Generating large Ising models with Markov structure via simple linear relations

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Abstract: We extend the notion of a tree graph to sequences of prime graphs which are cycles and edges and name these non-chordal graphs hollow trees. These structures are especially attractive for palindromic Ising models, which mimic a symmetry of joint Gaussian distributions. We show that for an Ising model all defining independences are captured by zero partial correlations and conditional correlations agree with partial correlations within each prime graph if and only if the model is palindromic and has a hollow-tree structure. This implies that the strength of dependences can be assessed locally. We use the results to find a well-fitting general Ising model with hollow-tree structure for a set of longitudinal data.

Keywords: Chain graph; Chordal graph; Chordless cycle; Concentration graph; Cut-set; Elimination scheme; Hollow tree; Log-linear interaction; Logit regression; Palindromic distribution; Prime graph; Probabilistic graph; Quadratic exponential distribution.

1 Introduction

After Maurice Bartlett had defined in 1935 log-linear interactions in trivariate contingency tables, it took almost thirty years until sets of minimal sufficient statistics for maximum-likelihood estimates (mle) were derived by Martin Birch in 1963, for the model without a 3-factor interaction and for a range of possible hypotheses of conditional independence for the discrete variables. Almost another 10 years passed until a general iterative-proportional fitting algorithm became available in published form as well as relations of log-linear to the so-called logit-regressions; Bishop (1972).

Since then, log-linear models became widely used, at the beginning helped by a Fortran Program distributed by Leo Goodman, called ‘Everybody’s Contingency Table Analysis (ECTA)’. But strong complaints emerged that some scientists continued to use methods of data analysis based on correlations. For instance in the preamble of a book by Goodman (1984), ‘correlationers’ are suggested to be in stark contrast to ‘crosstabbers’. The former were seen to rely on linear models and linear regressions and the latter on contingency tables and the corresponding log-linear models, logit regressions and odds-ratios. One main purpose of the current paper is to identify and characterize a large class of models for binary variables in which particular sequences of generating logit regressions are indeed equivalent to sequences of linear regression.

A theoretical discussion of linear versus log-linear models for contingency tables is by Darroch and Speed (1983). Recently, more methodological research was requested to come to a better understanding when linear relations might be appropriate; see Hagenaars (2015). In the 1970’s in Germany, it took data from an experiment carried out by psychologist Gustav Lienert, to convince the community that correlations could sometimes be extremely misleading; for an English data description see Wermuth (1998). The structure in Lienert’s data is very close to having a strong dependence among three binary variables in spite of three pairwise independences, that is when also the three simple Pearson’s correlation coefficients are zero.

So far, there appear to be not many results concerning linear relations for binary distributions. One is that directed acyclic graph models can be generated with linear main-effect regressions provided that all variables have mean zero, unit variance and they are symmetric;
see Wermuth, Marchetti and Cox (2009). However, these models have mainly been used to illustrate small graph-structured models and to demonstrate the possible equivalence of different types of such models. Relations between probabilities and correlations in Bernoulli distributions with special types of graph, named star graphs, see Figure 2 for the simplest example, are by Wermuth and Marchetti (2014) and Wermuth, Marchetti and Zwiernik (2014).

Another result is by Loh and Wainwright (2013). They prove that a conditional independence constraint, represented by the missing edge in an undirected graph, leads for binary variables to a zero partial correlation given all remaining variables if the graph is, what we name, a bulged tree. For an example of such a graph see Figure 3. Unfortunately, partial correlations may then also be zero when they correspond to edges present in the graph. In that case, one cannot use zeros in the matrix of partial correlations to recognize an independence structure.

This happens for instance, for the following two contingency tables with four variables. In the first, the graph structure is a paw graph, see Figure 2 with all edges present for the nodes 1, 2, 3 and one edge for 3, 4, but the only nonzero marginal correlation is $\rho_{34}$. In the second, no edge is missing in the graph since the log-linear 4-factor interaction, $\lambda_{1234}$ defined here with equation (1), is large, but nevertheless all six $\rho_{ij}$ are zero.

Such types of tables may describe sequences of bacterial genoms; see Radavičius, Recačiūnas and Židanavičiūtė (2017). For the analysis of such combinations of symmetric and antisymmetric sequences, logit regressions may be useful but linear regressions are clearly useless.

One might then be tempted to conclude that linear relations and hence correlations become relevant when all higher than 2-factor log-linear interactions vanish, that is when they are constrained to be zero. This is the case in the models proposed by physicist Ernst Ising in 1925 for binary variables in effect coding, $-1, 1$. In the statistical literature, Ising models have been studied as binary lattice models by Besag (1974), and as quadratic exponential distributions for binary variables by Cox and Wermuth (1994a).

But another feature is needed also for Ising models to make linear relations useful. It is a central symmetry property of joint continuous distributions, illustrated here for just two variables.

This points directly to a main property of the following binary distributions, called palindromic Ising models. The term palindromic had been introduced in linguistics to characterise special symmetric words or sentences. An English palindromic sentence is ‘step on no pets’.

For a single binary variable, the distribution is palindromic if it is symmetric, that is if both levels occur with probability $1/2$. For a Bernoulli distribution of binary variables $A_1, \ldots, A_d$ with effect coding, the distribution is palindromic if $\Pr(\omega) = \Pr(-\omega)$ for all $\omega$, where $\omega$ is a level combination and $-\omega$ is the complement of $\omega$ in which all signs are switched. For Ising models, this type of central symmetry is generated with the additional constraint that each variable taken alone is symmetric that is has uniform margins.

\footnote{lower levels are here indicated by ‘0’, also later, in order to save space or to simplify the notation}
When probabilities are denoted by $\alpha, \beta$ in such bivariate distributions or by $\alpha, \beta, \gamma, \delta$ in such trivariate distributions, then the probability tables can be written as

Table 1a)

| $A_1$ | $A_2$ | -1 | 1 | sum |
|-------|-------|----|---|-----|
| -1    | $\alpha$ | $\beta$ | $\frac{1}{2}$ |
| 1     | $\beta$  | $\alpha$ | $\frac{1}{2}$ |
| sum   | $\frac{1}{2}$ | $\frac{1}{2}$ | 1 |

Table 1b)

| $A_1$ | $A_2$ | -1 | 1 | 1 | 1 | sum |
|-------|-------|----|---|---|---|-----|
| -1    | $\alpha$ | $\gamma$ | $\delta$ | $\beta$ | $\frac{1}{2}$ |
| 1     | $\beta$  | $\delta$ | $\gamma$ | $\alpha$ | $\frac{1}{2}$ |
| sum   | $\alpha + \beta$ | $\gamma + \delta$ | $\gamma + \delta$ | $\alpha + \beta$ | 1 |

With the assumed effect coding of the levels, the variables have mean zero and unit variance, so that the covariance matrix $\Sigma$ coincides with the correlation matrix, having $\sigma_{ii} = 1$, $\sigma_{ij} = \rho_{ij}$.

From Table 1a) rewritten in terms of the simple correlation $\rho_{12}$, one gets also

$$
\pi_{11} = \frac{1 + \rho_{12}}{4}, \quad \pi_{-11} = \frac{1 - \rho_{12}}{4}, \quad \lambda_{12} = \frac{1}{2} \log \left( \frac{1 + \rho_{12}}{1 - \rho_{12}} \right) = \tanh^{-1} \rho_{12},
$$

so that $\lambda_{12}$ coincides here with the z-transformation of $\rho_{12}$ suggested by Ronald Fisher in 1922 for a different purpose. It opens the range $-1 < \rho_{12} < 1$ to the full line, $-\infty < \lambda_{12} < \infty$.

Note that for bivariate binary distributions with skewed margins, $\rho$ is not a function of the odds-ratio, it changes instead with the degree of skewness. In this case, the simple correlation coefficient is not relevant for assessing the strength of the dependence; see Edwards (1963).

When the column vector $\pi$, containing the probabilities $p(\omega)$, has a lexicographic order with the index of the first variable changing fastest, the index of the last changing slowest and $H_d$ is the Hadamard matrix defined by the following Kronecker product:

$$
H_d = \left(\begin{array}{c}
1 \\
1 \\
1 \\
1 \\
\end{array}\right) \otimes \cdots \otimes \left(\begin{array}{c}
1 \\
1 \\
1 \\
1 \\
\end{array}\right),
$$

then the log-linear interaction vector, $\lambda$, and linear interaction vector, $\xi$, are respectively:

$$
\lambda = H_d^{-1} \log \pi = (H_d \log \pi)2^{-d}, \quad \xi = H_d \pi.
$$

The second equality defining $\lambda$ is the matrix form of an adding-and-subtracting algorithms proposed by Frank Yates in 1937 for effect estimation in $2^d$ experimental designs. This was recognized and related to more general Fourier analyses by Good (1958).

A main result for palindromic Bernoulli distributions, proven in Marchetti and Wermuth (2016), is their characterization by vanishing elements in $\lambda$ and $\xi$ which involve an odd number of variables. Such distributions get even closer to joint distributions of standardized Gaussian variables, when they are also Ising models. In palindromic Ising models, the only terms of $\lambda$ permitted to be nonzero, are the overall effect $\lambda_{\emptyset}$ and the 2-factor terms $\lambda_{ij}$. For independence of variables $A_i, A_j$ given all remaining variables, we use a notation due to Dawid (1980):

$$
\lambda_{ij} = 0 \iff i \perp \! \! \! \! \! \! \perp j | N \setminus \{i, j\}, \quad (2)
$$

A set of such independence statements defines an independence structure, also called the Markov structure of the model, and shows in missing edges of the following type of graph.

We treat here only simple, finite, undirected graphs that is at most one $ij$-edge couples distinct nodes, $i, j$, taken from node set $N = \{1, \ldots, d\}$ having a finite $d$ and each edge present is undirected. In addition, all our starting graphs are connected so that each node can be reached from another by walking along a path, that is along a sequence of distinct edges. In the following, a ’graph’ is always a member of this class of graphs.

Essential for our discussions will be subgraphs, cut-sets and prime graphs. The subgraph of a node set $a \subseteq N$ has as edges those present in the graph among the nodes of $a$. A subgraph
in which all nodes are coupled is a complete graph, also called a simplex by Wagner and Halin (1962). We use their term even though it has a different meaning in geometry. A maximal simplex is a clique; it turns into an incomplete subgraph when one more node of the graph is added to it. A cut-set is the smallest simplex $c$ which separates disjoint subsets $a$ and $b$ of a graph, meaning that every path between $a$ and $b$ has a node in the complete subgraph $c$.

Prime graphs are characterised by having no cut-set. Prime graphs are either cliques or, if incomplete, each node has some uncoupled neighbours, we say equivalently: each node resides in at least two cliques. This is evident in chordless cycles, where each node has two uncoupled neighbours, but is more difficult to detect in the other more complex, incomplete prime graphs. For instance in the next to last prime graph of Figure 1 each of four nodes resides in a triangle and in a hidden chordless 4-cycle. This feature of prime graphs that are more complex than cliques or cycles has been explained early on by Rose (1970, Figure 1), long before the concept of probabilistic graphs was defined.

Figure 1: the three types of prime graph in connected graphs, from the left: complete graphs; chordless $h$-cycles, $h > 3$; other incomplete graphs, also with no node residing in a single clique

In probabilistic graphs, nodes represent random variables and different types of edge permit a broad range of conditional dependences for a given independence structure, also called Markov structure, defined by the missing edges. One early, nearly neglected, but most important result for probabilistic undirected graphs is the uniqueness of their set of prime graphs.

**Theorem 1.** Wagner and Halin (1962). *Every finite graph breaks into its prime graphs.*

Directly related to Theorem 1 is one characterization of the so-called chordal graphs: their set of prime graphs consists exclusively of cliques. For less than five nodes, Figure 2 shows all chordal, incomplete but connected graphs to which we get back later. The prime graphs of a diamond graph are its two triangles, of a paw graph they are a triangle and an edge. In all other graphs of Figure 2 they are just edges.

Figure 2: All chordal, incomplete graphs in three or four nodes from the left: a transmitting V; a diamond; a paw; a tripod or 3-leaf star; a single 3-edge path or 4-node Markov chain

After the publication of Theorem 1 it took another 30 years until an efficient algorithm became available to find a graph’s set of prime graphs; Leimer (1993), and until some proofs of properties of distributions with prime graph structure were given; Matúš (1994, App.).

In computer science and statistics, a strong emphasis is until today on chordal graphs and on their so-called decomposable models; see Tarjan and Yannakakis (1984), Darroch, Lauritzen and Speed (1980), Thomas and Green (2009), Studeny and Cussens (2016). One main reason is that the mle of models with a chordless-cycle structure is typically fitted using an iterative procedure, even for Gaussian distributions; Dempster (1972); Speed and Kiiveri (1986); Dahl, Vandenberghe and Roychowdhury (2008), Lauritzen, Uhler and Zwiernik (2017).

In this paper, we extend traditional trees, which are chordal graphs, to a subclass of non-chordal graphs with attractive properties for the corresponding palindromic Ising models. For this, we distinguish first four classes of simple, finite, incomplete and connected graphs using as illustration Figure 3. The traditional trees, called here also ‘thin trees’, form one class. The
other three types are extensions of thin trees. When one chooses the prime graphs of a hollow tree as the nodes of a new graph and the cut-sets as the edges in this new graph, then just as in a traditional tree, a ‘single path’ connects each pair of ‘nodes’.

![Figure 3: from the left: traditional or thin tree; bulged tree; hollow tree; fattened tree](image)

The prime graphs of a hollow tree are exclusively edges or cycles – triangles or chordless cycles – and the cut-sets are single nodes or edges. It is the only class which may contain cycles, the other classes consist exclusively of chordal graphs. Thin and bulged trees form subclasses of hollow trees. A thin tree has only edges as prime graphs and single nodes as cut-sets, a bulged tree consists of edges or triangles and has cut-sets which are still just single nodes. Finally, a chordal, fattened tree is obtained from a hollow tree by completing each chordless $h$-cycle with all of its missing chords.

The plan of the paper is to summarise first some notation and results for graphs in Section 2. These needed, solid justifications of the extended tree models may be skipped at a first reading. We give properties and different parametrisations for palindromic Ising models with the extended tree structures in Section 3, stressing in particular linear parametrisations and closed form relations between parameters. Again, the details for special models are essential for our arguments but may be skipped at a first reading. We continue with some general properties of palindromic Ising models with hollow-tree structure, possible transformations between general and palindromic Ising models and consequences for model selection. In Section 4, we illustrate the results by fitting a general Ising model to a set of longitudinal data. A discussion ends the paper. Detailed proofs and needed previous results are given in appendices.

2 Summary of some graph terminology and results

A finite, undirected graph has a set of nodes, $N = \{1, \ldots, d\}$, for a finite $d$. An $ij$-edge couples two distinct nodes and turns the nodes $i$ and $j$ into neighbours; such nodes are also said to be adjacent. The graph is simple if there is at most one edge coupling each node pair and there are no loops, that is no $ii$-edges. Each graph can be represented by a binary symmetric matrix with an $ij$-one if an $ij$-edge is present and an $ij$-zero if the pair $i, j$ is uncoupled in the graph. The matrix is called edge matrix, if its diagonal elements are ones and adjacency matrix if they are zeros. Only for edge matrices, $E$, there is a matrix operator which can capture changes in the graph due, for instance, to marginalising; see here App. E.

In probabilistic applications, the nodes in the graphs represent random variables, in this paper these are binary variables $A_1, \ldots, A_d$. If an uncoupled node pair $i, j$ means conditional independence of $A_i, A_j$ given all remaining variables, then this type of undirected graph is also called a concentration graph and each $ij$-edge present is drawn as a full line, $i \rightarrow j$.

A graph is said to be edge-minimal if every $ij$-edge indicates a deviation from the independence constraint for $A_i, A_j$, so that the pair is conditionally dependent given all remaining variables, written typically as $i \indep j \mid N \setminus \{i, j\}$; see Wermuth and Sadeghi (2012). The type of a dependence may be captured by parameters of a given probability model. In this paper, we
discuss Ising models for skewed and for symmetric binary variables, in both of which
\[ \lambda_{ij} \neq 0 \iff i \neq j \mod N \setminus \{i, j\}. \] (3)

Such a model is said to be generated over an edge-minimal graph if equations (2) and (3) hold.

A path is a sequence of distinct edges connecting its endpoint nodes. The path is a cycle if the endpoints coincide. A cycle has the same number of nodes as edges and by starting at any node of a \( h \)-cycle and walking along its \( h \) edges, one returns to the starting node. A cycle of more than three nodes is said to be chordless.

For \( a, b, c \) nonempty disjoint subsets of \( N \), the intersecting set \( c \) of \( a \cup c \) and \( b \cup c \) is a separator if every path between \( a \) and \( b \) has a node in \( c \). The subgraphs of separator sets may be incomplete, such as every separator in a chordless cycle, see Figure 1, or be complete, as all of them are in the so-called chordal graphs; for examples see Figure 2. The smallest separating simplex of two prime graphs is a cut-set of the graph. In Figure 2, only the diamond graph has an edge as a cut-set; all other cut-sets are single nodes.

Prime graphs are characterized by having no cut-set. For the unique set of prime graphs of an undirected graph, only maximal simplexes are used, that is the cliques. An edge is said to be incident to \( m \subset N \) if just one of its endpoints resides in \( m \). The elimination of \( m \) from a graph means to remove not only all nodes and edges within \( m \) but also all incident to \( m \).

Leafs or outer nodes have traditionally been defined for thin trees as those single nodes which have just one neighbour. For chordal graphs, outer nodes reside in a single clique. Such outer nodes have also been called external or simplicial. The notion extends directly to outer node-sets which reside in a single prime graph. After the elimination of an outer node set, the starting set of prime graphs is reduced by just one prime graph so that, in this paper, the remaining graph is again a hollow tree.

For chordal graphs, outer single nodes can be eliminated repeatedly until only one last edge is left. This is the essence of the Tarjan–Yannakakis algorithm which ends with a proper, also called perfect, single-node elimination scheme or the conclusion that the graph is not chordal. Similarly, outer node-sets can be repeatedly eliminated from the extended trees until only one last prime graph is left. Leimer’s algorithm gives such a proper node-set elimination scheme and the unique set of prime graphs. In the R-package ‘gRbase’, this algorithm is implemented; see Dethlefsen and Højsgaard (2005).

**Proposition 1.** The unique set of unlabelled prime graphs of a connected graph remains unchanged if and only if every two prime graphs are attached at one of the graph’s cut-sets.

**Proof.** For a given graph, the unique cut-sets are given by its prime graphs and a proper node-set elimination scheme. Conversely, when one attaches a prime graph to one which is already in a given sequence of prime graphs, at least one previous cut-set is destroyed and another prime graph is generated.

One example is a line of \( h \) edges in \( h + 1 \) nodes. It generates a chordless \( h \)-cycle when the two ending edges are attached at their endpoint nodes. Another example is a chain of four triangles. With an edge-to-edge tiling of the triangles to give the graph next to the last on the right of Figure 2, a new prime graph is generated.

In 1962, Gabriel Dirac proved that every incomplete chordal graph has at least two outer nodes; see also Blair and Peyton (1993), Lemma 3. Leimer’s algorithm implies that every incomplete, connected graph has at least two outer node sets; these outer sets cannot be empty but each may also contain just a single node.

For thin trees, it was derived by Camille Jordan in 1869 that in its center, there is a node or an edge from where the paths to the outer nodes are shortest; for an efficient algorithm see
Mitchell Hedetniemi, Cockayne and Hedetniemi (1981). For hollow trees, the following small modification of Leimer’s algorithm finds at its last step either a prime graph or a cut-set which is an edge: eliminate first all outer single nodes residing in an edge and all outer-edge nodes residing in a triangle until none are left. Then, eliminate stepwise all outer-node sets of the remaining prime graphs. For instance, after the first two steps have been applied to the hollow tree and to the fattened tree of Figure 1 the two tree trunks in Figure 4 remain.

Figure 4: left: hollow-tree trunk to Figure 3; right: fattened-tree trunk to Figure 3

We use Figure 4 to illustrate here how a proper node-set elimination scheme can be generated. If in these two graphs of Figure 4 the outer node-set on the left is eliminated first, its nodes are labelled as 1, 2. The other outer nodes in the 5-cycle may then get labelled as 3, 4, 5, 6. The remaining four nodes in set c = {7, 8, 9, 10} form then an inner prime graph and c separates sets a = {1, 2} and b = {3, 4, 5, 6}, that is every path from a to b has a node in c. But c it is here not a cut-set, since it is incomplete for the graph on the left and it not a smallest simplex for the graph on the right.

In statistics, undirected graphs were the first studied types of the broad class of probabilistic graphs. For many probabilistic graphs one knows now when they are Markov equivalent, that is when they define the same independence structure, just in a different way; see here App. F. One may for instance orient a hollow tree, that is change some of its full lines to arrows, by any proper node-set elimination scheme and obtain a special type of chain graph, one of those introduced by Lauritzen and Wermuth (1989) and Frydenberg (1990), called and studied later as discrete LWF chain graphs; see Drton (2009).

Thus, the hollow-tree trunk of Figure 4 may for instance be oriented as in Figure 5. These orientations mimic one important property of thin trees: each prime graph can be chosen as the undirected past, that is as the one from where arrows are starting.

Figure 5: Markov equivalent orientations of the hollow tree in Figure 4 with undirected cycles, left: the 4-cycle in the middle; middle: the 4-cycle on the left; right: the 6-cycle on the right

Factorisations of a distribution such as in equation (22) below relate to elimination schemes: the outer-node sets correspond to joint responses, each cut-set to a set of regressors.

Proposition 2. In a hollow tree and in its fattened tree, one obtains – after eliminating in sequence only outer node sets – a subset a ∪ b ∪ c where a and b are the outer nodes of two prime graphs and the smallest separator c is their cut-set or their inner prime graph.

Proof. By the uniqueness of the set of prime graphs and the existence of a proper node-set elimination scheme for all nodes, only the edges within and incident to N \ {a ∪ b ∪ c} are removed, hence no edge is added and none is removed in the subgraph of a ∪ b ∪ c. □

For Ising models, this is exploited in Section 3 by using covering models, which are chordal, and reduced models, which have cycles; see Cox and Wermuth (1990) for these notions. Thereby, we build heavily on the existence of proper node-set elimination schemes.
3 On the relevance of linear relations for Ising models

3.1 Measures of dependence in trivariate palindromic models

In the palindromic model for three binary variables, the 3-factor interaction is missing, hence it is an Ising model with symmetric marginal distributions and it has joint symmetries.

To relate different measures of dependence later, we take Table 1b) rewritten as

| $A_3$ | $A_1$ | $A_2$ | $A_{12}$ | $A_{13}$ | $A_{23}$ |
|-------|-------|-------|----------|----------|----------|
| $-1$ | $-1$ | $-1$ | sum      | $1$      | $1$      |

For this table, we define at level $-1$ of $A_3$ several standard and widely used measures of dependence as well as further measure, $\tau$, that we name the hypetan interaction since it is the hype(rbolic) tan(gent) of $\lambda$. It had been introduced and studied for $2 \times 2$ tables under the name ‘coefficient of colligation’ by Yudney Yule in 1912. The difference of the conditional probabilities for level $1$, taken at levels $1$ and $-1$ of another variable, is said to be the chance difference for success. It is used almost exclusively in the current literature on causal modelling.

Each of these measures remains unchanged when moving to level $1$ of $A_3$ and $1 \perp 2 \perp 3$ is reflected in a zero value of each measure except for the odds-ratio, which then equals one.

odd-ratio or cross-product ratio: $\text{odr}_{123} = (\alpha \delta) / (\beta \gamma)$,

chance difference for success: $\text{chd}_{123} = 16(\alpha \delta - \beta \gamma) / (1 - \rho_{23}^2)$,

conditional correlation: $\rho_{123} = 16(\alpha \delta - \beta \gamma) / ((1 - \rho_{13}^2)(1 - \rho_{23}^2))^{-1/2}$,

log-linear interaction: $\lambda_{12} = (\log \text{odr}_{123}) / 4$,

hypetan interaction: $\tau_{12} = (\text{odr}_{123}^{1/2} - 1) / (\text{odr}_{123}^{1/2} + 1) = \tanh(\lambda_{12})$.

As explained before, linear relations may in general not be relevant for contingency tables. But here, there is an invertible relation of the conditional probabilities to the simple correlations in terms of an anti-diagonal matrix, a Hankel matrix formed by $(-1, -1, 0)$ and $(0, -1, -1)$. With $\alpha = \frac{1}{2} - (\beta + \gamma + \delta)$, we have:

$$
\begin{pmatrix}
\rho_{12} \\
\rho_{13}
\end{pmatrix} =
\begin{pmatrix}
-1 & -1 & 0 \\
-1 & 0 & -1
\end{pmatrix}
\begin{pmatrix}
\beta \\
\gamma \\
\delta
\end{pmatrix}
- 1/2.
$$

By applying equation (4), one sees directly that there is no log-linear and no linear 3-factor interaction. Furthermore, as stated next in equations (5) and (6), chance differences coincide with linear regression coefficients, and conditional correlations with partial correlations.

For more general palindromic Ising models, linear regression coefficients are based on the covariance matrix $\Sigma$ which coincides with the correlation matrix. We write such a linear regression coefficient by indicating the response before a conditioning sign ‘|’, the regressor after ‘|’ and the remaining regressors of the given response after ‘|’.

For the trivariate palindromic Ising model, we have $16(\alpha \gamma - \beta \delta) = (\rho_{12} - \rho_{13} \rho_{23})$ so that

$$
\beta_{1|2,3} = (\rho_{12} - \rho_{13} \rho_{23}) / (1 - \rho_{23}^2) \quad \text{coincides with chd}_{1|2,3},
$$

$$
\rho_{12,3} = (\rho_{12} - \rho_{13} \rho_{23}) / ((1 - \rho_{13}^2)(1 - \rho_{23}^2))^{-1/2} \quad \text{coincides with } \rho_{12,3}.
$$
This makes it possible to study in the following changes in dependences for palindromic Ising models after marginalising or conditioning via well-known recursive, linear relations for Gaussian distributions; for general proofs when different equal measures remain unchanged after marginalising, that is when they are collapsible, see Xie, Ma and Geng (2008).

Recursive relations have been derived for linear regression coefficients by Bill Cochran in 1938, for covariances by Ted Anderson in 1958 and for concentrations by Arthur Dempster in 1969. For discussions of all three in connection with graphs see Wermuth and Cox (1998), Marchetti and Wermuth (2009), Wermuth (2015); for simple proofs of matrix forms see Wiedenbeck and Wermuth (2010).

\[ \beta_{1|2} = \beta_{1|2,3} + \beta_{1|3,2} \theta_{23}/\theta_{22}, \quad \sigma_{12|3} = \sigma_{12} - \sigma_{13} \rho_{23}/\sigma_{33}, \quad \sigma^{12,3} = \sigma^{12} - \sigma^{13} \rho_{23}/\sigma^{33}, \]

where for covariances, ‘|’ means again conditioning, while for concentrations, ‘.’ indicates marginalising. For more than three variables, an additional conditioning set, \( c \), is added to the regression coefficients and an additional marginalising set, \( m \), to the concentrations in each term of the above equations; as for instance for equation (15) below.

While the relevance of such linear measures for palindromic hollow trees will be shown later, the recursive relations for \( A_1, A_2, A_3 \) give for trivariate distributions directly:

\[ \beta_{1|2} = \beta_{1|2,3} \iff 1 \perp \perp 3|2 \text{ or } 2 \perp \perp 3, \]

\[ \sigma_{12|3} = \sigma_{12} \iff 1 \perp \perp 3 \text{ or } 2 \perp \perp 3, \]

\[ \sigma^{12,3} = \sigma^{12} \iff 1 \perp \perp 3|2 \text{ or } 2 \perp \perp 3|1, \]

expressing conditions for collapsibility in terms of independences.

There is also a recursive relation for \( \tau_{ij} \), which after marginalising over \( A_k \) turns into the simple correlation \( \tau_{ij}^b = \rho_{ij} \) of variables \( A_i, A_j \), as proven for equation (20) in App. A:

\[ \rho_{ij} = \tau_{ij}^b = (\tau_{ij} + \tau_{ik} \tau_{jk})/\text{const.}, \quad \text{with: const.} = 1 + \rho_{ij} \tau_{ik} \tau_{jk}. \quad (7) \]

Equation (7) leads directly to conditions for collapsibility for \( \tau_s, \lambda_s \) and the odds-ratios with:

\[ \tau_{12|3} = \tau_{12} \iff 1 \perp \perp 3|2 \text{ or } 2 \perp \perp 3|1. \]

For three variables, equations (1) show that there is no 3-factor interaction for the log-linear and for the linear interaction parameters. That linear-regression coefficients are positive multiples of \( \tau_s \) is derived in App. B and shown next:

\[ \beta_{1|2,3} = \tau_{12}(1 - \tau_{13}^2)/(1 - \tau_{12}^2 \tau_{13}^2), \quad \beta_{1|3,2} = \tau_{13}(1 - \tau_{12}^2)/(1 - \tau_{12}^2 \tau_{13}^2), \quad (8) \]

Since for instance \( \rho_{12,3} \) is a a positive multiple of \( \beta_{1|2,3} \), it follows that also partial correlations are positive multiples of the hypetan interaction \( \tau_{12} \).

By the definition of Pearson’s correlation coefficient for binary variables, see here equation (16), the probability \( \pi_{11|k=1} \) coincides with the probability when all signs are switched and is

\[ \pi_{11|k=1} = 2^{-3} \{\text{const.} \rho_{12,3} + (1 + \rho_{13}k)(1 + \rho_{23}k)\}, \quad \text{const.} = \{(1 - \rho_{12}^2)(1 - \rho_{23}^2)\}^{1/2}, \quad (9) \]

and, since \( \rho_{ijkl} = \rho_{ijk} \), all probabilities are also given by using the partial correlation matrix.

### 3.2 Palindromic Ising models with no independences and with diamond-graph structure

For \( d \) binary random variables \( A_1, \ldots, A_d \) taking values \(-1, +1\), the probability distribution \( \Pr(\omega) = \Pr(A_1 = \omega_1, \ldots, A_d = \omega_d) \) is a palindromic Ising model if

\[ \log \Pr(\omega) = \lambda_{\emptyset} + \sum_{s<t} \lambda_{st} \omega_s \omega_t, \quad -\infty < \lambda_{st} < \infty. \quad (10) \]
In such models with concentration graph structure, a missing edge for \( i, j \) in the graph indicates the conditional independence of equation (2) and an \( ij \)-edge present means the conditional dependence of equation (3). The interactions \( \lambda_{ij}, \xi_{ij} \) result as in equation (1).

By equation (10), the log-linear interactions, \( \lambda_{ij} \), and hence the \( \tau_{ij} = \tanh \lambda_{ij} \), are constant at all level combinations of the remaining variables. Similar to \( d = 3 \):

\[
\lambda_{ij} = \frac{1}{2} \log(1 + \tau_{ij})/(1 - \tau_{ij}), \quad \tau_{ij} = (\odr_{ij/N\{i,j\}}^{1/2} - 1)/(\odr_{ij/N\{i,j\}}^{1/2} + 1).
\]

But for \( d > 3 \), this does in general not imply a linear model with only 2-factor linear interactions. In particular, for \( \rho_{ij|N\{i,j\}} \neq 0 \) varying at several level combinations of the remaining variables, these conditional correlations cannot equal the single value of the partial correlation, \( \rho_{ij,N\{i,j\}} \); but see Proposition 3 as well as Theorem 3 below.

As an illustration, we choose the palindromic Ising model with the diamond graph structure shown in Figure 2, the smallest covering model for a chordless 4-chain. We denote the variables by \( A, B, C, D \), their levels by \( i, j, k, \ell \) and \( p(\omega) = \pi_{ijkl} \). Conditional probabilities, for instance for \( A \) given the level combinations of \( B, C, D \), are then \( \pi_{ijkl} = \pi_{ijk\ell}/\sum_i \pi_{ij\ell} \). We label the outer nodes of the diamond graph as 1, 2 and the cut-set nodes as 3, 4 so that the missing edge is for nodes 1, 2. An example is displayed in the next table:

| \( ijk\ell \) with \( l = 0 \) | 0000 | 1000 | 0100 | 1100 | 0010 | 1010 | 0110 | 1110 |
|-----------------------------|------|------|------|------|------|------|------|------|
| 302 \( \pi_{ijkl} \)        | 100  | 20   | 5    | 1    | 12   | 8    | 3    | 2    |

The following matrix on the left contains \( \lambda_{ij} \) in the lower and \( \tau_{ij} \) in the upper-triangular part, the matrix on the right has \( \rho_{ij} \) in the lower and \( \rho_{ij,\ell} \) in the upper-triangular part.

| 0   | 0   | 0.292 | 0.465 |
|-----|-----|-------|-------|
| 0   | 0   | 0.382 | 0.799 |
| 0.301 | 0.402 | 0    | 0.342 |
| 0.504 | 1.100 | 0.357 | 0     |
|-----|-----|-------|-------|
| 1   | 0   | 0.210 | 0.265 |
|     | 0.523 | 1   | 0.213 | 0.714 |
|     | 0.523 | 0.656 | 1    | 0.206 |
|     | 0.589 | 0.854 | 0.669 | 1     |

The linear regression of either \( A_3 \) or \( A_4 \) on all remaining variables induces a linear 4-factor-interaction in the joint distribution, so that the nonzero conditional correlations vary with the level combinations of \( A_1, A_2 \) and hence, can for these responses not coincide with the single value of the corresponding partial correlation in the joint distribution of all four variables.

But the 4-factor linear interaction is irrelevant, when this palindromic Ising model is generated by three logit equations, for which the nodes are ordered as 1,2,3,4, and each response has just two regressors. To simplify notation, we change again level \(-1\) to 0.

\[
\logit (\pi_{1|k\ell}) = \log \pi_{1+k\ell} - \log \pi_{0+k\ell} = 2(\lambda_{13} k + \lambda_{14} \ell) \quad \text{for response } A,
\]
\[
\logit (\pi_{1|k\ell}) = \log \pi_{1+k\ell} - \log \pi_{0+k\ell} = 2(\lambda_{23} k + \lambda_{24} \ell) \quad \text{for response } B, 
\]
\[
\logit (\pi_{1|\ell}) = \log \pi_{++1\ell} - \log \pi_{++0\ell} = 2(\lambda_{34} \ell) \quad \text{for response } C,
\]

where, for instance, for response \( A: \pi_{1+k\ell} = \sum_j \pi_{1j\ell} \), for response \( C: \pi_{++1\ell} = \sum_{ij} \pi_{ij\ell} \). Only term \( 2\lambda_{12} \) is missing compared to a model without any independence constraint.

The term ‘logit’ had been introduced for ratios of rates and in logit-regressions rates depend only on binary variables. For the above ratios of conditional probabilities, the terms conditioned upon cancel so that only the probabilities in the two 3-node triangles, for subsets \( \{1, 3, 4\}, \{2, 3, 4\} \), and within the cut-set of the graph, \( \{3, 4\} \), are used to generate the model.

A strongly condensed, common notation for densities and probabilities reflects both: independence structures and proper elimination schemes. For instance for the diamond graph and for the 4-node Markov chain in Figure 2, respectively, we can write:

\[
f_N = f_{1|34} f_{2|34} f_{3|4} f_A, \quad f_N = f_{1|2} f_{2|3} f_{3|4} f_4.
\]
This type of factorisation exists if and only if the model has a chordal graph structure. The reason is that for chordal graphs and only for those, every proper single-node elimination scheme results in a directed acyclic graph in which none of the previous Vs, $\circ \rightarrow \circ \rightarrow \circ$, corresponds to a sink $V$, that is to a subgraph of the type $\circ \rightarrow \circ \leftarrow \circ$; see here Theorem 6 in App. F and for its proof see Wermuth and Sadeghi (2012, Theorem 1).

The diamond graph distribution of equation (11) may, by its factorisation and by the inverse equation (4), equivalently be generated with the following linear regressions:

$$
\begin{align*}
\pi_{ijk\ell} &= \frac{1}{2} \{1 + \beta_{1[3,4]} i k + \beta_{1[4,3]} i \ell\}, \\
\pi_{jik\ell} &= \frac{1}{2} \{1 + \beta_{2[3,4]} i k + \beta_{2[4,3]} i \ell\}, \\
\pi_{ikj\ell} &= \frac{1}{2} \{1 + \beta_{3[4]} k \ell\}, \\
\pi_{kij\ell} &= \frac{1}{2}.
\end{align*}
$$

(12)

For each of $f_{134}, f_{234}$, the conditional correlations and the partial correlations coincide by definition, see the previous section. Hence, the strength of the dependences can be judged from the partial correlations for $A, C, D$ and $B, C, D$, while the independence for pair $(1,2)$ shows in the zero partial correlation $\rho_{123,4}$, the standardised version of the concentration $\sigma_{12}^2$.

Induced simple correlations result for $a \perp b | c$ – as in Gaussian distributions – from requiring $\Sigma_{abc} = 0$, here for $a = \{1\}$, $b = \{2\}$, and $c = \{3, 4\}$, with

$$
\Sigma_{ab}^* = \Pi_{a|c} \Sigma_{cb}, \quad \Pi_{a|c} = \Sigma_{ac} \Sigma_{cc}^{-1}
$$

(13)

where $\Pi_{a|c}$ denotes the matrix of linear regression coefficients for response nodes $a$ and regressor nodes $b$. More explicitly, after indicating a transposed vector by $(\ )^T$, equation (13) becomes for the diamond graph, labeled as above, $\rho_{12}^* = (\beta_{1[3,4]}, \beta_{1[4,3]})(\rho_{23}, \rho_{42})^T$.

It follows from equation (14), or more directly from equation (2.4) in Wermuth, Marchetti and Cox (2009), that the 4-factor linear interaction, $\xi_{ijk\ell}$, for $A, B, C, D$ with $e = (j, k, \ell)$ is:

$$
\xi_{ijk\ell} = \Pi_{i|e}(\rho_{k\ell}, \rho_{j\ell}, \rho_{jk})^T.
$$

(14)

This gives for the diamond graph, labeled as above, $\xi_{1234} = (\beta_{1[3,4]}, \beta_{1[4,3]})(\rho_{24}, \rho_{34})^T$. For response nodes 3 or 4, this interaction implies in regressions on all remaining nodes varying linear coefficients even though the logit-regression coefficients are constant.

In trivariate palindromic Ising models and in triangles as prime graphs, linear regression coefficients are constant by definition, but by Proposition 3 this constancy is impossible for a node chosen as response when it still has more than two neighbours.

**Proposition 3.** For palindromic Ising models, a main-effect logit-regression of response $A_i$ is equivalent to a main-effect linear regression of $A_i$ if and only if $A_i$ has at most two regressors.

*Proof.* The claim holds for three variables with equation (8) given the equivalence of the parametrizations in terms of $l$s and $t$s, in equations (10) and (27). For a response with three or more regressors, a 4-factor linear interaction is introduced in the joint distribution; see equation (14). It implies a 3-factor linear interaction in the conditional distribution of this response given more than two regressors, hence destroys the equivalence. 

Proposition 3 explains, for an inner node chosen as a response, when main-effect logit regressions can be replaced by main-effect linear regressions. This holds for instance, for the chordal graphs on the left and on the right of Figure 2 but not for the other three and stresses the importance of proper elimination schemes in order to obtain relevant linear regressions.
Relations of regression coefficients and partial correlations to concentrations, follow most directly with a matrix operator which extends the sweep operator and is defined here in App. E. For a partitioning of a node set as \( \{1, 2, c, m\} \), one has

\[
\rho_{12,c} = -\sigma_{12,m}^{11,m} / \sigma_{12,m}^{11,m} \sigma_{22,m}^{2,2,m} \] \begin{equation}
\beta_{1|2,c} = -\sigma_{12,m}^{11,m} / \sigma_{22,m}^{2,2,m} .
\end{equation}

By contrast, within each \( 2 \times 2 \) subtable, the conditional correlation is just a correlation coefficient for two binary variables. Here, we replace again level \(-1\) by \(0\), let \(e = N \setminus \{m, 1, 2\} \) denote a fixed level combination of the remaining variables and e.g. \(p_{i+1e} = \sum_i p_{i1e}\)

\[
\rho_{12|e} \left( \pi_{11e} - \pi_{1+1e} \pi_{1+e} \right) / \left( \pi_{1+1e} \pi_{1+0e} \pi_{1+1e} \pi_{10+e} \right) \}^{-1/2} .
\]

The following adapts a previous result to be used below for palindromic Ising models.

**Theorem 2.** Baba, Shibata and Sibuya (2004). The partial correlation \( \rho_{12,N \setminus \{m, 1, 2\}} \) coincides with the conditional correlation \( \rho_{ij|e} \) if and only if \( E(A_i, A_j | A_e) \) is a linear function of the vector variable \( A_e \) and \( \rho_{ij|e} \) is constant at all level combinations \(e\).

Theorem 2 and Proposition 3 imply for the equivalence of \( \rho_{ij|e} \) and \( \rho_{12,N \setminus \{m, 1, 2\}} \), that no node chosen as a response should have more than two neighbours. This is reached with any proper node-set elimination scheme for hollow trees and, as we shall see, only for these palindromic Ising models.

### 3.3 Palindromic Ising models generated over chordless cycles

We start this section with a 4-cycle having its nodes labelled as in the left graph of Figure 6.

![Figure 6: left: labeled 4-cycle; right: labeled 5-cycle](image)

Thus, the missing edges are for pairs \((1,2), (3,4)\). An example is in the next table.

\[
\begin{bmatrix}
ijkl \text{ with } l = 0 : & 0000 & 1000 & 0100 & 1100 & 0010 & 1010 & 0110 & 1110 \\
\text{556} \pi_{ijkl} & 180 & 36 & 5 & 1 & 20 & 15 & 12 & 9
\end{bmatrix}
\]

The following matrix on the left contains \( \lambda_{ij} \) in the lower and \( \tau_{ij} \) in the upper-triangular part, the matrix on the right has \( \rho_{ij} \) in the lower and \( \rho_{ij, k\ell} \) in the upper-triangular part.

\[
\begin{bmatrix}
0 & 0 & 0.319 & 0.442 \\
0 & 0.646 & 0.771 & 0 \\
0.330 & 0.768 & 0 & 0 \\
0.474 & 1.024 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
1 & 0 & 0.226 & 0.286 \\
0.511 & 1 & 0.459 & 0.648 \\
0.504 & 0.705 & 1 & 0 \\
0.561 & 0.806 & 0.597 & 1
\end{bmatrix}
\]

The two conditional independences \( 1 \perp 2 | \{3, 4\} \) and \( 3 \perp 4 | \{1, 2\} \) show as zeros in usual measures of dependence for the contingency table, \( \lambda_{ij}, \tau_{ij} \), and in the partial correlations, \( \rho_{ij, k\ell} \).

For the chordless cycle here, all elements of \( \Sigma^{-1} \) relate to joint linear regressions of two uncoupled nodes on their neighbours. For \( a = \{1, 2\} \) as in Figure 6, the neighbours of nodes 1, 2 are both in \( b = \{3, 4\} \). With \( N = (a, b) \) and \( m = \emptyset \), equation (15) gives for row 1 of \( \Sigma^{-1} \)

\[
\sigma_{11}^{11} = 1/\sigma_{11|b}, \quad (\sigma_{13}^{13}, \sigma_{14}^{14}) = -\sigma_{11}^{11}/\Pi_{1|b},
\]

where \( \Pi_{1|b} = (\beta_{1|3,4}, \beta_{1|4,3}) \), \( \sigma_{11|b} = 1 - \Pi_{1|b} \Sigma_{b1} \) and for row 2, the analogous results. It is shown in App. B that linear regression coefficients are positive multiples of the \( \tau \)s in an almost
unchanged form of equation (8) which holds for trivariate distributions. Similarly, partial correlations are then also positive multiples of the $\tau$s.

The following equations, (18) and (19), give the induced marginal correlations for pair $(1, 2)$ in both cycles of Figure 6 in terms of the hypetan interactions, $\tau_{ij}$. A formal proof for the 4-cycle is in App. A, while the following explanations are to provide some more intuitive insights.

In the labelled 4-cycle, we have $\tau_{13} = \tau_{134}$ and $\tau_{23} = \tau_{234}$ due to $3 \perp 4 \mid \{1, 2\}$. Marginalising over node 4 in the subgraph $1 \rightarrow 4 \rightarrow 2$, which is a so-called transmitting $V$, induces $\tau_{124} = \tau_{14} \tau_{24}$. By applying next equation (7) to the marginal table of $A_1, A_2, A_3$, one gets for the margin of $A_1, A_2$:

$$\rho_{12}^x = \tau_{1234} = (\tau_{14} \tau_{24} + \tau_{13} \tau_{23})/\text{const.}, \quad \text{with const.} \equiv 1 + \tau_{13} \tau_{14} \tau_{23} \tau_{24}. \quad (18)$$

The linear 4-factor interaction is instead a multiple of the sum of products of $\tau_{ij}$s for disjoint edges:

$$\xi_{1234} = (\tau_{13} \tau_{24} + \tau_{14} \tau_{23})/\text{const.}, \quad \text{with const.} \equiv 1 + \tau_{13} \tau_{14} \tau_{23} \tau_{24}. \quad$$

However, this interaction is not relevant if the undirected graph is oriented into a Markov-equivalent LWF chain graph, that is, for instance, by letting an arrow point from node 4 to 1 and from node 2 to 3. The distribution generated over this graph has factorisation $f_{13} f_{24}$ and satisfies for response nodes 1 and 3 the two independences $1 \perp 2 \mid 34$ and $3 \perp 4 \mid 12$.

For the labelled 5-cycle of Figure 6 a minor modification of the 4-cycle argument gives:

$$\rho_{12}^y = \tau_{12345} = (\tau_{14} \tau_{15} \tau_{25} + \tau_{13} \tau_{23})/\text{const.}, \quad \text{with const.} \equiv 1 + \tau_{14} \tau_{15} \tau_{25} \tau_{13} \tau_{23}. \quad (19)$$

One knows that $\tau_{j3} = \tau_{j345}$ for $j = 1, 2$ since $\{4, 5\} \perp 3 \mid \{1, 2\}$ and $\tau_{1245} = \tau_{14} \tau_{15} \tau_{25}$ by closing the transmitting $V$s along the path $1 \rightarrow 4 \rightarrow 5 \rightarrow 2$. Next, one applies equation (7), again as above, to the table of $A_1, A_2, A_3$, which remains after marginalising over 4, 5.

These arguments for the 4- and 5-cycle lead directly to the following result for all chordless cycles.

**Proposition 4.** In a chordless $h$-cycle of a palindromic Ising model, the induced $\rho_{k\ell}^*$ for an uncoupled node pair $(k, \ell)$ results by tracing the two paths, connecting $k, \ell$ in the cycle, in terms of products of $\tau$’s, attached to the $h$ edges present in the cycle.

A matrix form for induced correlations uses instead partial correlations. For this, we denote the overall matrix of partial correlations by $\theta$. The relation between $\Sigma$ and $\theta$ becomes transparent by using the identity matrix $I$ and standardising, that is, changing the elements $m_{ij}$ of a symmetric matrix $M$ to give with the elements of $M_{\text{std}}$ as $m_{ij}/\sqrt{m_{ii} m_{jj}}$:

$$\Sigma^* = K_{\text{std}} \quad \text{with} \quad K = (2I - \theta)^{-1}. \quad (20)$$

This holds in unchanged form for all larger chordless cycles.

With $|M|$ denoting the determinant of $M$, the product $\Sigma^{-1} |\Sigma|$ gives two equations in terms of marginal correlations which may be solved numerically for a set of given data to obtain $x = \rho_{12}^*$ and $y = \rho_{34}^*$:

$$x(y^2 - 1) - c_1 y + c_2 = 0, \quad y(x^2 - 1) - c_1 x + c_3 = 0, \quad (21)$$

where $c_1 = \rho_{13} \rho_{24} + \rho_{14} \rho_{23}$ is the sum of products of disjoint edges, $c_2 = \rho_{13} \rho_{23} + \rho_{14} \rho_{24}$ relates to the two paths connecting pair $(1, 2)$ and $c_3$ relates, analogously, to the two paths connecting $(3, 4)$. The five possible solutions reduce to one if one constrains them to be within a range,
say of ±0.2, of the given \( \rho_{12} \) and \( \rho_{34} \). For the example to a diamond graph in the previous section, the solution changes \( \rho_{12} = 0.523 \) to \( \rho_{12}^* = 0.545 \) and \( \rho_{34} = 0.669 \) to \( \rho_{34}^* = 0.590 \).

To generate the probabilities to the 4-cycle in Figure 6, there are then two main options. One may (1) fit the four sufficient two-way tables with some standard iterative procedure or (2) generate first the probabilities in the marginal tables for nodes 1, 3, 4 and 2, 3, 4 using the solutions of equations \((21)\) and exploit next that the independence constraint for pair \((1, 2)\) gives \( f_{1234} = f_{134}f_{234} \).

The two trivariate tables used in this expression may be obtained in terms of simple correlations and equation \((4)\), in terms of partial correlations and equation \((9)\) or simply as marginal three-dimensional tables when an observed table with skewed margins has been transformed into a saturated palindromic Ising model, as described in section 3.5. There are analogous, albeit a bit more complex extensions to larger chordless cycles, not given here.

### 3.4 Some properties of Ising models with hollow tree-structure

We recall from Section 1, how parameters of Bernoulli distributions are defined in equation \((1)\) and that in palindromic Ising models, the 1-factor terms are zero, in addition to all higher than 2-factor log-linear interactions. Equations \((2)\) define independences and equations \((3)\) point to the dependences in Ising models with an edge-minimal graph structure.

From Section 2, we remember that models with hollow-tree structure have a unique set of prime graphs which consists of edges or cycles, attached to each other at cut-sets which are single nodes or edges. The unique set of cut-sets arises with any proper node-set elimination scheme giving sequences of outer node sets as responses residing in a single prime graph.

Binary thin trees as well as bulged trees are a subclass of the hollow trees but contain exclusively chordal-graph models. For thin trees with non-symmetric margins, there is an extensive literature in graph theory, in phylogenetics and in machine learning. Bulged trees have been studied under the name ‘dino graphs’ by Loh and Wainwright (2013) for general multinomial and for Bernoulli distributions.

In general Bernoulli distributions with a thin or extended tree-structure, one may, by Proposition \(2\) reduce the concentration graph to subgraphs, such as to the tree trunks in Figure \(4\) which have a subset of nodes \( a \cup b \cup c \) satisfying the conditional independence constraint \( a \perp b | c \). The nodes in \( a \) and in \( b \) are then the outer nodes of two prime graphs, set \( c \) separates \( a \) and \( b \); the smallest remaining separator is either a cut-set or a prime graph. Then, the joint probability distribution in this marginal distribution, \( f_{a \cup b \cup c} \), factorises as

\[
\begin{aligned}
f_{a \cup b \cup c} &= f_{a | c} f_{b | c} f_{c}.
\end{aligned}
\]

For our extended trees, several special features, based on linear relations, are to be summarised next. In particular, we shall see that all conditional independence constraints – and only these – are reflected for the palindromic hollow trees in zero elements, \( \sigma^{ij} = 0 \), of \( \Sigma^{-1} \). Each \( ij \)-edge present in the graph shows instead as \( \sigma^{ij} \neq 0 \).

For palindromic Ising models with hollow tree-structure and factorisations as in equation \((22)\), there are block-triangular matrix decompositions of \( \Sigma^{-1} \) for \( N' = a \cup b \cup c \) just as for joint Gaussian distributions; see Wermuth (1992, equation (3.5)):

\[
\Sigma^{-1} = \varphi_a (\Sigma^{aa})^{-1} \varphi_a^T + \varphi_b (\Sigma^{bb.a})^{-1} \varphi_b^T + \varphi_c (\Sigma^{cc.ab})^{-1} \varphi_c^T
\]

with

\[
\begin{align*}
\varphi_a &= \begin{pmatrix} \Sigma^{aa} \\ \Sigma^{ba} \\ \Sigma^{ca} \end{pmatrix}, & \varphi_b &= \begin{pmatrix} 0_{ab} \\ \Sigma^{bb.a} \\ \Sigma^{cb.a} \end{pmatrix}, & \varphi_c &= \begin{pmatrix} 0_{ac} \\ 0_{bc} \\ \Sigma^{cc.ba} \end{pmatrix}.
\end{align*}
\]

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where for instance, $\Sigma^{ba}$ is the submatrix for $(b, a)$ in a concentration matrix for $a \cup b \cup c$, $\Sigma^{cb,a}$ is the submatrix for $(c, b)$ in a concentration matrix obtained after marginalizing over $a$ and $\Sigma^{cc,ba}$ is a concentration matrix for $c$ after marginalizing over $a$ and $b$.

When the nodes in $a$ and in $b$ are the outer nodes of two prime graphs of a hollow tree and $c$ is a prime graph or a cut-set separating $a$ and $b$, then $a \perp b | c$, is an ‘independence constraint between prime graphs’ and shows $\Sigma^{ab} = 0$, while, for instance, when $a$, $b$, and $c$ have more than three nodes, there are cycles within $a$, $b$ and $c$ in the graph, which represent ‘independence constraints within prime graphs’ and show as cycles within $\Sigma^{aa}$, $\Sigma^{bb,a}$ and $\Sigma^{cc,ab}$.

One consequence of this representation is the following result proven in App. C.

**Theorem 3.** A quadratic exponential distribution for symmetric binary variables is generated over an edge-minimal hollow tree if and only if (1) the Markov structure of its concentration graph is defined by the set of zeros in its overall partial correlation matrix and (2) within each of its prime graphs, all conditional correlations agree with the partial correlations.

Theorem 3 states essentially that such joint distributions are determined by linear relations. This implies that dependences along paths can be combined by marginalising since linear relations are traceable; for this notion see here App. D or Wermuth (2012). For instance in hollow trees with chordless cycles as prime graphs, the simple correlations induced for the missing edges within a cycle may be obtained in terms of partial correlations or, in a more compact way, in terms of the hypetan interactions, as in equations (18) and (19); see also Proposition 4. For a 4-cycle, the linear relations lead to equations (21), expressed in terms of the correlations for the edges present in the graph and give solutions for the induced correlations.

Theorem 3 is important for judging a hypothesized hollow-tree structure in a new sample for two main reasons. First, one can recognize the pairwise independences defining the Markov structure in the overall partial correlation matrix, $(2I - \Sigma^{-1})_{\text{std}}$, which is easily estimated for reasonably large sample sizes and contains elements ranging at most within $\pm 1$. Second, one can judge the strength of each pairwise dependence by the partial correlation computed from small submatrices of the estimated covariance matrix corresponding to the unique subset of prime graphs for the hollow tree.

Together with the equivalence in Proposition 3 for main-effect logit and main-effect linear regressions, Theorem 3 also leads to the following results.

**Corollary 1.** The joint distribution of a palindromic Ising model with thin- or bulged-tree structure can be generated with linear regressions by using any single-node elimination scheme.

**Corollary 2.** Palindromic Ising models with hollow-tree structure are traceable, but may contain cycles both in partial correlations and in marginal correlations.

![Figure 7: 4-cycle in concentrations; right: 4-cycle in covariances; i - - j indicates i \(\notin\) j](image)

The more restrictive requirement of a distribution to have no additional independences than those indicated by the graph, is not satisfied by general Gaussian distributions; see for an example Wermuth (2012, Section 2.5). Both cycles of Figure 7 hold also in the next table:

\[
\begin{bmatrix}
jkll \text{ with } \ell = 0 & 0000 & 1000 & 0100 & 1100 & 0010 & 1010 & 0110 & 1110 \\
80 \pi_{ijkl} & 9 & 9 & 1 & 1 & 1 & 9 & 1 & 9
\end{bmatrix}
\]
The following matrix on the left contains $\lambda_{ij}$ in the lower and $\tau_{ij}$ in the upper-triangular part, the matrix on the right has $\rho_{ij}$ in the lower and $\rho_{ij,kl}$ in the upper-triangular part.

\[
\begin{array}{ccc}
0 & 0 & 0.635 \\
0 & 0 & 0.635 \\
0.749 & 0.749 & 0 \\
-0.749 & 0.749 & 0
\end{array} \quad \begin{array}{ccc}
1 & 0 & 0.452 \\
0 & 1 & 0.452 \\
0.452 & 0.452 & 1 \\
-0.452 & 0.452 & 0
\end{array}
\]

Notice from equation (18) that a special parametric constellation induces here the zero marginal correlations $\rho_{12}^* = 0$ and $\rho_{34}^* = 0$. Such constellations have been named parametric cancellations, when they were discussed for Gaussian distributions by Wermuth and Cox (1998). It is an open question whether such constellations may characterise processes of special interest. Here, the marginal and the partial correlations coincide, in addition, and there is no 4-factor linear interaction. More generally, one knows for instance the following.

**Proposition 5.** If a palindromic hollow-tree Ising model has overall exclusively positive or zero partial correlations, then there are no path cancellations and no correlation is negative.

**Proof.** The claim follows with Theorem 3, Proposition 4 and results for the total positivity of joint distributions; see Fallat et al. (2017), Karlin and Rinott (1983), Bolviken (1982).

In Proposition 5, ‘correlation’ means all possible types of correlations, partial as well as simple ones. In such distributions, there will in particular never be any effect reversal, i.e. no Yule-Simpson paradox, and for our connected graphs, all simple correlations are positive.

### 3.5 Transformations between general and palindromic Ising models

For binary two-way tables with probabilities $\pi^T = [\alpha, \beta, \gamma, \delta]$, there is a unique way to move from the skewed margins to symmetric ones, preserving the odds-ratio; see Cox (2006, Sec. 6.4), Palmgren (1989). The next table divided by $2(\sqrt{\alpha\delta} + \sqrt{\beta\gamma})$ gives the transformed probabilities

\[
\begin{pmatrix}
\sqrt{\alpha\delta} & \sqrt{\beta\gamma} \\
\sqrt{\beta\gamma} & \sqrt{\alpha\delta}
\end{pmatrix}
\]  

(24)

This builds on the result by Edwards (1962) that the odds-ratio and only functions of this canonical parameter vary independently of moment parameters, here of the marginal frequencies. The transformation may equivalently be obtained in terms of log-linear parameters: $(\lambda_0, \lambda_1, \lambda_2, \lambda_{12}) \rightarrow (\lambda_0^*, 0, 0, \lambda_{12})$, where one recalls that for $-1, 1$ coding $\lambda_{12} = \frac{1}{4} \log(\alpha\delta)/(\beta\gamma)$.

The asymptotic variance, $\text{avar}$, of $\hat{\lambda}_{12}$ is best found with a Poisson-based formulation of the unconstrained maximum likelihood equations. One uses that for an estimate $\Sigma_k c_k^2 log(n_k/n)$ from $n$ observations with cell frequencies $n_k$, the asymptotic variance, derived with the delta method as $\Sigma_k c_k^2 / E(n_k)$; see Bishop, Fienberg and Holland (1975, p. 495). It turns out to be:

\[
n \text{avar}(\hat{\lambda}_{12}) = 4 + 4[\cosh(2\lambda_{12}) \{\cosh(2\lambda_1) + \cosh(2\lambda_2)\} + \cosh(2\lambda_1) \cosh(2\lambda_2)].
\]  

(25)

By setting $\lambda_1 = \lambda_2 = 0$ in (25), the palindromic case is obtained, where the correlation coefficient $\rho_{12}$ is a 1-1 function of $\lambda_{12}$. In the symmetric case, the variance is 16 under independence and typically not much larger, otherwise, while it can increase considerably for skewed margins. If a hollow-tree structure is well-fitting to a table which preserves all observed marginal odds-ratios, it might therefore happen that an edge is no longer significant for the original data. But, by removing any edge of a hollow tree the resulting structure is still a hollow tree.

We apply the transformation of equation (24) to all $2 \times 2$ tables and use the additional knowledge that for any hollow-tree Ising model, the two-way tables of edges present in the
graph, form the set of minimal sufficient statistics. But for any given set of data, one needs to check first whether it is close to an Ising model without any independence constraints. For this, all higher than 2-factor log-linear interactions have to be so small that they can be ignored.

With the transformed two-way tables, a palindromic Ising model without any independence constraints results with any iterative proportional fitting procedure. Next, one exploits the computationally attractive features of this distribution to find a possibly well-fitting hollow-tree structure. Given the selected subset of edges present, the set of minimal sufficient statistics for a hollow-tree structure in the original data is the same subset of the observed $2 \times 2$ tables.

It cannot be extended to more than two variables to symmetrise an observed table as above, such that the resulting palindromic Ising model preserves the marginal odds-ratios, or by setting to zero the main effects in a multivariate regression for categorical responses, due to Glonek (1986). One could use instead a multivariate logistic parametrization; see Glonek and McCullagh (1985), Bergsma and Rudas (2002), Marchetti and Wermuth (2017), but this would lead to considerably more demanding computations.

### 3.6 Model selection for Ising models with hollow tree-structure

As is known, for general Ising models, the set of minimal sufficient statistics consists of observed two-way tables for all edges present in the graph; see Birch (1963, equations (3.5) to (3.6)), while for palindromic Ising models, it contains the corresponding symmetrised two-way tables. The latter are averages of the observed counts for $p(\omega)$ and $p(-\omega)$; see Marchetti and Wermuth (2016, equation 4.6) or they are a subset of the two-way tables preserving the marginal odds-ratios of an observed general Ising model.

The mle-computation for a general, unconstrained trivariate Ising model requires already an iterative procedure. Therefore, computational complexity will increase for Ising models of bulged-tree structure with many triangles as prime graphs. By contrast, mle-fitting of a palindromic Ising model is in this class in closed form, provided only one uses a proper single-node elimination scheme; see Corollary [1].

In a palindromic Ising model with a fattened-tree structure, one gets with equations (22) and (8), the likelihood-ratio statistic for $a \perp \perp b | N \setminus \{a \cup b\}$ reduced to one for $a \perp \perp b|c$:

$$\chi^2 = 2(\log n_{a,b,c} - \log n_{a,c} - \log n_{b,c} + \log n_{c})$$

(26)

see the discussion of hypothesis $H_{d3}$ by Birch (1963). Thus, this type of goodness-of-fit test, a ‘test between prime graphs’, can be carried out in smaller tables and without computing the mle. This is an attractive property in general, but it is especially important for very large data sets, where it avoids working with extremely sparse tables.

Equation (26) becomes even more useful for Ising models with a hollow-tree structure.

**Proposition 6.** For an Ising model with hollow-tree structure, goodness-of fit tests are of two types: for conditional independences between and within prime graphs.

The ‘tests between prime graphs’ reduce for instance to closed-form tests between two covering, completed prime graphs, attached to each other at an edge or a single node. A ‘test within prime graphs’ is for a saturated Ising model in a triangle or for the fit of a chordless $h$-cycle for $h > 3$. Such smaller tables make estimation and testing much more reliable; see Altham (1984).

For data which are close to a palindromic Ising model, any standard iterative method estimates the 2-factor log-linear interactions even though it is a so-called non-hierarchical model. The mle of the probabilities relates to the mles of the log-linear interactions and the linear interactions via the same relation in equation (1), that hold for the parameters. This is an extremely attractive property of maximum-likelihood estimates.
There are further options when a hollow-tree structure is given as a hypothesis. Then, the estimates between and within prime graphs can be obtained with linear regressions on at most two regressors. One may alternatively first get the mle of $\Sigma^{-1}$ with any Gaussian estimation routine; see Speed and Kiiveri (1986), Sadeghi and Marchetti (2012), Lauritzen, Uhler and Zwiernik (2017). Given the selected subset of variable pairs which generate a joint Gaussian distribution with hollow-tree structure, one can estimates the same structure for Ising models by using the corresponding subset of two-way tables.

However, for sample sizes larger than the number of variables, the latter is not an option. In these cases, one might first try to learn a concentration graph structure as for Gaussian distributions but using the marginal correlations in all two-way tables, transformed to symmetry by preserving the observed odds-ratios as described in the previous section.

One robust search technique is due to Castelo and Roverato (2006) which assumes however that all independences of the graph and only these hold in the generated distribution. If the resulting graph is a hollow tree, then the block-triangular factorisation of the concentration matrix can again be exploited to estimate probabilities in the palindromic Ising model and in a starting general Ising model; see also the data example in the next section. For very large data sets this is especially important since it reduces the fitting to small subgraphs.

4 An Ising model with a hollow-tree, for symmetric and for skewed margins

We use data from a larger prospective study in Germany, designed to develop strategies for counselling prospective students; see Weck (1991). We apply first a standard graphical check, due to Cox and Wermuth (1994b), to reassure us that the data are close to an Ising model.

![Expected normal order statistics](image)

**Figure 8:** *left: achievement data; right: strong 3-factor interactions in the first table above*

The left plot of Figure 8 is for this set of data having six binary variables. The approximate $t$-values for linear 3-factor interactions lie well within the range of $(-2, 2)$, hence do not indicate any strong 3-factor interaction and we proceed with an analysis. By contrast, the corresponding plot for the counts given in the first table of this paper indicate strong interactions. There, the plot shows strong ones to be within subset $(1,2,3)$ and the weaker ones within $(1,2,4)$.

The five variables are the average grade reached in years 11 to 13 at high school in median-dichotomized form ($A_1$, level 1 means achievement above median: 50%). Further variables are $A_2$: poor integration into high-school classes (yes: 10.3%), $A_3$: high-school class repeated (yes: 34.2%), $A_4$: change of primary school (yes: 20.1%) and $A_5$: education of father (at least ‘Abitur’, i.e. high-school completed: 42.7%). Variables $A_2$ to $A_5$ are potential regressors for $A_1$. By the time-order, variables $A_4, A_5$ are further in the past than $A_2, A_3$. The observed
counts are in the next table.

\[
\begin{pmatrix}
  n_{ijklm} \text{ with } m = 0 : & 275 & 419 & 30 & 22 & 238 & 99 & 37 & 13 & 46 & 67 & 12 & 3 & 49 & 21 & 7 & 2 \\
  n_{ijklm} \text{ with } m = 1 : & 161 & 292 & 19 & 29 & 142 & 56 & 29 & 7 & 49 & 102 & 4 & 9 & 59 & 23 & 12 & 6
\end{pmatrix}
\]

After applying equation (24) to all two-way tables, an iterative proportional fitting algorithm gives probabilities of a saturated palindromic Ising model. For the above data, the following matrices contain \( \hat{\rho}_{ij} \) in the lower and \( \hat{\rho}_{ij,klm} \) in the upper-triangular part; on the left without, on the right with independence constraints.

\[
\begin{pmatrix}
  1 & -0.098 & -0.318 & 0.007 & 0.044 \\
  -0.138 & 1 & 0.108 & 0.029 & 0.058 \\
  -0.333 & 0.148 & 1 & 0.050 & -0.016 \\
  -0.007 & 0.045 & 0.052 & 1 & 0.166 \\
  0.042 & 0.056 & -0.015 & 0.167 & 1
\end{pmatrix}
\]

\[
\begin{pmatrix}
  1 & -0.096 & -0.319 & 0 & 0 \\
  -0.138 & 1 & 0.108 & 0 & 0.054 \\
  -0.333 & 0.148 & 1 & 0.047 & 0 \\
  -0.018 & 0.017 & 0.052 & 1 & 0.167 \\
  -0.010 & 0.056 & 0.017 & 0.167 & 1
\end{pmatrix}
\]

All partial correlations which are smaller than \(|0.045|\) in the left table have been set to zero in the right table: these are for pairs \((1,4), (1,5), (2,4), (3,5)\). The induced marginal correlations for these pairs differ from the unconstrained marginal correlations, while for all other pairs, the marginal correlations in the saturated model on the left match the marginal correlations on the right. This coincides with the defining property of a concentration graph model for Gaussian distributions; see Dempster (1972).

Figure 9 shows the well-fitting hollow tree on the left, an equivalent oriented version on the right. This hollow-tree structure fits also the original data where the set of minimal sufficient statistics are the observed two-way tables of the edges present in the graph. A split of the test into two parts, fitting first an Ising model without independence constraints gives a likelihood-ratio statistic of \(\chi^2 = 17.65\) on 16 degrees of freedom (df) and second, the additional independences contribute \(\chi^2 = 5.78\) on 4 df.

\[
\begin{pmatrix}
  1 & 2 & 3 & 4 & 5 \\
  1 & 1 & 1 & 1 & 1 \\
  2 & 2 & 2 & 2 & 2 \\
  3 & 3 & 3 & 3 & 3 \\
  4 & 4 & 4 & 4 & 4 \\
  5 & 5 & 5 & 5 & 5
\end{pmatrix}
\]

The same conclusion of a good fit can be reached by testing the `hypothesis between prime graphs’, here \(1 \perp \perp \{4,5\}\{\{2,3\}\), using equation (26) on the observed table and the two hypotheses within prime graphs in the smaller tables of variables \(1,2,3,4,5\). These give, respectively, \(\chi^2 = 16.75\) on 12 df, \(\chi^2 = 1.16\) on 1 df and \(\chi^2 = 5.52\) on 7 df. Of course, these types of decomposition become especially useful only in very large tables.

The next table shows of the fitted log-linear terms, all that are nonzero for the general Ising model. For the latter it also gives corresponding t-statistics.

| Int. type   | \(\emptyset\) | 1    | 2    | 3    | 4    | 5    | 12   | 13   | 23   | 25   | 34   | 45   |
|-------------|---------------|------|------|------|------|------|------|------|------|------|------|------|
| pal. Ising  | 4.204         | 0    | 0    | 0    | 0    | 0    | -0.102| -0.335| 0.116| 0.055| 0.051| 0.169|
| gen. Ising  | 3.458         | 0.198| 1.064| 0.245| 0.666| 0.003| -0.104| -0.342| 0.116| 0.056| 0.051| 0.169|
| t-statistics| -5.27 , 29.88 | 6.16 | 24.80| 0.00 | -2.81| -14.45| 3.20 | 2.34 | 1.92 | 7.09 |

The log-linear 2-factor terms agree closely but not fully for the palindromic and the general Ising model. To interpret the generally weak dependences, we use some of the time order.

High achievement is less likely when a high-school class had been repeated and when a student integrated poorly into high-school classes. To repeat a high-school class is more likely with such poor integration and with a previous change of primary school. The risk for poor integration increases in the case of better educated fathers and with repeating classes. Finally, the risk to change primary school is higher for better educated fathers.
5 Discussion

We have studied Ising models, which have simple, undirected and connected probabilistic graphs for a finite set of nodes. Each edge missing in these graphs represents a pairwise independence given all remaining variables and we let, in addition, each edge present indicate a corresponding pairwise dependence. Then, the removal of any edge from a given graph leads to a different model since an additional independence constraint is introduced.

Ising models form the subclass of lattice models, also called quadratic exponential distributions, that is defined for binary variables having levels $-1, 1$. For unconstrained marginal distributions of the binary variables, we speak of general Ising models and when all margins are symmetric of palindromic Ising models. The latter mimic a central symmetry property of joint Gaussian distributions and have the same probability for level combinations $\omega$ and $-\omega$.

In palindromic Ising models – as in mean-centered Gaussian distributions – there is only one parameter associated with an edge present in the graph. In general, this parameter is a log-linear interaction, not based on covariances. But, we have identified a subclass of graphs, named hollow trees, in which palindromic Ising models are generated over oriented graphs such that all main-effect logit regressions can be be replaced by linear main-effect regressions.

To characterize hollow trees, we used early graph theoretical results on the existence of unique sets of prime graphs, their smallest complete separators, called cut-sets, and corresponding node-set elimination schemes, as well as Markov-equivalence conditions for different types of chain graphs. The only types of prime graphs of a hollow tree are chordless cycles, triangles or edges and its cut-sets contain one or two nodes. To recognize the tree-like structure, one replaces nodes by prime graphs and edges by cut sets, then a ‘single path’ connects each pair of ‘nodes’.

General Ising models with hollow-tree structure contain as subclasses, for instance, Markov chains and tree-structures used in phylogenetics, connected star graphs which can represent subscales in item response studies and non-decomposable models with chordless-cycle structures. Due to their computational complexity in mle-fitting, the last have not been used intensively in the past even though they may capture important spatial research questions.

This may start to change now when the attractive computational properties of palindromic Ising models with hollow-tree structure are exploited for any set of data close to a general Ising model by applying a one-time transformations to a saturated palindromic Ising model which preserves all observed marginal odds-ratios. It may be necessary to check beforehand whether the data belong to a connected graph, when one wants to study single trees to understand a forest’s build-up; for a history of such network-flow algorithms see Dinitz (2006).

Once a well-fitting hollow-tree structure has been obtained for a palindromic Ising model, one knows the subset of symmetric two-way marginal tables which generates this joint distribution. One can then take the same subset of the observed two-way tables – with possibly strongly skewed margins – to estimate the probabilities of a general Ising with the selected hollow-tree structure. The factorisation of the joint distribution with hollow-tree structure into subsets corresponding to its prime graphs, will permit one to compare results for small subsets of the variables with the available knowledge in the field about these variables under study. This is always an essential step towards progress in substantive research, but especially so when data for large numbers of variables are to be analyzed.

Appendix A: Dependences induced by marginalising

Equivalent to the log-linear formulation of the palindromic Ising model in equation (10) is

$$
\Pr(\omega) = \text{const.}\prod_{s<t}(1 + \tau_{st}\omega_s\omega_t), \quad 1/\text{const.} = 2^d(1 + \prod_{s<t}\tau_{st}), \quad -1 < \tau_{st} < 1, \quad (27)
$$
where $\tau_{st} = \tanh(\lambda_{st})$ are the hypetan interactions.

Proof. The logarithm of equation (27) yields the sum $\sum_{s<t} \log(1 + \tau_{st}\omega_s\omega_t)$ where each summand can be expanded as

$$\log(1 + \tau_{st}\omega_s\omega_t) = \tau_{st}\omega_s\omega_t - (\tau_{st}\omega_s\omega_t^2)/2 + (\tau_{st}\omega_s\omega_t^3)/3 - \cdots$$

and by noting that $\omega^s = 1$ if $s$ is even and $\omega^s = \omega_s$ if $s$ is odd, this gives the explicit form

$$\log(1 + \tau_{st}\omega_s\omega_t) = \omega_s\omega_t \tanh^{-1}(\tau_{st}) + \log(1 - \tau_{st})/2 = \text{const.} + \omega_s\omega_t\lambda_{st},$$

so that finally $\log \Pr(\omega) = \text{const.} + \sum_{s<t} \omega_s\omega_t\lambda_{st}$.

We use equation (27) to derive several effects of marginalising in the following cycles:

To obtain $\pi_{+jk}$ and $\rho_{23} = \tau_{23\setminus 1}$, one best uses equation (27) in the form:

$$\pi_{ij} = \text{const.} (1 + \tau_{12}ij)(1 + \tau_{13}ik)(1 + \tau_{23}jk), \ 1/\text{const.} = 2^3(1 + \tau_{12}\tau_{13}\tau_{23}), \ (28)$$

to get the result via

$$\sum_i (1 + \tau_{12}ij)(1 + \tau_{13}ik) = \sum_i 1 + \tau_{12}j\sum_i 1 + \tau_{13}k\sum_i i + \tau_{12}\tau_{13}j\sum_i i^2 = 2(1 + \tau_{12}\tau_{13}jk),$$

$$\pi_{+jk} = \frac{1}{2}(1 + \rho_{23}jk), \ \rho_{23} = \tau_{23\setminus 1} = (\tau_{23} + \tau_{12}\tau_{13})/(1 + \tau_{12}\tau_{13}\tau_{23}). \ (29)$$

Similarly, when starting with the chordless 4-cycle, one uses best equation (27) in the form:

$$\pi_{ijk\ell} = \text{const.} (1 + \tau_{13}ik)(1 + \tau_{23}jk)(1 + \tau_{24}\ell\ell)(1 + \tau_{14}\ell\ell), \ 1/\text{const.} = 2^4(1 + \tau_{13}\tau_{14}\tau_{23}\tau_{24}),$$

where the $\tau$s are now functions of the conditional odds-ratios given two further variables.

To obtain $\pi_{+jk\ell}$, one argues in the same way as going from equation (28) to (29):

$$\pi_{+jk\ell} = \text{const.} (1 + \tau_{23}jk)(1 + \tau_{24}\ell\ell)(1 + \tau_{13}\tau_{14}\ell\ell), \ 1/\text{const.} = 2^5(1 + \tau_{13}\tau_{14}\tau_{23}\tau_{24}). \ (30)$$

This shows (1) that the constant is just changed by a factor of two, (2) that the form of the distribution remains unchanged and (3) that by marginalising over 1, one gets $\tau_{23\setminus 1} = \tau_{13}\tau_{14}$.

By marginalising in the trivariate distribution of equation (30) further over node 2, equation (18) results so that the two dependence-inducing paths are traced with hypetan interactions.

One may also trace the contribution of the $\tau$s for the marginal correlation of an edge present in the graph and obtains a similar effect as in equation (29). For instance,

$$\rho_{23} = \tau_{23\setminus 14} = \text{const.} (\tau_{23} + \tau_{24}\tau_{14}\tau_{13}), \ 1/\text{const.} = (1 + \tau_{13}\tau_{14}\tau_{23}\tau_{24}). \ (31)$$

These results extend directly to chordless cycles in more than four nodes which then prove (1) that the marginal distributions of a chordless-cycle stays a cycle up to any trivariate marginal distribution and for the marginal hypetan interaction induced in a bivariate distribution (2) that it results by tracing two paths if the edge is missing in the starting cycle and (3) that it coincides with the simple correlation if the edge is present.

With an added independence for pair (2,3), the discussed two cycles turn into 2-edge and 3-edge chains having $\tau$-parameters to each edge present in the graph which coincide with simple correlations. Equations (29), (31) replicate then, respectively, the well-known result that the induced dependence for the endpoints in a linear Markov chain is the product of the simple correlations along the chain: $\tau_{23\setminus 1} = \rho_{12}\rho_{13}$ and $\tau_{23\setminus 14} = \rho_{24}\rho_{14}\rho_{13}$.
Appendix B: Effects of conditioning

In addition, when going to equations (29), (31), one gets \( \pi_{i|jk} = \pi_{ijk} / \pi_{+jk} \) and \( \pi_{i|jk\ell} \) as:

\[
\pi_{i|jk} = \frac{1}{2}(1 + \tau_{12}ij)(1 + \tau_{13}ik)/(1 + \tau_{12}\tau_{13}jk), \quad \pi_{ij|k\ell} = \frac{1}{2}(1 + \tau_{13}ik)(1 + \tau_{14}i\ell)/(1 + \tau_{13}\tau_{14}k\ell).
\]

These have essentially the same form, stressing the similarity between the two types of cycles, the triangle and the chordless 4-cycle.

A standard factorisation of \( \pi_{ijk} \) and Cochran’s recursive relation for linear regression coefficients give a linear parametrization of the joint probabilities as

\[
\pi_{ijk} = \frac{1}{8}(1 + \rho_{12}ij + \rho_{13}ik + \rho_{23}jk), \quad \pi_{ij|k} = \frac{1}{2}(1 + \beta_{12}ij + \beta_{13}ik), \quad \pi_{ik|j} = \frac{1}{2}(1 + \rho_{23}jk).
\]

The expression for \( \pi_{ijk} \) in terms of \( \tau \)'s simplifies, using \( j^2k^2 = 1 \), by expanding the fraction with \( (1 - \tau_{12}\tau_{13}jk) \), to give:

\[
\pi_{i|jk} = \frac{1}{2}(1 + \tau_{12}ij + \tau_{13}ik + \tau_{12}\tau_{13}jk)(1 - \tau_{12}\tau_{13}jk)/(1 - \tau_{12}^2\tau_{13}^2)
\]

\[= \frac{1}{2}[1 + \{\tau_{13}(1 - \tau_{12}^2)/\text{const.}\}ik, \text{const.} = 1 - \tau_{12}^2\tau_{13}^2],
\]

so that equation (8) expresses the linear regression coefficients in terms of \( \tau \)s.

By similar arguments, one finds for the above chordless 4-cycle directly, for instance,

\[
\beta_{12} = 0, \quad \beta_{13} = \tau_{13}(1 - \tau_{14}^2)/(1 - \tau_{13}^2\tau_{14}^2)
\]

and for the joint conditional distribution of \( A_1, A_3 \) given \( A_4 \), one gets

\[
\text{cov}(A_1, A_3|A_4 = \ell) = \rho_{13} - \rho_{14}\rho_{34} \text{ since } E(A_1A_3|A_4 = \ell) = \rho_{13}, \quad E(A_i|A_4 = \ell) = \rho_{i4}\ell.
\]

Furthermore, since also \( \text{var}(A_i|A_4 = \ell) = 1 - \rho_{i4}^2 \) does not vary with \( \ell \) for \( i = 1, 3 \), the conditional correlations are constant at all combinations of \( k, \ell \) and Theorem 2 applies.

Appendix C: Proof of Theorem 3

**Theorem 3:** A quadratic exponential distribution for symmetric binary variables is generated over an edge-minimal hollow tree if and only if (1) the Markov structure of its concentration graph is defined by the set of zeros in its overall partial correlation matrix and (2) within each of its prime graphs, all conditional correlations agree with the partial correlations.

**Proof.** Assume first that an Ising model is palindromic and its edge-minimal graph is a hollow tree. Then, the joint distribution factorises according to its prime graphs and cut-sets, given any one of the proper node-set elimination schemes; see Theorem 1, Proposition 1 and equation (22). By definition, the prime graphs of a hollow tree are edges or cycles. Cycles are either triangles or chordless cycles and cut-sets contain at most two nodes.

In the marginal distribution within each prime graph, all conditional correlations coincide with the partial correlations; see Theorem 2, Proposition 3, and equation (20). In particular, independences are captured by zero log-linear 2-factor interactions and by zero partial correlations. The factorisation of the joint density implies, together with the independence constraints and the traceability of linear relations, that a zero overall partial correlation equals the zero partial correlation within a prime graph.

If nodes \( i, j \) belong to distinct prime graphs of a hollow tree, the smallest separating set, say \( S \), such that \( X_i \perp \perp X_j \mid X_S \) holds, is a cut-set of the graph. Then, the traceability implies for the conditional correlations, \( 0 = \rho_{ij|N \setminus \{ij\}} = \rho_{ij|S} \). As \( S \) contains at most two nodes, a conditional correlation equals also the partial correlation, hence also \( 0 = \rho_{ij|N \setminus \{ij\}} = \rho_{ij|S} \).
For the converse, note first that a graph without hollow-tree structure has either (i) a prime graph which is different from an edge and from a cycle or (ii) it has a cut-set containing more than two nodes. In case (i), there is a prime graph $P$ in which at least one node, say $i$, has more than two neighbours, since each node has exactly two neighbours only in a cycle. By definition, no cut set and hence no outer node exists if this prime graph $P$ is incomplete. Then, there is also no proper node-set elimination scheme by which the distribution of the variables of $P$ could be generated via a factorisation by which the logit main-effect regression with more than two regressors, could be avoided. Hence, by Theorem 2 and Proposition 3, conditional and partial correlations involving variable $X_i$ do not agree within $P$.

In case (ii), there are at least two prime graphs. Let $i$ and $j$ be nodes residing in different prime graphs and having cut-set $C$ containing more than two nodes. Then for the subset $\{i, j, C\}$ of the variables, there is a factorisation as $f_{i,j,C} = f_{i|C}f_{j|C}$. But by Proposition 3, the main-effect logit regression of $X_i$ on $X_C$ is then not equivalent to a main-effect linear regression of $X_i$ on $X_C$ with the consequence that $\rho_{i,j,C} \neq 0$ even though $\rho_{i|j|C} = 0$.

$\Box$

Appendix D: On traceability

A distribution is traceable if (i) its graph is edge-minimal, (ii) its independences combine downwards and upwards and (iii) it is dependence-inducing; Wermuth (2012).

To (i): for an edge-minimal concentration graph, every $ij$-edge present in the graph means $A_i, A_j$ are dependent given all remaining variables since equation (3) is satisfied.

To (ii): Combining independences for sets $a, b, c, d$ partitioning $N' \subseteq N \setminus (a \cup b \cup c \cup d)$ applies to equivalences of $a \perp \perp bd|c$. For palindromic Ising models with hollow-tree graphs:

$$(a \perp \perp b|dc \mbox{ and } a \perp \perp d|c) \iff (a \perp \perp b|dc \mbox{ and } a \perp \perp d|bc) \iff (a \perp \perp b|c \mbox{ and } a \perp \perp d|c).$$

The implications of $a \perp \perp bd|c$ hold for all probability distributions, as well as the converse of the first decomposition, since $f_{a|b|d|c} = f_{a|d|c}$ together $f_{a|d|c} = f_{a|c}$ implies the simplified factorisation $f_{a|b|d|c} = f_{a|c}$. The second and third equivalence are not satisfied in general. The downward and upward combinations result here with the recursive relation for concentrations and for covariances, respectively; see also Theorem 4 above.

To (iii). A concentration graph model has been said to be association- or dependence-inducing if for each $V$ in the graph with outer nodes $i, j$, common neighbour $k$ and $i \perp \perp j|\{k, c\}$ given for some $c \subseteq N \setminus \{i, j, k\}$, the independence changes to $i \perp \perp j|c$ by marginalising over the inner node $k$. From Theorem 3 and the discussion of equation (23), the recursive relation among concentrations applies also to palindromic Ising models with hollow-tree structure. The vanishing of $\rho_{ij,N\setminus c}$ indicates conditional independence for all $c$, which – based on a proper node-set elimination scheme – do not introduce a dependence in the corresponding marginal distribution; see Proposition 2 and App. D.

Properties (i) and (iii) have been attributed to Gaussian distributions by Lněnìčka and Matúš (2007). In some literature, distributions with properties (i) have been named compositional graphoids and those with property (iii) singleton-transitive: see for instance Sadeghi and Wermuth (2016). The dependence-inducing property (iii) applies to marginalising over single nodes but not to sets of variables; see the data to Figure 9.

Appendix E: On partial inversion and partial closure

Partial inversion generalises the Beaton sweep operator, Dempster (1972, App.) to non-symmetric matrices. Let $N = \{1, \ldots, d\}$ denote the rows and columns of a real-valued matrix $M$ having invertible leading principal submatrices. For $a \subset N$ and $b = N \setminus a$, one may obtain $M^{-1}$ with two partial inversion steps: $M^{-1} = \text{inv}_b(\text{inv}_a M)$.
The partial inversion operator is, with $a = \{1\}$:

$$M = \begin{pmatrix} s & v^T \\ w & m \end{pmatrix} \quad \text{inv}_{\{1\}} M = \begin{pmatrix} 1/s & -v^T/s \\ w/s & m - w v^T/s \end{pmatrix}. \quad (32)$$

For $t > 1$ elements in $a$, $\text{inv}_a M$ applies this same operation $t$ times, using permutations.

**Proposition 7.** Wermuth, Wiedenbeck and Cox (2006). The partial inversion operator is commutative, can be undone and is exchangeable with taking submatrices.

The first property shows for instance that $\text{inv}_b(\text{inv}_a M) = \text{inv}_a(\text{inv}_b M)$, the second that $\text{inv}_a M^{-1} = \text{inv}_b M$ and with the last, one derives equation (15) with $N' \subset N$. 

**Partial closure** is the analogue of the partial inversion operator defined for edge matrices $\mathcal{M}$. The operator derives the structural zeros after partial inversion on Gaussian parameter matrices, that is it takes independences into account but not any special parametric constellations. Let $N = \{1, \ldots, d\}$ denote the rows and columns of an edge matrix $\mathcal{M}$, zeros capture missing edges and ones edges of one type, such as full lines of a concentration graph in a unit symmetric matrix or arrows of a directed acyclic graph in a unit upper-triangular matrix. For $a \subset N$ and $b = N \setminus a$, one obtains e.g. the transitive closure of a directed acyclic graph with two partial closure steps: $\mathcal{M}^- = \text{zer}_b(\text{zer}_a \mathcal{M})$.

The partial closure operator is, with $a = \{1\}$ and ‘In’ denoting the indicator function:

$$\mathcal{M} = \begin{pmatrix} 1 & v^T \\ w & m \end{pmatrix} \quad \text{zer}_{\{1\}} \mathcal{M} = \begin{pmatrix} 1 & v^T \\ w & \text{In}[m + w v^T] \end{pmatrix}. \quad (33)$$

For $t > 1$ elements in $a$, $\text{zer}_a \mathcal{M}$ applies this same operation $t$ times, using permutations.

**Proposition 8.** Wermuth, Wiedenbeck and Cox (2006). The partial closure operator is commutative, cannot be undone and is exchangeable with taking submatrices.

The operator can be interpreted as tracing paths in the graph if the graph is edge-minimal. The exchangeability justifies, for instance, repeated closure of Vs in subgraphs. Matrix versions of both operators have been explicitly exploited, for instance, by Marchetti and Wermuth (2009, App.) and Wermuth (2011, 2012, 2015).

**Appendix F: On Markov equivalence**

Starting from any prime graph or a cut-set, a hollow tree may be oriented – based on a proper node-set elimination scheme – so that no sink $V$, that is no $\circ \rightarrow \circ \leftarrow \circ$, and no sink $U$ is generated, that is no $\circ \rightarrow \circ \leftarrow \circ \circ \rightarrow \circ \leftarrow \circ$. This avoids that any constraint $i \perp \perp j|N \setminus \{i, j\}$ gets the quite different meaning $i \perp \perp j$ and applies the following more general result where these $V$- and $U$-constellations have been called ‘minimal complexes’.

**Theorem 4.** Frydenberg (1990). Two LWF chain graphs, with identical sets of edges present, are Markov equivalent if and only if they have the same minimal complexes.

Similarly, there is a necessary and sufficient condition for the Markov equivalence of other types of chain graph. Chain graph models with so-called regression graphs have sequences of joint responses and one last component which is a concentration graph, hence has $i \rightarrow j$. Each component $i$ of a joint response may depend only on nodes $j$ in its past, drawn as $i \leftarrow j$, and the components within a given joint response may be dependent given their past, drawn as $i \leftrightarrow j$; for these models see also Wermuth (2015).
There are three types of $V$s which generalise the sink $V$ in a directed acyclic graph and are called collision $V$s: $i \rightarrow o \rightarrow j$, $i \leftarrow o \leftarrow j$, and $i \leftarrow o \rightarrow j$. In larger graphs, each of them states a conditional independence of the uncoupled nodes excluding the inner node. All other $V$s have been named transmitting $V$s since the are equivalent to $i \leftarrow o \leftarrow j$. All transmitting $V$s, including $i \leftarrow o \rightarrow j$, state conditional independence of the uncoupled nodes given the inner node and possibly other nodes conditioned upon.

**Theorem 5.** Wermuth and Sadeghi (2012). *Two regression graphs, with identical sets of edges present, are Markov equivalent if and only if their sets with collision $V$s coincide.*

Thus, an undirected graph is Markov-equivalent to another regression graph, if and only if the latter has no collision $V$. This holds by construction for every fattened tree. A distribution with a chordal fattened-tree structure is a covering model for the one with the hollow graph so that the independence structure of the former also holds for the latter.

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