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Restricted Graphical Log-linear Models

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Abstract

We introduce a new type of graphical log-linear model called restricted graphical log-linear model. This model is obtained by imposing equality restrictions on subsets of main effects and of first-order interactions. These restrictions are obtained through partitions of the variable and first-order interaction sets. The vertices or variables in the same class have the same main effects in all their categories, and the first-order interactions in the same class are equal. We study its properties and derive its associated likelihood equations and provide some applications. A graphical representation is possible through a coloured graph.

Keywords: graph colourings, graphical Gaussian models with symmetries, graphical log-linear models, iterative proportional fitting, log-linear models, symmetry and quasi-symmetry models.

1. Introduction

In this paper we introduce a new type of model for discrete variables called restricted or coloured graphical log-linear model (*RGLL model*), which combines symmetry with discrete graphical models. Symmetry is considered through specific parameter restrictions not used before, but inspired by those used in the continuous case. It can be seen as a tool to model symmetry and could help to get a better understanding of the data. In a specific model we may obtain improved knowledge about the distribution; for instance, conditional independences as in graphical models or the relationship between cells in a contingency table. RGLL can be fitted to different kinds of data such as panel data, where the variables have the same categories. The model may be useful for researchers of linear models, symmetry, and graphical models.

RGLL models are special cases of hierarchical log-linear models and can be represented graphically, including equality restrictions between certain parameters. Restrictions are imposed on two kind of parameters: the first ones correspond to main effects terms and the second ones to first-order interactions. For the former, restriction classes consist of variables; for the latter, the classes are defined by the parameters themselves. At the same time, marginal and

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conditional independences derived from a graph are considered. A graphical representation involves colouring the associated graph.

Symmetry and quasi-symmetry models for square contingency tables were introduced by Bowker (1948) and Caussinus (1965), respectively; and afterwards they were further studied by other authors; for instance, Agresti (2002, p. 423-431). For the same type of tables, Tahata, Yamamoto, Nagatani, and Tomizawa (2009) defined a measure and three types of symmetry through it and distinguished departures from usual symmetry assuming conditional symmetry, and Yamamoto, Iwashita, and Tomizawa (2007) studied alternative ways to decompose symmetry into models that include quasi-symmetry. More recently, Kateri, Mohammadi, and Sturmfels (2014) defined one model in the same two-dimensional case in which algebraic and graphical concepts are used, particular cases corresponding to quasi-symmetry and the Pearsonian quasi-symmetry model, the latter defined through a divergence measure. Lovison (2000) introduced generalized symmetry models (*GS models*), which are defined for any dimension when the same variable is observed several times and where some or even all interaction parameters of any order are invariant under any permutation of the associated index. The other parameters are free to vary and restrictions on the main effects as the ones derived from RGLL models are allowed. However, only GS models for the three-dimensional case are presented.

The relationship between graphical models and symmetry has not been studied as extensively in the discrete case. In the continuous case, Højsgaard and Lauritzen (2008) introduced Gaussian graphical models with symmetries; in one of them (*RCON model*), equalities are set among elements of the concentration matrix. In the discrete case, quasi-symmetric (*QS*) and symmetric and quasi-symmetric (*SQS*) graphical models were introduced by Gottard, Marchetti, and Agresti (2011) and Gottard (2009), respectively.

Symmetry and quasi-symmetry models for square contingency tables can be expressed as RGLL models with two variables. In this sense, RGLL models can be considered as a generalization of symmetry models. Any graphical log-linear model (e.g., Lauritzen 1996, ch. 4 and Edwards 2000, ch. 2) can be expressed as an RGLL model by considering that all parameters are unrestricted. Conditional symmetry (Andersen 1991, p. 328-329) is also a particular case of an RGLL model.

RGLL and RCON models are similar though they are defined for different data types. There is also a relationship between RGLL models and QS and SQS graphical models. Let $u_{XY}(ij)$ represent the first-order interaction between variables X and Y when they take the values i and j, respectively, and $u_X(i)$ a main effect. In SQS graphical models, the main effects restrictions are similar to those for RGLL models, and in SQS and QS models there are restrictions of the kind $u_{XY}(ij) = u_{RS}(ij)$ for all $i, j = 1, ..., L$ (considering L levels in each variable), for elements in the same class; including restrictions $u_{XY}(ij) = u_{XY}(ji)$ for all $i, j = 1, ..., L$, and $u_{RS}(ij) = u_{RS}(ji)$ for all $i, j = 1, ..., L$; and implying specific restrictions on the second-order interactions, i.e. on the parameters $u_{XYZ}(ijk)$. QS graphical models are similarly defined, but they allow even higher-order interactions. Unlike RGLL models, interactions of second or higher order are restricted. The first-order interaction restrictions in any SQS or QS graphical model are a particular case of the kind of restrictions defined for those terms in RGLL models. When these are the highest-order interactions, QS and SQS graphical models are RGLL models.

RGLL, SQS, and GS models are different and related as follows. In SQS models, restrictions of the kind $u_{XY}(ij) = u_{RS}(ij)$ are allowed besides invariance under permutation of the indexes, which are the only kind of restrictions allowed in GS models. However, in RGLL

models we allow any restriction on the indexes corresponding to first-order interactions, which do not necessarily have to be permutations or the kind of restriction given in SQS models, and higher-order interactions are not restricted. Hence, the three models are equivalent when (1) a model includes at most first order interactions, (2) the restrictions are of the kind $u_{XY}(ij) = u_{XY}(ji)$, and (3) there are no other first-order interaction restrictions.

Twins data. In order to motivate RGLL models, consider the data analyzed by Drton and Richardson (2008) (Table 1). The data consist of 597 observations for monozygotic twins indicating whether twin i ($i = 1, 2$) suffers from major depression (variable D_i, for $i = 1, 2$) or alcoholism (variable A_i, for $i = 1, 2$). The values associated with D_i and A_i correspond to 0 (*no*) and 1 (*yes*). Consider a model in which the parameters are obtained from the set

$$\mathbf{A} = \{\{A_1, A_2\}, \{A_1, D_1\}, \{A_2, D_2\}, \{D_1, D_2\}\}, \tag{1}$$

called the generating class. Hence, the expected frequency $m_{A_1A_2D_1D_2}(a_1, a_2, d_1, d_2)$ for a specific cell in the table (a_1, a_2, d_1, d_2) has the following log-linear expansion

$$\begin{aligned}\log m(a_1, a_2, d_1, d_2) =& u + u_{A_1}(a_1) + u_{A_2}(a_2) + u_{D_1}(d_1) + u_{D_2}(d_2) + \\ & u_{A_1A_2}(a_1a_2) + u_{A_1D_1}(a_1d_1) + u_{A_2D_2}(a_2d_2) + u_{D_1D_2}(d_1d_2).\end{aligned} \tag{2}$$

Let V be the set of variables or vertex set and E the set of first-order interactions. A model in which the values of variables A_1 and D_1 are permuted with those of variables A_2 and D_2, respectively, in such a way that the distribution is preserved corresponds to an RGLL model. It is the model with generating class $\mathbf{A}$ and graph G=(V, E) where V is partitioned into two sets $V = (V_1, V_2)$ and E= $(E_1, E_2, ..., E_{10})$. Here, $V_1 = \{A_1, A_2\}$ and $V_2 = \{D_1, D_2\}$; and E_1= $\{u_{A_1D_1}(00),\ u_{A_2D_2}(00)\}$, E_2= $\{u_{A_1D_1}(01),\ u_{A_2D_2}(01)\}$, E_3= $\{u_{A_1D_1}(10),\ u_{A_2D_2}(10)\}$, E_4= $\{u_{A_1D_1}(11),\ u_{A_2D_2}(11)\}$, E_5= $\{u_{A_1A_2}(01),\ u_{A_1A_2}(10)\}$, E_6= $\{u_{D_2D_1}(01),\ u_{D_2D_1}(10)\}$, E_7= $\{u_{A_1A_2}(00)\}$, E_8= $\{u_{A_1A_2}(11)\}$, E_9= $\{u_{D_2D_1}(00)\}$, and E_{10}= $\{u_{D_2D_1}(11)\}$. The partition in V means that the main effects for all the values taken by the variables in each set V_1 and V_2 are the same, whereas the partition in E means that the first-order interactions in each class are the same. The associated graph G is given in Figure 1, in which the partitions are represented by using colours; for instance, variables A_1 and A_2 have the same colour. Observe that one edge of the graph is associated with each first-order interaction. To avoid using too many colours, lines in black represent unrestricted first-order interactions.

The distribution is preserved after the permutation of the values of the variables because the expected frequency $m_{A_1A_2D_1D_2}(a_1, a_2, d_1, d_2)$, given the log-linear expansion in equation (2) and the equality restrictions given by the partitions, is equal to the expected frequency for the cell (a_2, a_1, d_2, d_1); thus $m_{A_1A_2D_1D_2}(a_1, a_2, d_1, d_2)$= $m_{A_1A_2D_1D_2}(a_2, a_1, d_2, d_1)$. The model also implies that A_1 and D_2 are conditionally independent given D_1 and A_2, $A_1 \perp D_2 | D_1, A_2$, and $A_2 \perp D_1 | A_1, D_2$.

The remainder of the paper is organized as follows. In Section **2** we formally define RGLL models. Section **3** is devoted to symmetry and quasi-symmetry models and their representation as RGLL models including an example. In Section **4** we derive the likelihood equations and consider model selection. Finally, in the Appendix we provide a method for getting a numerical solution.

Table 1: Alcohol dependence and major depression for 597 pairs of female twins. Left panel: Observed counts. Right panel: Fitted frequencies under an RGLL model.

		A_2				A_2			
		0		1		0		1	
		D_2				D_2			
A_1	D_1	0	1	0	1	0	1	0	1
0	0	288	80	15	9	285.29	84.87	12.60	11.24
	1	92	51	7	10	84.87	55.97	3.75	7.41
1	0	8	4	3	2	12.60	3.75	3.52	3.14
	1	8	9	4	7	11.24	7.41	3.14	6.21

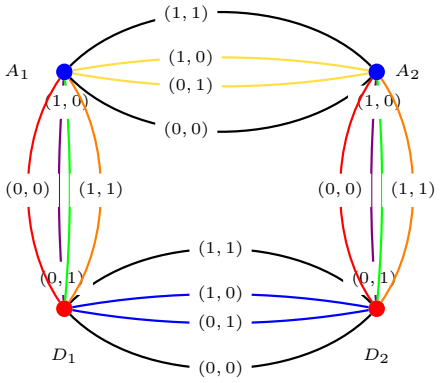


Figure 1: An RGLL model with generating class $\mathbf{A}$= $\{\{A_1, A_2\}, \{A_1, D_1\}, \{A_2, D_2\}, \{D_1, D_2\}\}$ associated with the twins data.

2. Preliminaries and definition

Consider V as a set of variable labels or a set of vertices. For each element δ in V we associate a discrete random variable I_δ, so that the set of random variables can be expressed as a vector $I = (I_\delta)_{\delta \in V}$. The values taken by those variables, known as levels or categories, are included in a set I_δ. Then all possible values that I takes are given by I, with $\mathrm{I} = \times_{\delta \in V} \mathrm{I}_\delta$. A cell i corresponds to one of these values, i.e. $i \in \mathrm{I}$. Seen as a q-way contingency table, a specific cell can be denoted as $i = (i_1, i_2, ..., i_q)$. A subvector of I is denoted as I_a, where $a \subseteq V$, and a value taken by it is denoted as i_a, where $i_a \in \mathrm{I}_a = \times_{\delta \in a} \mathrm{I}_\delta$.

We denote a parameter associated with a set a, $a \subseteq V$, which depends on the corresponding values i_a, as $u_a(i_a)$. When $a = \emptyset$ it corresponds to a constant term, when $|a| = 1$ to a main effect, and when $|a| > 1$ to an interaction. We also denote $m(i)$ as the expected frequency in a cell $i \in \mathrm{I}$, for instance in a two-way contingency table it is $m(i_1, i_2)$.

A saturated log-linear model can be written as

$$\log m(i) = \sum_{a \subseteq V} u_a(i_a). \tag{3}$$

By setting specific parameters $u_a(i_a)$, for all i_a, to zero in (3), different models are obtained. For example, a log-linear model is called hierarchical when the presence of an interaction $u_a(i_a)$ implies the presence of all those interactions $u_b(i_b)$ with $b \subset a$. The parameters included in this model depend on a generating class $\mathbf{A}$, which is a set of subsets of V. The model can be

written as

$$\log m(i) = \sum_{a \in K} u_a(i_a), \tag{4}$$

where K is the set of subsets of the elements in the generating class $\mathbf{A}$.

Definition 1. A hierarchical log-linear model,

$$\log m(i) = \sum_{a \in K} u_a(i_a),$$

is a *restricted graphical log-linear model (RGLL model)* with associated graph $G = (V, E)$ if it satisfies two properties: (a) its generating class is C, the cliques set in the associated graph, and (b) the set of variables V and the set of first-order interactions E are partitioned as follows: the set V is partitioned into $V_1, ..., V_T$, with $T \in \{1, 2, ..., |V|\}$, such that the main effects of the variables in the subset V_t, for t=1,..., T, are equal in all their levels in I^{V_t}, where I^{V_t} is the level set associated with $I_{V_t} = (I_\delta)_{\delta \in V_t}$, for t=1,..., T. The set E is partitioned into $E_1, ..., E_S$, with $S \in \{1, 2, ..., |E|\}$, such that the interactions in every subset E_s, for s=1,..., S, are equal.

RGLL models can be defined assuming that all variables have the same categories, i.e. the level set I_δ is the same for all $\delta \in V$ or I^{V_t} is the same for all V_t, for $t = 1, ..., T$. This implies that the number of categories is the same for any variable, i.e. $|\mathrm{I}_\delta| = L$, for all $\delta \in V$. The advantages of such a restriction are the following: (1) it allows for symmetry interpretations, and (2) it simplifies some of the computational programming. This condition could have been relaxed assuming that only those variables in the same vertex class V_t with $|V_t| > 1$ for every $t = 1, ..., T$ should have the same number of categories or even the same categories; however, interpretation of such models might not be straightforward. The interpretation of an RGLL model depends on the equality restrictions. Some RGLL models have a symmetry interpretation; for instance, in Section 1 this was discussed through an example.

Even though RGLL models could be represented through a graph, this representation might be too complex, for instance when there are six or more variables with three or more levels each one. However, a graphical representation is optional, in the sense that it helps to represent a model but does not define it. In fact, this also happens for any graphical model, so that concepts from graph theory are used, but a graphical representation is not necessary.

Consider an RGLL model with set of variables V and set of first-order interactions E. We define the associated diagram $G = (V, E^*)$ as a graph with vertex and edge set V and E^*, respectively. The set E^* is formed by elements $\{X_k, Y_k\}$, for k= 1,..., $|\mathrm{I}_X|\,|\mathrm{I}_Y|$, where $|\mathrm{I}_X|\,|\mathrm{I}_Y|$ corresponds to all combination of categories of X and Y, considering that $u_{XY}(ij) \in E$ for every (i, j), where $i \in \mathrm{I}_X$ and $j \in \mathrm{I}_Y$, for any $\{X, Y\} \in V$. By definition, there is a one-to-one correspondence between the sets E^* and E so that the graph (V, E) is the same as the graph (V, E^*). As a consequence, the first graph is also denoted as G. For example, if we define a model including two binary variables X and Y, so that $\mathrm{I}_X = \mathrm{I}_Y = \{1, 2\}$, and the associated first-order interactions $u_{XY}(ij)$; i, j =1, 2, then the set E contains the elements $u_{XY}(11)$, $u_{XY}(12)$, $u_{XY}(21)$, $u_{XY}(22)$. As a consequence, E^* contains the edges $\{X = 1, Y = 1\}$, $\{X = 1, Y = 2\}$, $\{X = 2, Y = 1\}$, and $\{X = 2, Y = 2\}$, which are multiple edges joining X with Y. The graph G= (V, E) is a multigraph, a graph with multiple edges without loops, which is determined by the first-order interactions. Clearly, there is a one-to-one correspondence between the first-order interactions and the edges, so that it is equivalent to partition

over the parameters or over the edges.

The representation of $G = (V, E)$ consists of circles representing the variables, two of which may be united with an edge when a first-order interaction including those variables is part of the model. There are multiple edges between vertices according to the possible combinations of values of the associated variables. We note that the underlying simple graph G^u associated with the graph G obtained from an RGLL model is the independence graph associated with a graphical log-linear model (e.g., Bondy and Murty 1976, p. 103).

Symbolically, X and Y are in the same vertex class if and only if $u_X(l) = u_Y(l)$, for all $l = 1, ..., L$, where u_X and u_Y are main effects and L is the number of categories for variables X and Y. Similarly, two first-order interactions or their corresponding edges, one joining variable X with variable Y at the values (i_1, j_1) and another joining variable Z with variable R at the values (k_1, l_1), are in the same class if and only if $u_{XY}(i_1 j_1) = u_{ZR}(k_1 l_1)$, where $X, Y, Z, R \in V$; with $i_1 \in \mathrm{I}_X$, $j_1 \in \mathrm{I}_Y$, $k_1 \in \mathrm{I}_Z$, and $l_1 \in \mathrm{I}_R$; and where $u_{XY}(i_1 j_1)$ and $u_{ZR}(k_1 l_1)$ are first-order interactions.

To represent an RGLL model, the graph G is coloured using a different colour for each class, as in Figure 1, i.e. using a vertex and edge colouring. Given any coloured multigraph, we can identify the parameter restrictions corresponding to the associated RGLL model. Then all restrictions in an RGLL model can be identified with a vertex and edge colouring.

We have the following observations concerning Definition 1:

a) In the graphical representation of RGLL models, there are multiple edges between variables, so that if there is a clique, it is not important which edges are used to obtain it. For instance, if there is a clique corresponding to a triangle and there are 4 multiples edges between each pair of edges on it, then there are 64 possible different cliques.

b) When $|V_t| = 1$ or $|E_s| = 1$ for some s or t, where $t = 1, ..., T$ and $s = 1, ..., S$, we have atomic classes; otherwise, they are composite. Atomic classes are those where the corresponding parameters are not restricted, and an RGLL model with only atomic classes is a graphical log-linear model.

c) Independences between variables can be read off from the graph by using separator sets as in graphical log-linear models.

d) Interactions of order higher than one are not restricted.

It is important to notice that we are not assuming any identification constraint on the parameters. As it is defined, any set of restrictions is possible even though they may generate redundant equations among the likelihood equations. However, there are specific RGLL models that do not generate such redundant equations, for instance when the parameter restriction do not change when the identification constraint is effect coding instead of using the parameters without such a constraint. This occurs, for example, when the restrictions on the model are of the form $u_{XY}(ij) = u_{ZR}(ij)$ or $u_{XY}(ij) = u_{ZR}(ji)$ or when the restrictions are imposed on the main effects.

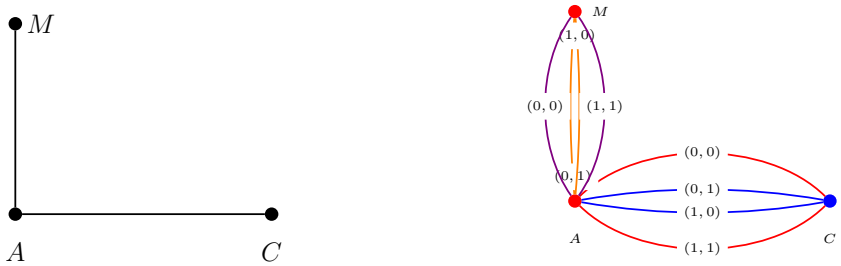
Example 1. Consider three binary variables A, C, and M with categories coded as 0 and 1 and the hierarchical log-linear model with generating class $\mathbf{A} = \{\{A, C\}, \{A, M\}\}$:

$$\log m(i, j, k) = u + u_A(i) + u_C(j) + u_M(k) + u_{AC}(ij) + u_{AM}(ik), \; i, j, k = 0, 1; \qquad (5)$$

and the equality restrictions

$$u_A(0) = u_M(0),\ u_A(1) = u_M(1),$$
$$u_{AM}(0,1) = u_{AM}(1,0),\ u_{AC}(0,1) = u_{AC}(1,0),$$
$$u_{AM}(0,0) = u_{AM}(1,1),\ u_{AC}(0,0) = u_{AC}(1,1).$$

Observe that model (5), without equality restrictions, is a graphical log-linear model with graph $G^u = (V^u, E^u)$, where $V^u = \{A, C, M\}$ and $E^u = \{\{A, C\}, \{A, M\}\}$, shown in Figure 2(a).



(a) Graphical model (b) RGLL model

Figure 2: Two hierarchical log-linear models for Example 1: (a) a graphical log-linear model; (b) an RGLL model.

According to the parameter restrictions, we see that the vertex set $V = \{A, C, M\}$ in the restricted model is partitioned as $V = (V_1, V_2)$, with $V_1 = \{A, M\}$ and $V_2 = \{C\}$. The set of first-order interactions or its corresponding edge set E is partioned as (E_1, E_2, E_3, E_4), where

$E = \{u_{AM}(00), u_{AM}(01), u_{AM}(10), u_{AM}(11), u_{AC}(00), u_{AC}(01), u_{AC}(10), u_{AC}(11)\}$, and $E_1 = \{u_{AM}(01), u_{AM}(10)\}$, $E_2 = \{u_{AC}(01), u_{AC}(10)\}$, $E_3 = \{u_{AM}(00), u_{AM}(11)\}$, and $E_4 = \{u_{AC}(00), u_{AC}(11)\}$.

We obtain the corresponding graph $G = (V, E)$ shown in Figure 2(b) whose underlying simple graph $G^u = (V^u, E^u)$ is shown in Figure 2(a). Using any of these graphs, we see that the generating class corresponds to the cliques set, which together with the restrictions on the parameters of the model define an RGLL model.

The following section shows symmetry and quasisymmetry as instances of RGLL models.

3. Symmetry and quasi-symmetry models as RGLL models

Symmetry and quasi-symmetry models were introduced to analyze square contingency tables with a symmetrical pattern. A square table formed by cells (i, j); for $i,\ j = 1, 2, ..., L$, satisfies symmetry if

$$m(i, j) = m(j, i),\ \text{for all } i \neq j.$$

If we consider two variables X and Y, symmetry can be represented using the log-linear model

$$\log m(i, j) = u + u_X(i) + u_Y(j) + u_{XY}(ij) \tag{6}$$

with additional restrictions

$$u_X(i) = u_Y(i),\ i = 1, 2, ..., L;$$
$$u_{XY}(ij) = u_{XY}(ji),\ i, j = 1, 2, ..., L.$$

Quasi-symmetry is used to analyze cases where there is no symmetry due to marginal heterogeneity, which means that the main effects in the symmetry model differ. Such a model can be written as (6) with restrictions

$$u_{XY}(ij) = u_{XY}(ji),\ i, j = 1, 2, ..., L.$$

The parameterization used to define these models is not unique (e.g., Meiser, von Eye, and Spiel 1997), some parameterizations can be obtained through those log-linear models classified as non-standard as discussed by Mair (2007).

Example 2. Migration patterns data. For a sample of U.S. residents, Agresti (Agresti 2002, p. 423) presents some data given in Table 2 based on data by the U.S. Census Bureau that compare region of residence in 1985 with that of 1980. The variables involved are place of residence in 1980 and 1985. Each variable has four possible values: Northeast, Midwest, South and West. We can see from the observed counts that the table is more or less symmetric; however, the symmetry model is rejected because we get a deviance of 243.55 with 6 degrees of freedom so that the deviance is greater than the associated χ^2 quantile at a significance level $\alpha = 0.05$.

A closer look at the table reveals that 366 people moved from Northeast to South whereas only 172 people moved from South to Northeast. A model which fits well these data according to the deviance is the quasi-symmetry model. It means that the lack of symmetry in the table is caused by some marginal heterogeneity. In other words, the number of people emigrating from region i in 1980 to region j in 1985 would be similar to the one entering to i in 1985 from j in 1980 if the number of people in each region for 1980 were the same as the number of people in the same region in 1985. RGLL models fitted for these data are presented in section 4.

Table 2: Observed counts[1] and fitted expected frequencies under symmetry[2] and quasi-symmetry[3] models for the data described in Example 2.

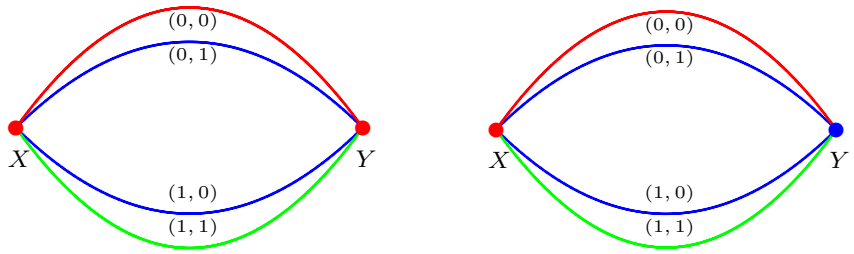
Residence	**Residence in 1985**			
in 1980	Northeast	Midwest	South	West
	11607[1]	100	366	124
Northeast	11607[2]	93.50	269.00	93.50
	11607[3]	95.79	370.44	123.77
	87	13677	515	302
Midwest	93.50	13677	370.00	239.00
	91.21	13677	501.68	311.11
	172	225	17819	270
South	269.00	370.00	17819	278.00
	167.56	238.32	17819	261.12
	63	176	286	10192
West	93.50	239.00	278.00	10192
	63.23	166.89	294.88	10192

Symmetry and quasi-symmetry models can be expressed as RGLL models as follows. In the symmetry model there is only one vertex colour class formed by both vertices and there are L atomic edge colour classes, one for every $u_{XY}(ii)$ interaction, and $\binom{L}{2}$ edge colour classes for the interactions $u_{XY}(ij) = u_{XY}(ji)$, for $i \neq j$. In the quasi-symmetry model there are the same edge colour classes as in symmetry models, but every vertex belongs to a different atomic class.

As an example, consider two binary variables X and Y with categories 0 and 1, and the saturated log-linear model given in (6) for i,j= 0, 1.

Now consider the RGLL model with graph $G = (V, E)$ given in Figure 3(a). From G, we observe that $E = (E_1, E_2, E_3)$, where $E_1 = \{u_{XY}(00)\}$, $E_2 = \{u_{XY}(11)\}$, and $E_3 = \{u_{XY}(01), u_{XY}(10)\}$. Edges in E_3 belong to the same class, indicating that the corresponding interactions are identical. The remaining edges belong to different atomic colour classes. The vertex set, $V = \{X, Y\}$, is not partitioned. Then, the main effects corresponding to X and Y are the same for all the categories. The model associated with Figure 3(a) can be expressed as (6), for i,j= 0, 1, with restrictions

$$u_{XY}(ij) = u_{XY}(ji),\ i, j = 0, 1;$$
$$u_X(i) = u_Y(i),\ i = 0, 1.$$



(a) Symmetry model (b) Quasi-symmetry model

Figure 3: Colourings for models with two binary variables: (a) symmetry model and (b) quasi-symmetry model.

Hence, the symmetry model for V=$\{X, Y\}$ is the RGLL model generated by $\mathbf{A}$= $\{\{X, Y\}\}$ with vertex class V and edge set E partitioned into $E_1 = \{u_{XY}(00)\}$, $E_2 = \{u_{XY}(11)\}$, and $E_3 = \{u_{XY}(01),\ u_{XY}(10)\}$, whose graph is given in Figure 3(a).

On the other hand, consider the RGLL model whose graph $G = (V, E)$ is shown in Figure 3(b). From G, we have the same edge or first-order interactions partition as in the symmetry model. The vertex set $V = \{X, Y\}$ is partitioned into V_1 and V_2, with $V_1 = \{X\}$ and $V_2 = \{Y\}$, so that the main effects are not restricted. Then, the quasi-symmetry model for V=$\{X, Y\}$ given in (6), for i,j= 0, 1, with restrictions

$$u_{XY}(ij) = u_{XY}(ji),\ i, j = 0, 1;$$

is the RGLL model generated by $\mathbf{A}$= $\{\{X, Y\}\}$ with vertex set $V = (V_1, V_2)$, where $V_1 = \{X\}$ and $V_2 = \{Y\}$, and edge set $E = (E_1, E_2, E_3)$, where $E_1 = \{u_{XY}(00)\}$, $E_2 = \{u_{XY}(11)\}$, and E_3= $\{u_{XY}(01),\ u_{XY}(10)\}$, whose associated graph is given in Figure 3(b).

4. Likelihood equations

There is some additional notation that has to be introduced before obtaining the likelihood equations. We denote by n the vector of observed or cell counts $n(i)$, for $i \in \mathrm{I}$, and m corresponds to a vector containing the expected frequencies for each cell $m(i)$, for $i \in \mathrm{I}$, i.e. $m' = (m(i))_{i\in \mathrm{I}}$.

Consider an RGLL model with associated graph $G = (V, E)$ in which V is partitioned into T classes $V = (V_1, ..., V_T)$ with $T \in \{1, 2, ..., |V|\}$. It is useful to identify each variable within a vertex class V_t, for $t = 1, ..., T$, as v_k^t, with k= 1,..., $kver(t)$, where $kver$ is a vector identifying the number of vertices included in each class. Hence, $V_t = \left\{v_1^t, ..., v_{kver(t)}^t\right\}$. We assume that each variable has L levels and define the associated parameters as

$u_{v_k^t}(l)$: main effect for variable v_k^t in category l, for t=1,..., T; k=1,..., $kver(t)$, and l=1,..., L.

For each vertex class V_t, for t=1,...,T, we obtain the following equality restrictions

$$u_{v_1^t}(l) = ... = u_{v_{kver(t)}^t}(l) = u_{V_t}(l), \text{ for } l = 1, ..., L;$$

where $u_{V_t}(l)$ is the parameter representing all the equated parameters associated with colour class V_t and level l.

We define the marginal total for the k-th variable in class V_t for level l, $n(v_k^t = l)$, as the sum of observed counts in all cells in which v_k^t takes value l:

$$n(v_k^t = l) = \sum_{z:z_{v_k^t}=l} n(z),\ l = 1, ..., L;\ k = 1, ..., kver(t);\ t = 1, ..., T.$$

We similarly define the corresponding marginal total for the expected frequencies $m(v_k^t = l)$.

Consider an RGLL model in which the first-order interactions set E is partitioned into S classes E_1,..., E_S. Each class $E_s = \left\{e_1^s, ..., e_{ked(s)}^s\right\}$ for s=1, 2,..., S, where e_r^s corresponds to the r-th element within class E_s, for $r = 1, 2, ..., ked(s)$, with s=1,..., S, where ked is a vector consisting of the number of edges in each class. We denote $u_{l_r^s m_r^s}(i_r^s j_r^s)$ as the first-order interaction associated with the edge e_r^s, so that e_r^s is an edge joining variable l_r^s to variable m_r^s at the values (i_r^s, j_r^s). That is, l_r^s and m_r^s are the r-th variables for the class E_s in the first and second entries, respectively, of $u_{l_r^s m_r^s}(i_r^s j_r^s)$, whose associated values are i_r^s and j_r^s, respectively.

For each class E_s, for $s = 1, ..., S$, we obtain the following equality restrictions

$$u_{l_1^s m_1^s}(i_1^s j_1^s) = ... = u_{l_{ked(s)}^s m_{ked(s)}^s}(i_{ked(s)}^s j_{ked(s)}^s) = u_{E_s},$$

where u_{E_s} denotes the parameter representing all parameters in class E_s for levels i_r^s and j_r^s, with $r = 1, 2, ..., ked(s)$ and $s = 1, ..., S$.

The marginal total for e_r^s is defined as the sum of observed counts in all cells in which l_r^s and m_r^s take the values i_r^s and j_r^s, respectively:

$$n(l_r^s = i_r^s, m_r^s = j_r^s) = \sum_{\substack{z:(z_{l_r^s}, z_{m_r^s}) \\ =(i_r^s, j_r^s)}} n(z),\ r = 1, ..., ked(s);\ s = 1, ..., S.$$

The corresponding marginal total for the expected frequencies $m(l_r^s = i_r^s, m_r^s = j_r^s)$ is similarly defined. Finally, the marginal counts for a subset b of the set of variables V, $b \subset V$, for a specific slice i_b corresponds to

$$n_b(i_b) = \sum_{j:j_b=i_b} n(j).$$

Cell counts n may follow a Poisson, multinomial, or multinomial with fixed marginals sampling scheme. The first one corresponds to having independent Poisson-distributed random variables for each cell $i \in \mathrm{I}$. The second one corresponds to having a fixed sample size $|n|$, random counts, and observations that independently belong to cell i with probability $p(i)$, for $i \in \mathrm{I}$, where $p(i) \geq 0$ and $\sum_{i\in\mathrm{I}} p(i) = 1$. The third one corresponds to having counts in specific slices i_b which are independent and multinomially distributed.

Independently of the sampling scheme, the logarithm of the kernel of the likelihood function $L(m)$ is (e.g., Lauritzen 1996, p. 71)

$$\sum_{i\in\mathrm{I}} n(i) \log m(i) - \sum_{i\in\mathrm{I}} m(i). \tag{7}$$

When a hierarchical log-linear model (4) is considered, expression (7) becomes

$$\sum_{a\in K} \sum_{i_a} n_a(i_a) u_a(i_a) - \sum_{i\in\mathrm{I}} \exp\left(\sum_{a\in K} u_a(i_a)\right). \tag{8}$$

This expression is used to obtain the likelihood equations corresponding to an RGLL model by including the corresponding parameter restrictions.

For an RGLL model, expression (8) becomes

$$\begin{aligned}\sum_{t=1}^{T}\sum_{l=1}^{L}\sum_{k=1}^{kver(t)} n(v_k^t = l) u_{V_t}(l) + \sum_{s=1}^{S}\sum_{r=1}^{ked(s)} n(l_r^s = i_r^s, m_r^s = j_r^s) u_{E_s} + \\ \sum_{a\in K, |a|\neq 1,2} \sum_{i_a} n_a(i_a) u_a(i_a) - \sum_{i\in\mathrm{I}} \exp\Big(\sum_{a\in K} u_a(i_a)\Big).\end{aligned} \tag{9}$$

When expression (9) is differentiated with respect to each parameter and equated to zero, we obtain an equation system as follows:

$$\begin{aligned}\sum_{k=1}^{kver(t)} n(v_k^t = l) &= \sum_{k=1}^{kver(t)} m(v_k^t = l),\ t = 1, ..., T;\ l = 1, ..., L; \\ \sum_{r=1}^{ked(s)} n(l_r^s = i_r^s, m_r^s = j_r^s) &= \sum_{r=1}^{ked(s)} m(l_r^s = i_r^s, m_r^s = j_r^s),\ s = 1, 2, ..., S; \\ n_a(i_a) &= m_a(i_a),\ \text{for all } a \in K,\ |a| \neq 1, 2;\end{aligned} \tag{10}$$

where, $m_a(i_a)$ denotes the marginal expected frequency for the slice i_a, i.e. $m_a(i_a) = \sum_{j:j_a=i_a} m(j)$.

Redundant equations can be eliminated by replacing the last equation in (10) with

$$n_a(i_a) = m_a(i_a), \text{ for all } a \in A, \ |a| \neq 1, 2.$$

Hence, the corresponding equation system is solved to obtain the maximum likelihood estimators of the expected frequencies m.

4.1. Solution of likelihood equations

There is a closed expression that solves the likelihood equations for a symmetry model; however, for a general RGLL model an approximated solution through numerical methods is necessary. Log-linear models are fitted using iterative proportional fitting, IPF (e.g., Bishop, Fienberg, and Holland 1975, p. 83-102), or the Newton Raphson (Fisher scoring) method (e.g., Agresti 2002, p. 143-146, p. 342-343). We have written programs to fit an RGLL model based only on the IPF method. The Newton Raphson method can be directly used when the restrictions can be equivalently used for parameters without identification constraints that consider all possible values of the variables (full parameters) or for the parameters under a parametrization. Instances of restrictions of such kind were described before Example 1 in Section **2**. In these cases, an RGLL model and its associated design matrix can be obtained using such a parameterization, and the associated design matrix has full rank. This is straightforward on models with vertex colouring only (main effects restrictions), but when there is an edge colouring (first-order interactions restrictions), equalities between parameters with different parameterizations are not always represented in the same way by simply changing the parameter. When we can not easily find such parametrization, we use the full parameters to obtain a system of equations where some of them are redundant. Hence, we can solve a subset corresponding to linearly independent equations and the rest are automatically solved. The modified IPF method described in the Appendix depends on those equations and can always be used.

A group of Fortran programs has been written to fit and select RGLL models, we refer to them as REGRAPH and are available upon request from the first author. The modified IPF method was implemented using some subroutines from Haberman (1972, 1976) to fit log-linear models, but most of the subroutines used were specifically written for RGLL models. Fitted expected frequencies, deviance, the associated design matrix, and the number of degrees of freedom for the associated asymptotic chi square distribution was also calculated. The number of degrees of freedom is calculated from the design matrix and is corrected when necessary, for instance, when an estimated expected frequency has a value of zero. Numerical results obtained with REGRAPH have been compared with those obtained by using *MIM 3.2.0.6* (Edwards 2000) or *R* for models in which the comparison is possible, e.g. quasi-symmetry and symmetry models.

4.2. Model selection

In order to fit an RGLL model to some data, three components have to be considered: (1) the graph structure given by the generating class, (2) the colouring or partition of the sets V and E, and (3) the estimated expected frequencies. Usually, the generating class is obtained performing a model search looking for a graphical log-linear model that fits the data using software like *MIM*. Then we apply a model search method to get a colouring, defining in this way an updated RGLL model. We obtained a method to see whether it is convenient to join colour classes using the deviance. Two classes are joined whenever its p value is greater than a significance level. With this method, we implemented an iterative search in REGRAPH to get, from any initial RGLL or graphical log-linear model, a new RGLL model that fits some data. Hence, only the last two components can be obtained through REGRAPH. The iterative search consists of joining pairs of vertex (or edge) classes from an initial model. We iteratively try to join all pairs of classes until a pair is significant according to its p value, ob-

taining new updated classes. The process is repeated with the new classes and so on until it is not possible to join more classes. We can first apply a model search for the vertex classes and use the final model obtained through this process as an initial model to obtain the edge classes.

Example 2 (continued). First, we label residence in 1980 and residence in 1985 as vertices 1 and 2, respectively. The four possible values, Northeast, Midwest, South and West, are coded as 1, 2, 3, and 4, respectively. The quasi-symmetry model fits these data and corresponds to an RGLL model with generating class **A**={{1, 2}} with V=(V_1, V_2), E=(E_1,...,E_{10}), where

$$V_1 = \{1\},\ V_2 = \{2\};\ E_i = \{u_{12}(ii)\}, i = 1, .., 4,\ E_5 = \{u_{12}(12), u_{12}(21)\},$$
$$E_6 = \{u_{12}(13), u_{12}(31)\},\ E_7 = \{u_{12}(14), u_{12}(41)\},\ E_8 = \{u_{12}(23), u_{12}(32)\},$$
$$E_9 = \{u_{12}(24), u_{12}(42)\},\ E_{10} = \{u_{12}(34), u_{12}(43)\}.$$

The deviance for this model obtained with REGRAPH is 2.99 with three degrees of freedom and a p-value of 0.39, indicating that we do not reject the null hypothesis that the model fits the data.

Starting from the quasi-symmetry model, we apply a selection method that preserves the vertex colour classes using REGRAPH. Assuming a significance level of 0.05, we get an RGLL model with generating class **A**={{1, 2}} with $V = (V_1, V_2)$ and E=(E_1,E_2,...,E_7), where

$$V_1 = \{1\}, V_2 = \{2\};\ E_1 = \{u_{12}(22)\},\ E_2 = \{u_{12}(12), u_{12}(21)\},\ E_3 = \{u_{12}(13), u_{12}(31)\},$$
$$E_4 = \{u_{12}(14), u_{12}(41)\},\ E_5 = \{u_{12}(23), u_{12}(32)\},\ E_6 = \{u_{12}(33), u_{12}(11), u_{12}(34), u_{12}(43)\},$$
$$E_7 = \{u_{12}(44), u_{12}(24), u_{12}(42)\}.$$

This model has a deviance of 2.98 with three degrees of freedom, p-value of 0.39, while the value of the Pearson X^2 statistic is 2.98. Of these classes, only two differ with respect to those in the quasi-symmetry model. The class containing $u_{12}(34)$ and $u_{12}(43)$ now also contains $u_{12}(11)$ and $u_{12}(33)$ and the class containing $u_{12}(24)$ and $u_{12}(42)$ now also contains $u_{12}(44)$. The graphs associated with this and the quasi-symmetry model are not presented here because they involve too many edges and colours to be helpful.

Example 2 shows the fitting of a quasi-symmetry model as an RGLL model and offers a second fitting of another RGLL model. Both indicate that the expected cell frequencies in the same class would be equal if the marginal effects were not considered or that the variables and values in the same class are equally associated.

Example 3 (twins data, continued). In Section 1 we defined an RGLL model with two vertex and ten edge colour classes. The associated restrictions are as usual for the main effects and of the kind $u_{XY}(ij)$=$u_{ZR}(ij)$ or $u_{XY}(ij)$=$u_{ZR}(ji)$ for the first-order interactions. This allows us to equivalently apply the restrictions on the full parameters or on those under effect coding as described in Section **4.1**. Hence, the model can be fitted with R using the *glm* function by generating the effect coding variables and summing those whose associated full parameters are equal. Similar statistics were obtained with REGRAPH, which uses an IPF algorithm, and R, where a Newton-Raphson algorithm is used. Using R we got a residual deviance of 9.49 with 10 degrees of freedom, and p value of 0.49, while using REGRAPH the statistic is 9.18 with the same degrees of freedom, and a p value of 0.51. When compared with the graphical model (the unrestricted model defined only by the generating class) whose deviance is 4.75 with seven degrees of freedom, the deviance between models is 4.74 (or 4.43 with REGRAPH) with three degrees of freedom and associated p value of 0.19 (or 0.21 with

REGRAPH). Hence, the model fits the data well when compared with both the saturated or graphical models. It improves the inference because it allows the symmetric interpretations discussed earlier. The associated fitted expected values are shown in Table 1.

5. Discussion and perspectives

We have introduced RGLL models mainly as a way of generalizing symmetry in graphical log-linear models. We have used both the parameterization and the kind of restrictions used by Agresti (Agresti 2002, p. 423-426) for symmetry and quasi-symmetry models. We could have used any other parameterization to define the parameter restrictions in RGLL models; for example, parameters under effect coding. In some particular cases, the restrictions with any kind of parameter are exactly the same. The graphical representation can be helpful when there are few variables and levels. RGLL models can be fitted to specific panel data, which can be represented using contingency tables as discussed by Lovison (2000).

RGLL models can be fitted using REGRAPH. Care should be taken with the interpretation of a fitted model. Indeed, in some cases the fitted model could be too complex to be interpreted in terms of the relationship between the cells. We have to be careful with which restrictions are imposed, for instance if all first-order interactions are in one class, then the corresponding parameter becomes a constant term and the model is non-hierachical. Even though we proved in Ramírez-Aldana (2010) that the IPF method converges to the estimators, we have to be careful with the initial values. The problem with this type of numerical methods is that for higher-dimension contingency tables, the solution can slightly differ depending on those values. This can be more evident on contingency tables in which there are cells with very small counts and others with very large counts. Future work could include to improving the computational algorithm in this sense.

There are two types of models defined in Ramírez-Aldana (2010) for graphical log-linear models with associated triangle-free graphs called label and level invariant graphical log-linear models. They represent four types of symmetry: (a) graph symmetry, (b) model and distribution preservation after permuting subsets of variables, (c) expected frequencies equalities, and (d) scale invariance. They can be expressed as RGLL models though they have different properties. The RGLL model associated with a label invariant model can be easily obtained using graphical and algebraic concepts. The example given in Section **1** corresponds to a particular level invariant graphical log-linear model, which is almost equivalent to a label invariant model but without scale invariance. The advantage of such a model is that its associated RGLL model can be obtained using similar concepts as the ones used for a label invariant model. The classes for the RGLL model in Section 1 can be obtained in this way.

We could extend RGLL models by setting equality restrictions not only on the main effects and first-order interactions, but also on higher-order interactions. This generalization requires additional work in both computational and theoretical terms. A graphical representation of these models, even with multi-graphs, is not possible, much less when we consider that the equalities involve not only variables but also their values. If we obtained these generalizations, more symmetry generalizations, for example complete symmetry or quasi-symmetry (Bishop *et al.* 1975, p. 299-306), would be particular cases.

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A. Solution to the likelihood equations

The IPF method (e.g., Lauritzen 1996, p. 83-84) consists of three steps applied to every cell i, for $i \in \mathrm{I}$. For RGLL models, there are likelihood equations that have to be solved in addition to the ones for the generating class $\mathbf{A}$. These equations correspond to first-order interactions and main effects, first and second equations in (10). The algorithm then solves RGLL models similarly to the IPF method; however, in step 2 we add transformations corresponding to the restrictions or colourings. The usual IPF method consists of the following steps:

1. Assign an initial value, $m_0(i)$, for $i \in \mathrm{I}$. For instance, $m_0(i)$ can be one.

2. Take all the elements in the generating class $\mathbf{A}$, and order them in a set $(b_1, b_2, ..., b_z)$. Define the transformation $T_v = T_{b_v}$, for $v = 1, 2, ..., z$, as

$$(T_{b_v} m)(i) = m(i) \frac{n(i_{b_v})}{m(i_{b_v})}, \ i \in \mathrm{I}.$$

   Define recursively

$$m_{r+1}(i) = (T_1 T_2 ... T_z) m_r(i), \ r = 0, 1, 2, ...$$

   In every step, we adjust all the elements in the generating class, so that there are z sub-steps for every step.

3. The process continues until the maximal difference between the marginal counts and the marginal adjusted expected frequencies reaches a predetermined error δ.

For RGLL models, we add other transformations. Considering that all variables have the same categories, L levels in each, we define for every vertex class V_t, where $t = 1, 2, ..., T$ and $l = 1, ..., L$, the following transformations

$$(T_{V_t(l)} m)(i) = m(i) \frac{\sum_{v_k^t \in V_t} n(v_k^t = l)}{\sum_{v_k^t \in V_t} m(v_k^t = l)}, \ i \in \{(i_1, i_2, ..., i_{|V|}) \in \mathrm{I} | i_{v_k^t} = l, \text{ for some } v_k^t \in V_t\}.$$

For each edge or first-order interaction class E_s, with $s = 1, 2, ..., S$, we define the following transformations for $i \in \{(q_1, q_2, ..., q_{|V|}) \in \mathrm{I} | q_{l_v} = i_v, \ q_{r_v} = j_v, \text{ for some } \{l_v = i_v, r_v = j_v\} \in E_s\}$

$$(T_{E_s} m)(i) = m(i) \frac{\sum_{\{l_v = i_v, r_v = j_v\} \in E_s} n(l_v = i_v, r_v = j_v)}{\sum_{\{l_v = i_v, r_v = j_v\} \in E_s} m(l_v = i_v, r_v = j_v)}.$$

We define $0/0 = 0$. The element $\{l_v = i_v, r_v = j_v\} \in E_s$ denotes an edge on E_s joining the variable l_v to r_v for the value combination (i_v, j_v), for $v = 1, ..., ked(s)$, where $s = 1, ..., S$.

Then, we define for r, where $r = 0, 1, 2, ...$

$$m_{r+1}(i) = (T_1 T_2 ... T_z T_{V_1(1)} T_{V_1(2)} ... T_{V_1(L)} ... T_{V_T(1)} T_{V_T(2)} ... T_{V_T(L)} T_{E_1} T_{E_2} .... T_{E_S}) m_r(i).$$

We emphasize that the transformation $T_{b_v} = T_v$ is applied for $|b_v| \neq 1, 2$ and that not all transformations associated with the colourings are applied to every cell, it depends on the class and cell. For example, if we have a cell whose entries corresponding to all the variables

in a colour class V_t are all different from l, then there is no sense in applying to this cell the transformation $T_{V_t(l)}$.

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