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On Some Representations and Modifications of Markov Chains

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Abstract: Two new representations of Markov chains are proposed. One of them uses the novel concept of Index Matrix (IM) which has greater modelling capabilities in comparison to the standard matrix. A new normalization operator over IMs is introduced. The other new representation proposed in the present paper uses Generalized Nets (GNs). Two GN models of Markov chain are described. It has been made an attempt to classify them with respect to the DM techniques (neural networks, genetic algorithms, etc.) and the tools used, as well as on the basis of the different areas of DM application (education, medicine, genetics, etc).

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1 Introduction

Markov Chain (MC) is one of the important concepts in the modelling of stochastic processes as a sequence of events, the probability of which depends only on the previous event [6–8]. Usually, a MC with n vertices is represented by a matrix:

$$\begin{Vmatrix} a_{1,1} & \dots & a_{1,j} & \dots & a_{1,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{i,1} & \dots & a_{i,j} & \dots & a_{i,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{n,1} & \dots & a_{n,j} & \dots & a_{n,n} \end{Vmatrix},$$

where for every i $(1 \leq i \leq n)$:

$$\sum_{j=1}^{n} a_{i,j} = 1. \tag{1}$$

The MC can be represented also by a graph. For example, a MC with 5 vertices $v_1, v_2, ..., v_5$ can have (standard) matrix representation

$$\begin{Vmatrix} 0.0 & 0.3 & 0.7 & 0.0 & 0.0 \\ 0.0 & 0.2 & 0.3 & 0,5 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ 0.6 & 0.0 & 0.0 & 0.0 & 0.4 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{Vmatrix},$$

and the graph representation shown in Fig. 1.

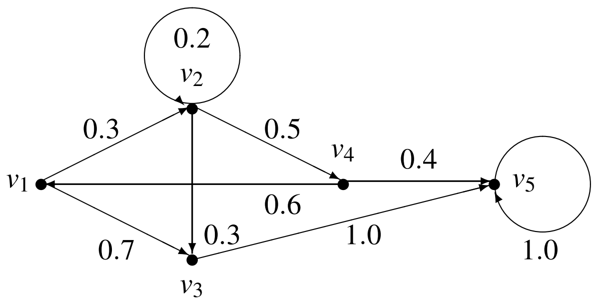

Figure 1.

If we do not like condition (1) to be valid for vertex v_5 as a final vertex, element $a_{5,5}$ of the matrix will obtain value 0.0 and Fig. 1 obtains the form in Fig. 2.

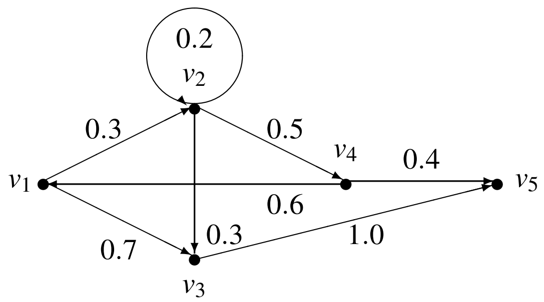

Figure 2.

In the present paper, representations of MC will be constructed by two comparatively new and not well-known mathematical objects - Index Matrices (IM, see [2,5]) and Generalized Nets (GNs, see [1,3,4]).

2 Index Matrix Representations of Markov Chains

Let I be a fixed set of indices and $\mathscr{R}$ be the set of the real numbers. By IM with index sets K and L $(K, L \subset I)$, we denote the object:

$$[K, L, \{a_{k_i,l_j}\}] \equiv \begin{array}{c|cccc} & l_1 & l_2 & \ldots & l_n \\ \hline k_1 & a_{k_1,l_1} & a_{k_1,l_2} & \ldots & a_{k_1,l_n} \\ k_2 & a_{k_2,l_1} & a_{k_2,l_2} & \ldots & a_{k_2,l_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ k_m & a_{k_m,l_1} & a_{k_m,l_2} & \ldots & a_{k_m,l_n} \end{array},$$

where $K = \{k_1, k_2, ..., k_m\}$, $L = \{l_1, l_2, ..., l_n\}$, for $1 \leq i \leq m$, and $1 \leq j \leq n$: $a_{k_i,l_j} \in \mathscr{R}$ – the set of real numbers.

Different operations, relations and operators are defined over IMs in [5]. For the needs of the present research, we will introduce the definition of the operation addition.

Let the IMs $A = [K, L, \{a_{k_i,l_j}\}]$ and $B = [P, Q, \{b_{p_r,q_s}\}]$ be given. Let $*$ be one of the operations "+", "-", ".", ":", between a- and b-elements of both IMs. Then,

$$A \oplus_{(*)} B = [K \cup P, L \cup Q, \{c_{t_u,v_w}\}],$$

where

$$c_{t_u,v_w} = \begin{cases} a_{k_i,l_j}, & \text{if } t_u = k_i \in K \text{ and } v_w = l_j \in L - Q \\ & \text{or } t_u = k_i \in K - P \text{ and } v_w = l_j \in L; \\ & \\ b_{p_r,q_s}, & \text{if } t_u = p_r \in P \text{ and } v_w = q_s \in Q - L \\ & \text{or } t_u = p_r \in P - K \text{ and } v_w = q_s \in Q; \\ & \\ a_{k_i,l_j} * b_{p_r,q_s}, & \text{if } t_u = k_i = p_r \in K \cap P \\ & \text{and } v_w = l_j = q_s \in L \cap Q; \\ & \\ 0, & \text{otherwise.} \end{cases}$$

Now, the IM for the MC from the example in Fig. 2 will have the form

$$\begin{array}{c|ccccc} & v_1 & v_2 & v_3 & v_4 & v_5 \\ \hline v_1 & 0.0 & 0.3 & 0.7 & 0.0 & 0.0 \\ v_2 & 0.0 & 0.2 & 0.3 & 0.5 & 0.0 \\ v_3 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ v_4 & 0.6 & 0.0 & 0.0 & 0.0 & 0.4 \\ v_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{array}.$$

At first sight, we can see that the IM is more complex than the standard one. The question: *Why we like to complicate the form of the first matrix?* is sound. But, as it is shown in [5], IMs can be used to describe things which cannot be described by standard matrices. For example, let us have another, for brevity – simpler, MC with 5 vertices w_1, w_2, w_3, w_4, w_5, the (standard) matrix

$$\left\| \begin{array}{ccccc} 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.4 & 0,6 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{array} \right\|,$$

without condition (1) for its vertex w_5, and with the graph-representation in Fig. 3.

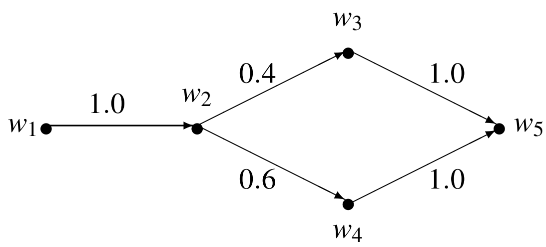

Figure 3.

If we know that the pairs of vertices v_2 and w_1, v_4 and w_2, v_5 and w_4 coincide, and if we would like to unite both of the MCs, matrix algebra does not allow us to construct a united MC, while if A is the IM which corresponds to the first MC (in Fig. 2) and

$$B = \begin{array}{c|ccccc} & w_1 & w_2 & w_3 & w_4 & w_5 \\ \hline w_1 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ w_2 & 0.0 & 0.0 & 0.4 & 0.6 & 0.0 \\ w_3 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_4 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{array}$$

is the IM for the MC in Fig. 3, then we can construct IMs in respect to the form of the operation between the matrix elements, as follows:

$$C = A \oplus_{(+)} B = \begin{array}{c|ccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & w_3 & w_5 \\ \hline v_1 & 0.0 & 0.3 & 0.7 & 0.0 & 0.0 & 0.0 & 0.0 \\ v_2 & 0.0 & 0.2 & 0.3 & 1.5 & 0.0 & 0.0 & 0.0 \\ v_3 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ v_4 & 0.6 & 0.0 & 0.0 & 0.0 & 1.0 & 0.4 & 0.0 \\ v_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_3 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{array}$$

and

$$D = A \oplus_{(\max)} B = \begin{array}{c|ccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & w_3 & w_5 \\ \hline v_1 & 0.0 & 0.3 & 0.7 & 0.0 & 0.0 & 0.0 & 0.0 \\ v_2 & 0.0 & 0.2 & 0.3 & 1.0 & 0.0 & 0.0 & 0.0 \\ v_3 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ v_4 & 0.6 & 0.0 & 0.0 & 0.0 & 0.6 & 0.4 & 0.0 \\ v_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_3 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{array}$$

that represent the union of both MCs.

Now, we can see that the condition (1) is violated for the rows indexed by v_2 and v_4. So, we can normalize the values in these rows, using the formula

$$a_{s,i} = \frac{a_{s,i}}{\sum\limits_{j=1}^{7} a_{s,j}}, \tag{2}$$

where $s = 2, 4$.

The IM C obtains the normalized form

$$C = \begin{array}{c|ccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & w_3 & w_5 \\ \hline v_1 & 0.0 & 0.3 & 0.7 & 0.0 & 0.0 & 0.0 & 0.0 \\ v_2 & 0.0 & 0.1 & 0.15 & 0.75 & 0.0 & 0.0 & 0.0 \\ v_3 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ v_4 & 0.3 & 0.0 & 0.0 & 0.0 & 0.5 & 0.2 & 0.0 \\ v_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_3 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{array}$$

and the IM D – the form

$$D = A \oplus_{(\max)} B = \begin{array}{c|ccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & w_3 & w_5 \\ \hline v_1 & 0.0 & 0.3 & 0.7 & 0.0 & 0.0 & 0.0 & 0.0 \\ v_2 & 0.0 & 0.13 & 0.2 & 0.67 & 0.0 & 0.0 & 0.0 \\ v_3 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ v_4 & 0.38 & 0.0 & 0.0 & 0.0 & 0.24 & 0.38 & 0.0 \\ v_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_3 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ w_5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{array}.$$

In these IMs, all rows without the last ones, indexed by w_5 (the final vertex) satisfy condition (1). The graphical form of the new MC in $+$-form, before normalization is shown in Fig. 4 and after it – in Fig. 5. The max-forms of non-normalized and normalized MCs have similar forms.

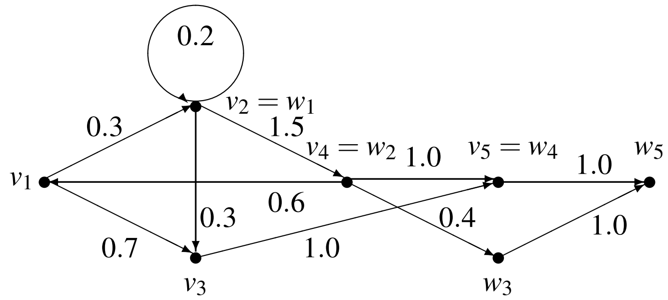

Figure 4.

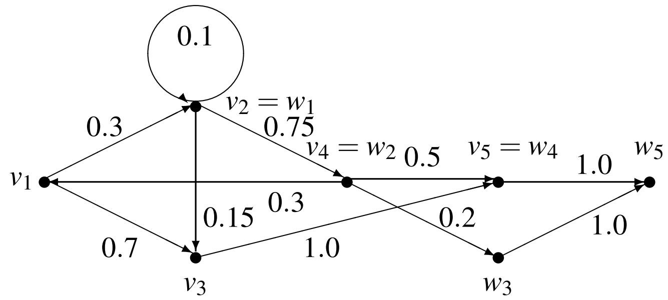

Figure 5.

The necessary condition for normalization of values in rows indexed by v_2 and v_4 described above, motivated us to introduce a normalization operator over IMs in the form:

$$N(A) = N([K, L, \{a_{k_i,l_j}\}]) = \left[K, L, \left\{ \frac{a_{k_i,l_j}}{\sum\limits_{s=1}^{n} a_{k_i,l_s}} \right\} \right].$$

3 Generalized Net Representations of Markov Chains

Generalized Nets (GNs, see [3,4]) are extensions of Petri nets and their modifications and extensions, like E-nets, Time Petri nets, Colour Petri nets, Stochastic Petri nets, Predicative-Transition nets, etc. GNs have a part of the components of the rest Petri nets types of nets, e.g., transitions, places, tokens, temporal components. But they have also some specific components, as transition condition predicates that are elements of IM, initial and current tokens characteristics and others. The existing of the predicates and characteristics increase essentially the modelling abilities of the GNs. So, for each type of Petri net extension or modification there exists a GN which describes the process of functioning and the results of the work of each net from the respective type.

For example, the colours of the tokens of the Coloured Petri nets are represented by the GN-tokens' characteristics; the time-components of the E-nets and of the Time Petri nets are represented by the GN-time components. In the GN case, however, there are two types of time-components which are similar to the components of the two Petri net modifications. As an illustration that the GNs have higher modelling powers than, e.g. the two discussed types of nets, we mention that the E-nets time-components can describe the continuation of a cinema projection, the time-components of the Time Petri nets - moments of the beginning of projection, but only both of the GN-time components give information for the interval between two projections. In addition, we mention that there is a GN that describes the process of functioning and the results of the work of each Turing machine. Another GN describes the process of functioning and the results of the work of the Kolmogorov's algorithm, etc. The possibilities of using GNs as a tool for describing Data Mining processes and objects are discussed in [9, 10].

When a GN-component is not necessary for a given model, it can be omitted and the GN without this component is called a reduced GN. For the models in the present paper, we will use a reduced GN with transitions of the following form

$$Z = \langle L', L'', r \rangle,$$

where $L' = \{k_1, ..., k_m\}$ is the set of the input places of the transition, $L'' = \{l_1, ..., l_n\}$ is the set of its output places and r is the IM

$$r = \begin{array}{c|ccccc} & l_1 & \ldots & l_j & \ldots & l_n \\ \hline k_1 & & & & & \\ \vdots & & & r_{i,j} & & \\ k_m & & & & & \end{array},$$

where $r_{i,j}$ is the predicate that corresponds to the i-th input and j-th output place $(1 \leq i \leq m, 1 \leq j \leq n)$. When its truth value is "*true*", a token from the i-th input place transfers to the j-th output place; otherwise, this is not possible.

The complete reduced GN, that we will use here, has the formal definition

$$\langle A, K, X, \Phi \rangle,$$

where A is the set of all GN-transitions, K - the set of the GN-tokens, which enter the GN or stay in certain GN-places with initial characteristics, given by the function X; Φ is the characteristic function that assigns new characteristics to each token when it makes a transfer from an input to an output place of a given transition.

Different operations, relations and operators are defined over GNs. The operations are union, intersection and subtraction of two GNs. The relations are used to compare the structure and the results of the work of two GNs. The operators are global (that can change the GN-global components), local (that can change the transitions components), hierarchical (used to replace a sub-GN with a transition or a place, or the opposite - to replace a place or a transition of a given GN with a sub-GN; to replace a sub-GN with another sub-GN and to replace a GN-token with a sub-GN), reduced (to omit some GN-components or to determine which GN-components of a given GN are omitted), extending (to extend a given GN to an extended GN of a given type) and dynamical (used to change the algorithms of tokens' transfer, to determine the possibility for a token to be split or united, and to determine the way of calculating the truth-values of the transition condition predicates).

The concept of stochastic Petri nets has been introduced practically in parallel by S. Shapiro [13] and S. Natkin [12]. In [11], Molloy has shown that each Markov chain can be represent by a stochastic Petri net.

Below, we will illustrate the GN capabilities to represent each Markov chain. For example, the chain in Fig. 4 can be represented by the GN in Fig. 6, but this is only one of the possible GN-representations.

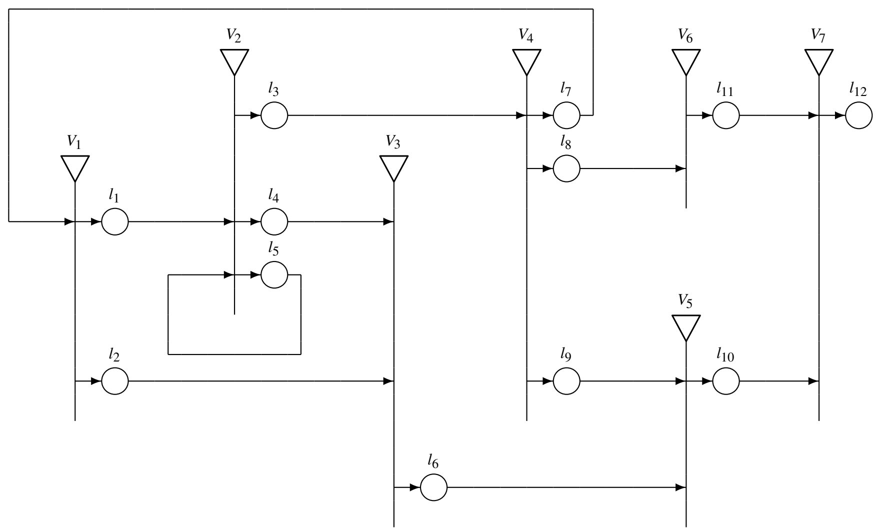

Figure 6. Generalized Net model of the MC from Fig. 4

We can juxtapose a GN-transition to each vertex of the Markov chain. In one of the GN-representations, when the token, which represents the process of functioning of the Markov chain, enters a place, it can have as a current characteristic the value of the variable $r \in [0,1]$. In Fig. 6, the GN has 7 transitions and 12 places, and the form in Fig. 6.

The formal forms of the transitions are the following.

$$V_1 = \langle \{l_7\}, \{l_1, l_2\}, \begin{array}{c|cc} & l_1 & l_2 \\ \hline l_7 & r_{7,1} & r_{7,2} \end{array} \rangle,$$

where
$r_{7,1} =$ "$r \in [0.0, 0.3]$",
$r_{7,2} =$ "$r \in (0.3, 1.0]$".

$$V_2 = \langle \{l_1, l_5\}, \{l_3, l_4, l_5\}, \begin{array}{c|ccc} & l_3 & l_4 & l_5 \\ \hline l_1 & r_{1,3} & r_{1,4} & r_{1,5} \\ l_5 & r_{5,3} & r_{5,4} & r_{5,5} \end{array} \rangle,$$

where
$r_{1,3} = r_{5,3} =$ "$r \in [0.0, 0.75]$",
$r_{1,4} = r_{5,4} =$ "$r \in (0.75, 0.9]$".
$r_{1,5} = r_{5,5} =$ "$r \in (0.9, 1.0]$".

$$V_3 = \langle \{l_2, l_4\}, \{l_6\}, \begin{array}{c|c} & l_6 \\ \hline l_2 & true \\ l_4 & true \end{array} \rangle.$$

$$V_4 = \langle \{l_3\}, \{l_7, l_8, l_9\}, \begin{array}{c|ccc} & l_7 & l_8 & l_9 \\ \hline l_3 & r_{3,7} & r_{3,8} & r_{3,9} \end{array} \rangle,$$

where
$r_{3,7} =$ "$r \in [0.0, 0.3]$",
$r_{3,8} =$ "$r \in (0.3, 0.5]$",
$r_{3,9} =$ "$r \in (0.5, 1.0]$".

$$V_5 = \langle \{l_6, l_9\}, \{l_{10}\}, \begin{array}{c|c} & l_{10} \\ \hline l_6 & true \\ l_9 & true \end{array} \rangle.$$

$$V_6 = \langle \{l_8\}, \{l_{11}\}, \begin{array}{c|c} & l_{11} \\ \hline l_8 & true \end{array} \rangle.$$

$$V_7 = \langle \{l_{10}, l_{11}\}, \{l_{12}\}, \begin{array}{c|c} & l_{12} \\ \hline l_{10} & true \\ l_{11} & true \end{array} \rangle.$$

Initially, the token can stay, e.g., in place l_7. It can have some initial characteristic related to the specifics of the model based on a Markov chain and the above mentioned variable r. Entering next places, the token can obtain as a characteristic not only the new value of r, but other information of interest for the model. Therefore, we can see directly that the GN represents the functioning of the Markov chain in Fig. 5. However, the GN can do additional things.

First, the token can collect additional information in its current characteristics.

Second, which is really important: we can put in the GN not one token, but a set of tokens to determine the way of the functioning of the Markov chain, and each of them can go through the GN with respect to its own characteristics (its own values of the variable r). If the place capacities are, e.g, infinity, then the tokens can go through the GN independently, but if these capacities or at least a part of them are finite, there will be situations in which different conflicts between the separate tokens, or between the separate parallel processes flowing in the given Markov chain will arise.

Third, in [15], a Markov chain in which the development of the process is a function of not only the current values of the r-variable, but of the events in the previous steps of the process is studied. Obviously, this idea can be realized by the present GN, if the token's characteristic function has the form of the function of the Markov chain. So, it will depend on the respective number of the previous characteristics of a given token. Moreover, it can depend on the respective number of the previous characteristics of all other GN-tokens. Obviously, this is a serious extension of the standard Markov process that is inspired by the GN properties.

Fourth, the GN can have another form, e.g., this in Fig. 7.

Now, each transition has an additional place, marked by m, with an additional token in it. The token obtains as a current characteristic the additional information related to the modelled process, which is different from the one, the tokens obtain during the functioning of the first model. Let us denote the first tokens as α-tokens and the new ones - as β-tokens. Now, the β-tokens can obtain as a current characteristic the random values that are generated in the Markov chain, which values can be functions of all events which have arisen in the GN-model.

Fifth, we can change the variable that determines the directions of the development of the processes (or the directions of tokens' transfers) with predicates, that will be evaluated when the transitions are activated as a result of collecting enough tokens in their input places. In the particular case, when the predicates have the form shown above as elements of the IM related to the separate transitions, we obtain the first GN-model. But these predicates can have essentially general form giving the possibility to describe more general processes.

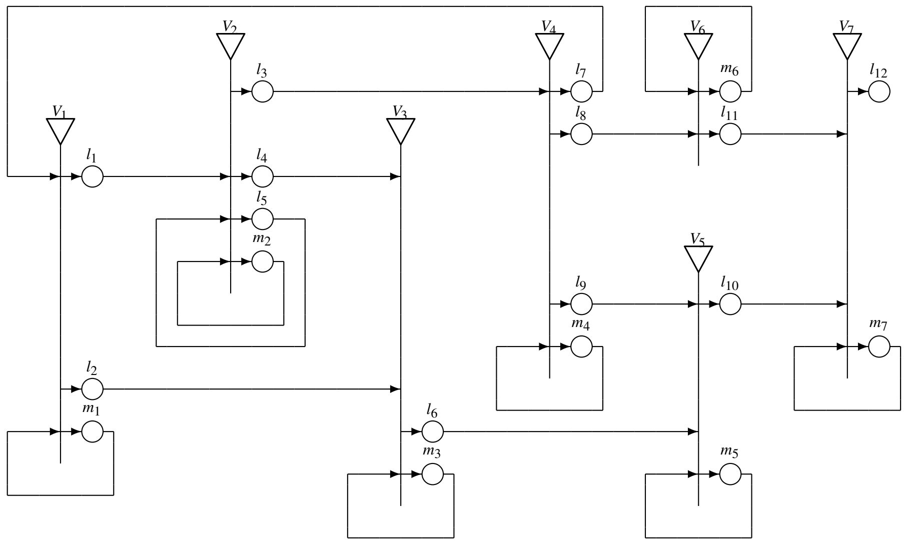

Figure 7. A more detailed GN of a MC.

We will illustrate this last possibility with the following example. Let us for simplicity use the GN from Fig. 6 and let us have the token α in place l_3. Let the values of the variables or of the predicates determine that it must go to place l_9. But let the predicate $r_{10,12}$ is not *true* as above, but, e.g., it is the predicate *"there is a token in place l_2"*. If this predicate is not true, then the token from place l_3 cannot go to place l_{12}. In the frames of the GN-model we can change the trajectory of token α so to direct it to place l_8 and then to place l_{12} through place l_{11}.

If we use the more detailed GN from Fig. 7, the solution for change of the trajectory will be obtained in the *m*-place of the transition V_4.

4 Conclusion

Markov chains have wide applicability and are an important area of mathematics. In particular, they are used in the modelling and evaluation of Human-Cyber-Physical Systems. The results presented here can be used in the modelling of telecommunication networks to assess the security level.

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