

$$P(D_1 = i, D_2 = j, D_3 = k) = \frac{1}{8}(1 + \xi_{12}ij + \xi_{13}ik + \xi_{23}jk).$$

Example 4.2. The following example gives the orthant probabilities of a trivariate, mean-centred Gaussian distribution having equal correlations: $-1/2 < \rho < 1$. The joint probability vector of the median-dichotomized variables is:

$$8\pi = (1 + 3\xi, \quad 1 - \xi, \quad 1 + 3\xi)$$

and the explicit transformations between the three types of parameters result with

$$\xi = \frac{2}{\pi} \arcsin \rho, \quad \lambda = \frac{1}{4} \log \frac{1 + 3\xi}{1 - \xi}, \quad \eta = \operatorname{atanh} \xi. \tag{4.4}$$

The arcsin transformation is due to Sheppard (1898) and the obtained distribution is a *concentric ring model*; see Wermuth, Marchetti & Zwiernik (2014).

Proposition 4.3. *If X has a d -variate Gaussian distribution with mean zero and correlation matrix $R = [\rho_{st}]$ for $s, t = 1, \dots, d$ and A is the binary random vector obtained by median dichotomizing X , with linear interaction parameters ξ_b , then R can be reconstructed from the correlation matrix $R_A = [\xi_{st}]$ between the binary variables A by*

$$\rho_{st} = \sin\{(\pi/2)\xi_{st}\}, \quad s, t = 1, \dots, d.$$

The proof results by inverting the arcsin transformation of the quadrant probability

$$\xi_{st} = 4 \Pr(X_s \leq 0, X_t \leq 0) - 1 = 2\pi^{-1} \arcsin \rho_{st}.$$

As a consequence one may reconstruct the original correlations from the palindromic Bernoulli distribution derived via the orthant probabilities.

4.2. Maximum likelihood estimation

For a palindromic Bernoulli distribution, given a random sample of size n , one has as counts, that is as observed cell frequencies: $n(a)$, $a \in \mathcal{I}$. The likelihood is

$$\prod_{a \in \mathcal{I}} p(a)^{n(a)} = \prod_{a \in \mathcal{I}_0} p(a)^{n(a)} p(\sim a)^{n(\sim a)} = \prod_{a \in \mathcal{I}_0} p(a)^{n(a) + n(\sim a)} \quad (4.5)$$

where \mathcal{I}_0 is the set of half of the cells a such that $a_1 = 0$. The sufficient statistics are thus the set of the 2^{d-1} frequencies $n(a) + n(\sim a)$, obtained by summing each cell and its complement image. The maximum likelihood estimate of a cell probability (or of a cell count) is the average of the two proportions (or of counts):

$$\hat{p}(a) = \{n(a) + n(\sim a)\}/(2n), \quad \hat{n}(a) = \{n(a) + n(\sim a)\}/2. \quad (4.6)$$

This produces a symmetrized vector of counts.

For palindromic Bernoulli distributions, Wilks' likelihood ratio test statistic is

$$w = 2 \sum_{a \in \mathcal{I}} n(a) \log \left(\frac{2n(a)}{n(a) + n(\sim a)} \right). \quad (4.7)$$

It has an asymptotic χ^2 distribution with 2^{d-1} degrees of freedom; see Edwards (2000, app. C). The maximum likelihood estimates of the linear interaction parameters are

$$\hat{\xi}_b = \begin{cases} 0 & \text{if } |b| \text{ odd,} \\ \sum_{a \in \mathcal{I}} (-1)^{a \cdot b} n(a)/n. & \text{if } |b| \text{ even.} \end{cases}$$

Thus, the estimated $\hat{\xi}_b$, for $|b|$ even, matches the observed moment statistic and for $|b|$ odd is zero. For $|b| = 2$, the estimated marginal correlation, $\hat{\xi}_{12}$

coincides with the correlation coefficient in the fitted table $\hat{p}(a)$, hence is a cross-sum difference of the counts

$$\hat{\xi}_{12} = (n_{00} + n_{11}) - (n_{01} + n_{10}). \quad (4.8)$$

Since the log-linear and the multivariate logistic parameters are in a one-to-one relation to the linear interactions, the maximum likelihood estimates of their parameter vectors, result by the same transformations that hold for the parameters; see Fisher (1922). For the special transformations that apply here, see equations (2.3), (2.5).

In the following, we speak of maximum likelihood estimates simply as ‘estimates’. Estimates may simplify further, when the distribution satisfies independence constraints in such a way that they lead to a graphical Markov model; see, for an overview of these models, e.g., Darroch, Lauritzen & Speed (1980), Haberman (1973), Wermuth (2015).

Example 4.4 (A Markov chain). Let A_1, A_2 and A_3 be three binary random variables where A_1 and A_3 are conditionally independent given A_2 , so that the probabilities satisfy

$$p_{ijk} = p_{+j+}^{-1} p_{ij+} p_{+jk} \text{ for } i, j, k = \pm 1.$$

Its undirected graph, called a concentration graph, $1 \text{ --- } 2 \text{ --- } 3$, has a missing edge for nodes 1 and 3, representing A_1 and A_2 , and it is a simplest type of a graphical Markov model, a Markov chain in 3 variables; see also Example 3.1.

The log-linear parameters are constrained by $\lambda_{13} = \lambda_{123} = 0$ for the conditional independence of pair (1, 3). If, in addition, the distribution is palindromic, the odd-order parameters are zero so that also $\lambda_1 = \lambda_2 = \lambda_3 = 0$. In general Bernoulli distributions, the minimal sufficient statistics are the observed counts corresponding to the *cliques* of the graph, i.e., the maximal complete subsets of the nodes, here just the node pairs (1,2) and (2,3). However for a palindromic Bernoulli distribution, the minimal sufficient statistics are the estimated counts \hat{n}_{ij+} and \hat{n}_{+jk} for margins (1, 2) and (2, 3), defined as in equation (4.6) from the symmetrized table, so that

$$\tilde{p}_{ijk} = n^{-2} \hat{n}_{ij+} \hat{n}_{+jk} \text{ for } i, j, k = \pm 1.$$

where \tilde{p}_{ijk} is the estimate of p_{ijk} under the Markov chain model.

This example illustrates how independence constraints, conditionally given all remaining variables, simply add to the linear constraints on canonical parameters of a palindromic Bernoulli distribution. Moreover, when the model is decomposable, since its concentration graph is chordal, see Darroch, Lauritzen & Speed (1980), it can be generated by a linear triangular system; see end of Section 2.

As far as the maximum likelihood estimation of palindromic graphical models is concerned, the hierarchical constraints of conditional independence and the non-hierarchical constraints of central symmetry are well compatible with one another. Thus one can fit a given graphical model to the symmetrized counts or equivalently symmetrize the fitted counts under the model.

5. Palindromic Ising models

We now introduce palindromic Ising models, especially when combined with conditional independence constraints. Ising models are joint Bernoulli distributions without any higher than two-factor log-linear interactions. An Ising model is palindromic if it has also uniform margins. As mentioned before, this leads for the $(-1, 1)$ coding to binary variables which have zero means, unit variances and covariances coinciding with Pearson's correlations. General Ising models have, for instance, been studied as lattice systems, Besag (1974), and as binary quadratic-exponential distributions, Cox & Wermuth (1994b).

The concentration graph of an Ising model in d variables has d nodes and at most one undirected edge coupling a node pair. The edge (i, j) in this concentration graph is missing if the two-factor log-linear interaction of pair (i, j) vanishes. Each missing edge (i, j) means $i \perp\!\!\!\perp j \mid \{1, \dots, d\} \setminus \{i, j\}$. Simpler independence statements such as $i \perp\!\!\!\perp j \mid C$, for $C \subset \{1, \dots, d\} \setminus \{i, j\}$ result if every path between i and j has a node in C ; see for instance Darroch, Lauritzen & Speed (1980). Recall that nodes and edges of the cliques of the graph form its maximal complete subgraphs, that is those node subsets without any missing edge which become incomplete when one more node is added.

Proposition 5.1. *If the concentration graph of a palindromic Bernoulli distribution has largest clique size three, then it is a palindromic Ising model.*

Proof. An unconstrained palindromic Bernoulli distribution has a complete concentration graph in nodes $\{1, \dots, d\}$. Each removed edge introduces an independence and reduces the size of a generating clique. If the largest clique-size is three, then each of the 2^3 generating probabilities for the joint palindromic distribution has no 3-factor log-linear interaction. \square

Proposition 5.2. *Palindromic Ising models are closed under marginalizing for $d \leq 4$.*

Proof. In an Ising model, all higher than 2-factor log-linear interactions are zero and all trivariate and bivariate marginal distributions are Ising models because palindromic distributions are closed under marginalizing. \square

For palindromic Ising models of more than four variables, cliques of even order may get induced by marginalizing and they may lead to corresponding even-order log-linear interactions. This happens, for instance, if the concentration graph is a star graph with edges is , for $i = 1, \dots, 4$, and marginalizing is over the common source $s = 5$. Notice however that, in any case, the bivariate and trivariate marginal probabilities remain palindromic Ising models.

Proposition 5.3. *For a decomposable palindromic Ising model with largest clique size three, the maximum likelihood estimates are obtained in closed form from the marginal correlations in the symmetrized 2×2 tables within its 2-node and 3-node cliques.*

Proof. If a model is decomposable, then an ordering of the cliques C_t , $t = 1, \dots, T$ can be found, such that the joint probability factorizes and estimation simplifies; see Sundberg (1975). This ordering satisfies the *running intersection property* meaning that the sets $S_1 = C_1 \cap (\cup_{t>1} C_t)$, $S_2 = C_2 \cap (\cup_{t>2} C_t)$, \dots , $S_{T-1} = C_{T-1} \cap C_T$, called separators, are all complete, that is all nodes are coupled by an edge. Then, the joint probability $p(a)$ factorizes into the product of the marginal distributions over cliques C_t divided by the product of the the marginal distributions over the separators S_t .

As cliques and separators have largest size ≤ 3 , and the associated marginal distributions are palindromic Ising models, they are fitted in closed form directly from the marginal 2×2 tables of the symmetrized counts by using for instance the marginal correlations of such tables, that is the cross-sum differences. \square

Example 5.1 below gives three non-decomposable palindromic Ising models having a so-called chordless four-cycle. They have maximal clique size two and edges for $(1, 3)$, $(1, 4)$, $(2, 3)$, $(2, 4)$. They differ in that all nonzero log-linear interactions are positive in the first and negative in the second case. In the third one, there is a chordless cycle in the concentration graph as well as in the covariance graph, that is not only the two independences of the concentration graph hold, $1 \perp\!\!\!\perp 2|34$ and $3 \perp\!\!\!\perp 4|12$, but, in addition, $1 \perp\!\!\!\perp 2$ and $3 \perp\!\!\!\perp 4$.

Example 5.1

| | | | | | | | | |
|--------------------------------|------|------|------|------|------|------|------|------|
| lev. of A_1, A_2, A_3, A_4 : | 0000 | 1000 | 0100 | 1100 | 0010 | 1010 | 0110 | 1110 |
| 336π : | 75 | 15 | 15 | 3 | 15 | 15 | 15 | 15 |
| 336π : | 3 | 15 | 15 | 75 | 15 | 15 | 15 | 15 |
| 336π : | 35 | 35 | 7 | 7 | 7 | 35 | 7 | 35 |

In these chordless cycles, the missing edges in the concentration graph show also as zeros in the matrix of partial correlations given all remaining variables that is in $-\rho^{ij} / \sqrt{\rho^{ii} \rho^{jj}}$. This points to the possible extension of a result by Loh & Wainwright (2013) to include chordless cycles for palindromic Ising models.

Proposition 5.4. *There is no effect reversal in a palindromic Ising model if all its nonzero log-linear interactions are positive.*

This result is a direct consequence of Proposition 3.4 (ii) in Fallat et al. (2016) for totally positive palindromic Ising models. We conjecture that the same holds, when all nonzero log-linear interactions in a palindromic Ising model are negative, such as in our second case of Example 5.1.

6. A case study

The following case study illustrates some of the obtained results. For a sample of grades obtained at the University of Florence, we aim at predicting grades in Physics in terms of given grades in Algebra, Analysis and Geometry. The passing grades range in each subject from 18 to 31. We use sums of grades over exams in three successive years and have data for $n = 78$ students who reached in each of the subjects a sum of at least 60 points. Instructors expect positive

correlations for each pair of these grades and no sign reversal for the correlations at fixed level combinations of the other variables. The data are in Appendix B.

The four summed grades are closely bell-shaped, each of their scatter plots shows a nearly elliptic form as well as the plots of residual pairs obtained after linear least squares regression of each grade on the other three. There is also no evidence for nonlinear relations in the probability plots of Cox & Wermuth (1994a). Thus, there is substantive and empirical support for assuming a joint Gaussian distribution.

After replacing for pairs (1,4) and (2,4) the observed correlations by $\hat{r}_{14} = r_{13}r_{34}$, $\hat{r}_{24} = r_{23}r_{34}$, in Table 3 we have the estimate of the correlation matrix, which has zeros for pairs (1,4) and (2,4) in its inverse, in its concentration matrix; see e.g. Wermuth, Marchetti & Cox (2009), equation (2.8).

TABLE 3

For four fields and 78 students, observed marginal correlations, r_{ij} (below the diagonal), concentrations on the diagonal and partial correlations, $r_{ij,kl}$ (above the diagonal).

| | Analysis | Algebra | Geometry | Physics |
|-------------|----------|---------|----------|---------|
| 1:=Analysis | 2.64 | 0.27 | 0.34 | 0.17 |
| 2:=Algebra | 0.72 | 3.03 | 0.51 | 0.04 |
| 3:=Geometry | 0.76 | 0.80 | 4.07 | 0.38 |
| 4:=Physics | 0.62 | 0.60 | 0.71 | 2.09 |

Wilks' likelihood-ratio test statistic on 2 degrees of freedom shows with a value of $w = 2.8$ a good fit to the model with generating sets $\{\{1, 2, 3\}, \{3, 4\}\}$. This implies conditional independence of the grade in Physics from those in Analysis and Algebra given the grade in Geometry. This follows directly, for instance, with the corresponding concentration graph, on the left of Fig. 3. It has the cliques $\{1, 2, 3\}$ and $\{3, 4\}$ for which node 3 separates node 4 from nodes 1,2 since to reach nodes 1,2 from node 4, one has to pass via node 3.

Similarly, after replacing the marginal correlations for pairs (1, 2), (1, 3) and (2, 3) by their average $\hat{r} = 0.76$, we have for the submatrix of (1,2,3) the conventional estimate of an equicorrelation matrix; see Olkin and Pratt (1958, Section 3). This is here well-fitting since $w = 3.4$ on 2 degrees of freedom. The grade in Physics, correlates with this sum score as 0.706, even slightly less than with the grade in Geometry alone, where $r_{34} = 0.709$. This is plausible in view of the well-fitting Markov structure.

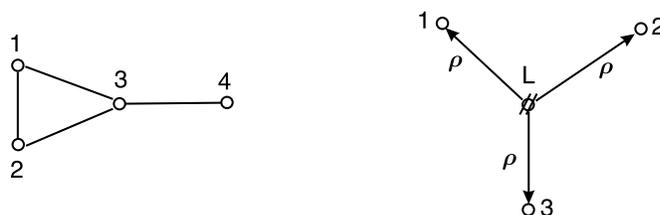


FIG 3. Left: the well-fitting concentration graph for the Florence grades; right: a possible generating graph for grades 1, 2, 3.

A possible generating graph for the Gaussian equicorrelation matrix is the star graph displayed on the right of Fig. 3. In it, mathematical ability is represented by the unobserved inner node, L , and the three grades are the outer nodes of the graph, shown as responses to L by arrows starting at L and pointing to the uncoupled nodes 1,2,3; each arrow has assigned to it the same positive correlation ρ . After marginalizing over L , each outer pair is correlated like ρ^2 . We shall see next how well these results are reflected in the dichotomized data.

After median-dichotomizing the grades with jittering, we generate precisely uniform binary variables, the marginal distributions of which differ only little from those obtained by simple median-dichotomizing. One obtains the estimate of a palindromic contingency table in closed form using equation (4.6) and as we shall see, the same well-fitting concentration graph as on the left of Fig. 3.

The observed contingency table is given next together with — in the additional rows and in the following order — the estimates of palindromic counts, the estimates of the counts after imposing, in addition, conditional independences for the model of Fig. 3 on the left, and the estimates of the corresponding log-linear interactions.

TABLE 4
Cells $ijkl$, levels of interactions, counts n_{ijkl} , estimates of palindromic counts, of the palindromic concentration graph counts and of the log-linear interactions under the latter model

| 0000 | 1000 | 0100 | 1100 | 0010 | 1010 | 0110 | 1110 | 0001 | 1001 | 0101 | 1101 | 0011 | 1011 | 0111 | 1111 |
|-------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| \emptyset | 1 | 2 | 12 | 3 | 13 | 23 | 123 | 4 | 14 | 24 | 124 | 34 | 134 | 234 | 1234 |
| 22 | 3 | 3 | 0 | 1 | 0 | 1 | 9 | 6 | 2 | 2 | 1 | 3 | 2 | 1 | 22 |
| 22 | 2 | 2.5 | 1.5 | 1 | 1 | 1.5 | 7.5 | 7.5 | 1.5 | 1.0 | 1.0 | 1.5 | 2.5 | 2.0 | 22.0 |
| 21.2 | 2.5 | 2.5 | 1.8 | 0.7 | 1.0 | 1.0 | 8.3 | 8.3 | 1.0 | 1.0 | 0.7 | 1.8 | 2.5 | 2.5 | 21.2 |
| 0.90 | 0 | 0 | 0.45 | 0 | 0.62 | 0.62 | 0 | 0 | 0 | 0 | 0 | 0.47 | 0 | 0 | 0 |

The palindromic concentration graph model fits well, with $w = 10.3$ on 11 degrees of freedom. This decomposes into $w = 9.1$ on 8 degrees of freedom for the saturated palindromic model and $w = 1.2$ on 3 degrees of freedom for the additional independence constraints.

Values of the studentized log-linear interactions are 2.5, 3.5, 3.5 and 3.7 for λ_{12} , λ_{13} , λ_{23} and λ_{34} , respectively. Thus, the same independences as for the underlying joint Gaussian distribution fit also the median-dichotomized data and further simplifications are not compatible given the sizes of the remaining studentized interactions. The partial correlations implied by the well-fitting palindromic Markov structure has also zeros for pairs (1,4) and (2,4).

The sum score of the median-dichotomized grades 1,2,3 leads as in the underlying Gaussian distribution not to an improved prediction of grades in Physics. To our starting question, we get two summarizing answers. Given a grade below the median in Geometry, one predicts that 72% of these students will have a grade below the median in Physics and, similarly, given a grade above the median in Geometry, one predicts that 72% will have a grade above the median in Physics.

7. Discussion

We say that centrally-symmetric Bernoulli distributions are palindromic since their probabilities, at the fixed level of one of the variables repeat in reverse order for the second level of this variable and thereby mimic palindromic sequences of characters as introduced in linguistics.

A palindromic Bernoulli distribution is characterized by the vanishing of all odd-order log-linear interactions. Hence, such zero constraints lead to a non-hierarchical, log-linear model which give centrally symmetric probabilities. Until now, it was only known that in centrally-symmetric Bernoulli distributions, all odd-order log-linear parameters vanish; see Edwards (2000, app. C). With these linear constraints, distributions result which are in the regular exponential family.

Palindromic Bernoulli distributions may also be parameterized with all odd-order interactions vanishing in a linear-in-probability model and in a multivariate-logistic model. The parameters in the three types of model are in one-to-one relations; see Section 2. These relations are now available in closed form for the linear and the log-linear formulations, while in general, iterative procedures are needed when the multivariate logistic formulation is involved. In any case, equivalent parameterizations assure that the maximum-likelihood estimates of the parameters are in the same one-to-one relation; see Fisher (1922).

It is remarkable that a palindromic Bernoulli distribution can be expressed precisely as a log-linear and as a linear model, since log-linear parameters use the notion of multiplicative interactions and the linear-in-probability models are based instead on the notion of additive interactions as discussed, for instance by Darroch & Speed (1983).

The log-linear parameterization shows that positive palindromic Bernoulli distributions are in the regular exponential family with and without additional independence constraints in its concentration graph. A palindromic Ising model may have only log-linear two-factor interactions as non-vanishing canonical parameters, while in their linear-model formulations higher-order interactions may be present. The palindromic property is preserved under marginalizing over any subset of the variables; see Proposition 2.1, even though one may no longer have an Ising model after marginalizing over some of the variables.

Another property is important for applications. In palindromic Bernoulli distributions, many other measures of dependence of a variable pair are one-to-one functions of the odds-ratio; in particular the relative risk, used mainly in epidemiology, and the risk difference, employed almost exclusively in the literature on causal modelling. Only if a measure of dependence is a function of the odds-ratio, it varies independently of its margins; see Edwards (1963) and only then, measures of bivariate dependence become directly comparable under different sampling schemes, for instance when the overall count is fixed as in a cross-sectional study or one of the margins is fixed as in a prospective study or the other margin is fixed as in a retrospective study.

We expect that with a direct extension of the palindromic property to discrete variables of more levels, similar attractive properties can be obtained as for the palindromic Bernoulli distribution.

Appendix A: Proofs

Proof of Proposition 2.5. The proof is by induction. We know that A_1 has a palindromic distribution. For $s = 2, \dots, d$ we assume that the random vector $A_{[s-1]} = (A_1, \dots, A_{s-1})$ has a palindromic distribution, and then we show that the distribution of $A_{[s]} = (A_1, \dots, A_s)$ is palindromic. Let $\mathcal{I}_{\text{even}}$ denote the subset of $\{0, 1\}^s$ with even order and split it in two parts

$$\mathcal{I}_0 = \{a \in \mathcal{I}_{\text{even}} : a_s = 0\}, \quad \mathcal{I}_1 = \{a \in \mathcal{I}_{\text{even}} : a_s = 1\}.$$

We then start from the identity

$$\Pr(A_{[s]} = a_{[s]}) = \Pr(A_{[s-1]} = a_{[s-1]})\Pr(A_s = a_s \mid A_{[s-1]} = a_{[s-1]})$$

and after substituting equations (2.5) and (2.13) and taking into account that by assumption $A_{[s-1]}$ has a palindromic distribution and thus $\xi_b = 0$ for all $b \in \mathcal{I}_1$, we have

$$\Pr(A_{[s]} = a) = 2^{-s} \sum_{b \in \mathcal{I}_0} \xi_b (-1)^{a \cdot b} \cdot \{1 + \sum_{j=1}^{s-1} \beta_{sj} (-1)^{a \cdot e_{s,j}}\}$$

where $e_{s,j}$ is a binary vector of dimension s with ones exactly in positions s and j . After multiplying and collecting terms we get with

$$\xi_b = \sum_{v \in \mathcal{I}_0 : v \Delta \{s,j\} = b} \xi_v \beta_{s,j}, \quad \text{for } b \in \mathcal{I}_1, \quad (\text{A.1})$$

$$\Pr(A_{[s]} = a) = 2^{-s} \left(\sum_{b \in \mathcal{I}_0} \xi_b (-1)^{a \cdot b} + \sum_{b \in \mathcal{I}_1} \xi_b (-1)^{a \cdot b} \right),$$

where Δ denotes the symmetric difference of sets. Therefore $A_{[s]}$ has a linear parameterization with exclusively even order interactions and hence is palindromic. Thus, by induction, the distribution of $A_{[d]} = A$ is palindromic. From the recursive equation (A.1), each linear interaction is a linear function of the regression parameters $\beta_{s,j}$. \square

Proof of Prop. 3.1. It is known that in a strictly positive 2^3 table $A_1 \perp\!\!\!\perp A_2 \mid A_3 \iff (\lambda_{12} = 0 \text{ and } \lambda_{123} = 0)$. As in a trivariate palindromic table the three-factor interaction is always zero the single condition $\lambda_{12} = 0$ is necessary and sufficient. This is in turn equivalent to a single condition on the partial correlation $\rho_{12.3} = 0$.

With no constraints other than those of palindromic distributions, there is a smooth one-to-one transformation $(\lambda_{12}, \lambda_{13}, \lambda_{23}) \longleftrightarrow (\rho_{12}, \rho_{13}, \rho_{23})$ where the marginal correlations are the free parameters of vector ξ .

In addition, there is a one-to-one smooth transformation between the simple correlations and the partial correlations $(\rho_{12}, \rho_{13}, \rho_{23}) \longleftrightarrow (\rho_{12.3}, \rho_{13.2}, \rho_{23.1})$,

since the conditional and partial correlations coincide. Also, the function $g: \mathbb{R} \rightarrow [-1, 1]: \lambda_{12} \mapsto r_{12.3}$ is strictly monotone increasing for any values of λ_{13} and λ_{23} and has a single zero in the origin, so that the partial correlation $r_{12.3}$ has the same sign as the log odds-ratio λ_{12} .

In more detail, the three variable table of Section 1, supplemented by both margins for the two conditional tables of A_1, A_2 can be written in terms of simple correlations as

| A_1 | $A_2 A_3$: | 00 | 01 | sum | 10 | 11 | sum |
|-------|-------------|------------------------------|------------------------------|------------------------------|------------------------------|------------------------------|------------------------------|
| 0 | | α | γ | $\frac{1}{4}(1 + \rho_{13})$ | δ | β | $\frac{1}{4}(1 - \rho_{13})$ |
| 1 | | β | δ | $\frac{1}{4}(1 - \rho_{13})$ | γ | α | $\frac{1}{4}(1 + \rho_{13})$ |
| sum | | $\frac{1}{4}(1 + \rho_{23})$ | $\frac{1}{4}(1 - \rho_{23})$ | $\frac{1}{2}$ | $\frac{1}{4}(1 - \rho_{23})$ | $\frac{1}{4}(1 + \rho_{23})$ | $\frac{1}{2}$ |

The probabilities in the two 2^2 tables, expressed with margins and $\rho_{12|3}$ give e.g.

$$8\alpha = (\rho_{12} - \rho_{13}\rho_{23}) + \{(1 + \rho_{13})(1 + \rho_{23})\},$$

$$8\delta = (\rho_{12} - \rho_{13}\rho_{23}) + \{(1 - \rho_{13})(1 - \rho_{23})\},$$

since the product of all four margins is in both tables $(1 - \rho_{13}^2)(1 - \rho_{23}^2)/16^2$ and

$$(\rho_{12} - \rho_{13}\rho_{23})/16 = \{\frac{1}{2} - (\beta + \gamma + \delta)\}\delta - \beta\gamma = \alpha\delta - \beta\gamma.$$

Thus, $\rho_{12|3} = \rho_{12.3}$ and $\alpha\delta - \beta\gamma = 0$ if and only if $\lambda_{12} = 0$. The above 2^3 table shows also directly that under the independence constraint $1 \perp\!\!\!\perp 2|3$, we have

$$\tilde{\alpha} = \{1 + \rho_{13}\}(1 + \rho_{23})/8, \quad \tilde{\delta} = \{(1 - \rho_{13})(1 - \rho_{23})\}/8$$

$$\tilde{\beta} = \{1 - \rho_{13}\}(1 + \rho_{23})/8, \quad \tilde{\gamma} = \{1 + \rho_{13}\}(1 - \rho_{23})/8$$

so that e.g. $\tilde{\alpha}\tilde{\delta}$ and the probability $\tilde{\alpha} + \tilde{\delta}$, induced in the marginal table of A_1, A_2 for $(1, 1)$, are

$$\tilde{\alpha}\tilde{\delta} = (1 - \rho_{13}^2)(1 - \rho_{23}^2)/8^2, \quad \tilde{\alpha} + \tilde{\delta} = (1 + \rho_{13}\rho_{23})/4. \quad \square$$

Appendix B: The data for the case study

The columns of Table 5 contain sums of grades of three exams in four subjects for $n = 78$ mathematics students at the University of Florence.

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TABLE 5

Summed grades over 3 exams in the order: Analysis, Algebra, Geometry and Physics.

| | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 78 | 78 | 74 | 80 | 88 | 77 | 79 | 85 | 82 | 82 | 74 | 89 | 85 | 77 | 93 | 85 | 79 | 85 | 74 | 69 | 78 | 88 | 67 | 92 | 85 | 69 |
| 76 | 75 | 71 | 77 | 81 | 79 | 77 | 90 | 79 | 72 | 62 | 90 | 75 | 83 | 92 | 88 | 80 | 88 | 68 | 80 | 75 | 88 | 70 | 89 | 88 | 75 |
| 82 | 81 | 74 | 71 | 85 | 74 | 81 | 83 | 73 | 73 | 71 | 86 | 84 | 84 | 93 | 82 | 78 | 90 | 70 | 79 | 71 | 89 | 68 | 91 | 91 | 62 |
| 85 | 77 | 80 | 80 | 79 | 80 | 75 | 82 | 71 | 71 | 72 | 87 | 82 | 69 | 90 | 75 | 75 | 82 | 70 | 78 | 72 | 77 | 69 | 93 | 87 | 68 |
| 79 | 92 | 76 | 88 | 73 | 91 | 76 | 71 | 65 | 74 | 80 | 71 | 78 | 77 | 70 | 83 | 89 | 72 | 82 | 77 | 91 | 92 | 75 | 90 | 90 | 93 |
| 78 | 92 | 78 | 87 | 68 | 85 | 78 | 79 | 68 | 76 | 89 | 74 | 81 | 74 | 68 | 89 | 81 | 76 | 81 | 74 | 92 | 92 | 69 | 79 | 82 | 93 |
| 71 | 92 | 84 | 88 | 64 | 83 | 82 | 69 | 71 | 75 | 80 | 71 | 85 | 69 | 67 | 88 | 83 | 75 | 83 | 82 | 93 | 92 | 72 | 90 | 89 | 93 |
| 79 | 90 | 86 | 78 | 69 | 75 | 82 | 71 | 63 | 72 | 78 | 74 | 81 | 67 | 66 | 72 | 82 | 75 | 79 | 76 | 92 | 87 | 75 | 79 | 78 | 89 |
| 92 | 87 | 81 | 82 | 76 | 86 | 92 | 87 | 79 | 91 | 88 | 90 | 90 | 92 | 89 | 83 | 77 | 69 | 89 | 92 | 86 | 76 | 68 | 79 | 76 | 88 |
| 93 | 83 | 69 | 70 | 75 | 71 | 80 | 70 | 70 | 77 | 88 | 92 | 85 | 92 | 84 | 83 | 82 | 74 | 83 | 92 | 74 | 71 | 62 | 68 | 66 | 89 |
| 93 | 87 | 74 | 67 | 80 | 69 | 87 | 77 | 69 | 92 | 83 | 91 | 82 | 91 | 86 | 83 | 80 | 83 | 83 | 90 | 78 | 71 | 65 | 74 | 83 | 91 |
| 89 | 77 | 81 | 79 | 84 | 72 | 80 | 81 | 70 | 79 | 77 | 72 | 88 | 81 | 86 | 81 | 78 | 76 | 77 | 79 | 73 | 69 | 69 | 72 | 80 | 85 |

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