PAPER

Structure Learning of Bayesian Networks Using Dual Genetic Algorithm*

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SUMMARY A new structure learning approach for Bayesian networks (BNs) based on dual genetic algorithm (DGA) is proposed in this paper. An individual of the population is represented as a dual chromosome composed of two chromosomes. The first chromosome represents the ordering among the BN nodes and the second represents the conditional dependencies among the ordered BN nodes. It is rigorously shown that there is no BN structure that cannot be encoded by the proposed dual genetic encoding and the proposed encoding explores the entire solution space of the BN structures. In contrast with existing GA-based structure learning methods, the proposed method learns not only the topology of the BN nodes, but also the ordering among the BN nodes, thereby, exploring the wider solution space of a given problem than the existing method. The dual genetic operators are closed in the set of the admissible individuals. The proposed method is applied to real-world and benchmark applications, while its effectiveness is demonstrated through computer simulation.

key words: Bayesian network, genetic algorithms, structure learning, dual chromosomes

1. Introduction

The Bayesian network (BN) is one of the most popular formalisms for reasoning under uncertainty in Artificial Intelligence (AI). The BN is a graphical model that denotes joint probabilistic distribution among variables of interest based on the variables' probabilistic relationships. The structure of the BN is represented as a directed acyclic graph (DAG). In a DAG, each node represents a variable that takes on a value over both continuous and discrete data set of domain and is connected with its parent's nodes. Each arc represents the conditional dependency between the two nodes so connected. With the development of large-scale database systems, the BN has become a popular knowledge representational scheme for probabilistic knowledge in data mining and knowledge discovery [1]–[3].

In building the BN, which represents the conditional dependencies in a database of cases, the problem of searching for the structure of the BN is both important and difficult. A large number of possible DAG structures could be determined from a small number of nodal connections. To

solve this problem, several methods have been reported [4]–[10] for the structure learning of the BN. The most popular method for BN structure learning from a database is the K2 algorithm [10]. The K2 algorithm assumes that an ordering on the variables is given and searches for an appropriate structure heuristically. But this method is heuristic and does not guarantee that an optimal structure will be found.

On the other hand, GAs have been successfully applied to various optimization problems in real world applications. They are well suited to the exploration of complex search spaces. As an alternative scheme to K2, the learning methods based on the GAs have been reported [7]–[9], [11], [12]. The GA, however, is not a ready made optimization tool for BN structure learning. The plain GA cannot be applied to the structure learning of BN and there is no general way to find the optimal structure in the entire DAG space because the plain genetic operations are not closed in the set of the possible BN structures. Thus, in the existing methods, the GAs also restrict the ordering on the variables, in which initially a search is conducted for the solution in the directed graph space, including cyclic and acyclic, and then the cyclic solutions are removed.

In this paper, a new structure learning method of the BNs based on a dual genetic algorithm (DGA) is proposed. In the proposed method, a BN structure is represented as paired chromosomes. One represents the ordering among the BN nodes and the other represents conditional dependencies among the ordered BN nodes. In contrast with the existing GA-based structure learning methods of the BN [7], the proposed method learns not only the topologies of the BN nodes, but also the ordering among the BN nodes, thereby, exploring the entire solution space of a given problem. The proposed method is somewhat similar to [18] but the contribution of this paper is twofold: (1) It is *rigorously* shown that the dual chromosome can represent all the possible BN structures, thereby exploring the entire BN structure space and (2) the proposed method uses slightly different genetic operators from [18].

This paper is organized as follows. In Sect. 2, a brief introduction to BNs and GAs is given. In Sect. 3, the DGA for structure learning of the BN is proposed and the new genetic operations are introduced. In Sect. 4, the proposed method is applied to real-world and benchmark problems: a database of virtual home network systems [13], a database of car diagnosis problems as suggested by Norsys [14], and a database of ALARM networks constructed by Beinlinch *et al.* [10]. Finally, some conclusions are drawn in Sect. 5.

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2. Preliminary Fundamentals: Bayesian Networks and Genetic Algorithms

2.1 Bayesian Network

The Bayesian network and associated schemes constitute a probabilistic framework for reasoning under uncertainty and in recent years have gained popularity in the community of artificial intelligence. The BN is composed of a network structure and a set of parameters associated with the structure. The structure of the BN is a directed acyclic graph (DAG), in which each node represents a random variable that can take on a finite set of values and each arc represents the conditional dependency (topology) between the two nodes [15]. In this paper, we assume that each node takes only discrete values.

To specify the BN completely in conjunction with the DAG, the user must give prior probabilities for all root nodes (nodes with no predecessors) and conditional probabilities for all the other nodes. The joint probability of any particular instantiation of all n variables in the BN can be calculated with

$$P(U) = \prod_i P(A_i | pa(A_i)) \quad (1)$$

where $U = A_1, A_2, \dots, A_n$ represents n nodes of the BN and $pa(A_i)$ is the parent set of the variable A_i . For example, the probability of the BN shown in Fig. 1 is computed by:

$$P(U) = P(A_1)P(A_2)P(A_3)P(A_4|A_1, A_2) \cdot P(A_5|A_2, A_3)P(A_6|A_4)P(A_7|A_5) \quad (2)$$

The process of building the BN can be separated into two tasks: structure learning and parameter learning. Structure learning is a search for an appropriate structure for the BN such that the BN accommodates the given set of samples. Parameter learning is computation of the conditional probabilities for the given BN structure such that the output of the BN approximates the distribution of the given set of samples. The most popular parameter learning method is the expectation maximization (EM) algorithm [16]. In this paper, the focus is structure learning of the BN and building an appropriate BN structure such that the BN structure accommodates the given set of samples.

Fig. 1 An example of a Bayesian network.

2.2 Genetic Algorithms

The genetic algorithm (GA) is the implementation of a biological metaphor. In the algorithm, learning is viewed as a competition among a population of evolving individuals. The fitness, or goodness, of each individual is evaluated and, according to the computed fitness value, it is determined which one will survive in the next generation. Through operations analogous to gene transfer in sexual reproduction, a new population of candidate solutions is created [17]. The general procedure for GA is summarized as follows. An initial population of individuals called chromosomes is created by random selection and the goodness of each individual is evaluated by a fitness function. Then, a new population of reproduced individuals is selected according to the fitness values. In the selection, the individuals with high fitness values are more likely to reproduce offspring than those with low fitness values. Finally, the selected individuals are mated with others and sometimes mutated. If the new population includes an individual that produces a satisfactory performance or fitness level, then the algorithm stops and the problem is solved. If not, then the algorithm is repeated until a termination condition is satisfied. The pseudo code of a simple genetic algorithm (SGA) is shown below:

procedure SGA()

```

initialize(Population);
evaluate(Population);
While (Not termination-condition) Do
    MatingPool=reproduce(Population);
    MutationPool=crossover(MatingPool);
    Population = mutation(MutationPool);
    evaluate(Population);
end
end

```

3. Structure Learning of Bayesian Networks Based on the Dual Genetic Algorithm

In this section, a new approach for structure learning of BNs based on the dual genetic algorithm is proposed. The proposed method explores a wider solution space than the existing GA-based structure learning method.

3.1 The Conventional Method for BN Structure Learning

In this subsection, the conventional method that uses the GA for the structure learning of the BN is explained briefly [7]. The BN structure with n variables is represented by an $n \times n$ connectivity matrix $C = (c_{i,j})$, where

$$c_{i,j} = \begin{cases} 1 & \text{if } i \text{ is a parent of } j \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

and each individual of the population is encoded as a chromosome,

$$c_{1,1}c_{1,2} \cdots c_{1,n}c_{2,1}c_{2,2} \cdots c_{2,n} \cdots c_{n,1}c_{n,2} \cdots c_{n,n} \quad (4)$$

With this representation, the plain crossover and mutation operators would produce illegal BN structures. In the previous method, to overcome this problem, the connectivity matrix was assumed to be upper triangular and the connectivity matrix,

$$C = \begin{pmatrix} 0 & c_{1,2} & c_{1,3} & \cdots & c_{1,n-1} & c_{1,n} \\ 0 & 0 & c_{2,3} & \cdots & c_{2,n-1} & c_{2,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & c_{n-1,n} \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \quad (5)$$

was encoded as a chromosome,

$$X = c_{1,2} \cdots c_{1,n}c_{2,3} \cdots c_{2,n} \cdots c_{n-2,n-1}c_{n-2,n}c_{n-1,n} \quad (6)$$

In other words, the ordering among the variables of the BN was fixed and a node A_i was allowed to have another node A_j as a parent node only if the node A_j comes before the node A_i in the ordering. This scheme restricts the values of $c_{i,j}$ ($i \geq j$) to 0 and narrows the search space to the extent that the GA will find only a suboptimal solution, if the fixed ordering of the nodes is wrong.

3.2 Dual Genetic Algorithm for BN Structure Learning

The conventional method has the limitation that the ordering between the nodes is predetermined and the nodal connections are upper triangular. The conventional genetic encoding cannot represent all the possible BN structures and the search space was not fully explored to determine the fittest structure of BNs. If there is no prior knowledge about the ordering between variables, which is usually the case, the resulting structure will not be satisfactory.

This paper describes a proposed new genetic method that can be applied to the structure learning of the BNs. In the proposed method, the connectivity matrix is assumed to be upper triangular, but it is not exactly the same as that of the conventional method. The ordering of the nodes is not fixed and it is also learned by the GA. Thus, the entire solution space is searched for the fittest structure of the BN.

3.2.1 Encoding

In order to encode all of the information related to the structure learning of the BN into a chromosome and search the entire solution space for the fittest structure, a dual chromosome is proposed, which is composed of an *ordering chromosome* and a *connectivity chromosome*: The ordering chromosome is integer-coded and denotes the ordering among the BN nodes. The connectivity chromosome is binary-coded and denotes the upper triangular connectivity matrix, which represents the connection among the nodes with respect to the ordering chromosome. The ordering chromosome X_o and the connectivity chromosome X_c are encoded as follows:

$$X_o = x_1x_2 \cdots x_n$$

$$X_c = c_{1,2} \cdots c_{1,n}c_{2,3} \cdots c_{2,n} \cdots c_{n-2,n-1}c_{n-2,n}c_{n-1,n} \quad (7)$$

where

x_i is an integer and $x_i \in \{1, \dots, n\}$, $x_i \neq x_j$, iff $i \neq j$

$$C = \begin{pmatrix} 0 & c_{1,2} & c_{1,3} & \cdots & c_{1,n-1} & c_{1,n} \\ 0 & 0 & c_{2,3} & \cdots & c_{2,n-1} & c_{2,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & c_{n-1,n} \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \quad (8)$$

$$c_{i,j} = \begin{cases} 1 & \text{if } x_i \text{ is a parent of } x_j \\ 0 & \text{otherwise} \end{cases}$$

The ordering chromosome consists of the indices of the variables. If there are n root nodes (nodes without parents) and they have m children nodes, the first n genes of this chromosome are the indices of the root nodes. The next m genes are the indices of nodes which can be the children of the root nodes. This structure is repeated until all of the variables are visited. The connectivity chromosome denotes the connectivity matrix, which defines the dependency relation among the variables. For the evolution of the connectivity chromosome, the plain GA operators are applied. For the evolution of the ordering chromosome, however, the plain GA operators do not work and some genetic operators used in traveling salesman problem (TSP) are applied to find the best ordering of the variables [17]. In [18], several GA operators used in TSP were applied under the K2 algorithm and it was shown that their performances are almost the same. In the proposed method, the GA operators similar to those of [18] are used. The following examples show the basic idea of the suggested dual genetic encoding. The GA operators for the dual genetic encoding will be explained in detail in the subsequent section.

Example 1 (Encoding of the dual chromosome):

Consider two BN structures as shown in Fig. 2.

Each BN is represented by a dual chromosome (X_{io}, X_{ic}) , in which $i = 1, 2$ and the subscripts o and c denote an ordering chromosome and a connectivity chromosome, respectively. These chromosomes are explicitly shown in (9).

$$X_{1o} = 126354$$

$$X_{1c} = 110000100010010$$

$$X_{2o} = 543126$$

Fig. 2 Two BNs (Example 1).

$$X_{2c} = 110001100010011 \quad (9)$$

C_i and $\bar{C}_i$ denote the connectivity matrices, as shown in (10), created by the proposed dual chromosome (X_{io}, X_{ic}) and by the conventional method [7], respectively.

$$C_1 = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \bar{C}_1 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$C_2 = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \bar{C}_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (10)$$

□

The proposed method can explore a much wider solution space than the existing GA-based method because the proposed dual chromosome encoding can represent all the possible structures of the BNs. The subsequent theorems show that there is no BN structure that cannot be encoded by the proposed dual genetic encoding and the proposed encoding explores the entire solution space of the BN structures. First, we define two terminologies that will be used in the theorems. The *root* indicates a node that has no parent nodes and a *leaf* indicates a node that has no child nodes.

Theorem 1:

Any DAG has at least one root and one leaf. There is no DAG which does not have a root or a leaf.

Proof. Consider a DAG with n nodes. If there is no leaf in the DAG, then all nodes in the DAG have at least one child node. So if we select any node in the DAG and traverse from the node to one of its child nodes $n + 1$ times, then we would encounter the same node at least one time. That means that there is at least one loop in the DAG and this is a contradiction. Therefore, any DAG has at least one leaf. Similarly, if there is no root in the DAG, then all nodes have at least one parent node. If any node in the DAG is selected and movement is in the reverse direction from the node to one of its parent nodes $n + 1$ times, then the same node will be encountered at least one time. That means that there is at least one loop in the DAG and this is a contradiction. Therefore, any DAG has at least one root. □

Theorem 2:

Consider a DAG with $n + 1$ nodes. The DAG can be decomposed as a connection of a root (or a leaf) and a small DAG with n nodes.

Proof. Consider the DAG G with $n + 1$ nodes. Then, by theorem 1, G has at least one root and one leaf. If we remove the root R and the connected arcs from G , then the resulting graph G' will have n nodes. Assume that the resulting graph

G' is not the DAG. Then, there is at least one loop in G' . Even if the deleted node R is appended to G' and the disconnected arcs are restored, the resulting graph still has a loop. Since the resulting graph is the original graph G and it has a loop, it is a contradiction. Therefore, G' is also the DAG and we can conclude that a DAG with $n + 1$ nodes can be decomposed as a connection of a root and a small DAG with n nodes. In the same way, it can be shown that if a leaf L and the connected arcs are removed from G , the resulting graph G' becomes the DAG and it can be concluded that a DAG with $n + 1$ nodes can be decomposed as a combination of a leaf L and a small DAG with n nodes. □

Hence, a discussion follows that reveals that there is no BN structure which cannot be encoded by the proposed dual genetic encoding.

Theorem 3:

Any DAG with n nodes can be represented by a certain ordering among n nodes and an upper triangular connectivity matrix with respect to the given ordering.

Proof. Here, mathematical induction is utilized. When the number of nodes is two, the theorem trivially holds. Assume that x_1 is a root and x_2 is a leaf. If the ordering is “12”, the connectivity matrix $C = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ for the DAG is upper triangular. Next, assume that this theorem holds when the number of nodes is n and consider a DAG G with $n + 1$ nodes. By theorem 2, DAG G with $n + 1$ nodes can be decomposed as a connection of a root (or a leaf) and a small DAG with nodes. If G is decomposed as a connection of a root and a small DAG G' , the root and the connected arcs can be removed. Then, by the assumption, we can find a proper ordering O among n variables and upper triangular connectivity matrix C with respect to the ordering O .

$$O = a_1 a_2 \cdots a_n$$

$$C = \begin{pmatrix} 0 & c_{1,2} & c_{1,3} & \cdots & c_{1,n-1} & c_{1,n} \\ 0 & 0 & c_{2,3} & \cdots & c_{2,n-1} & c_{2,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & c_{n-1,n} \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \quad (11)$$

where

$$a_x \text{ is an integer and } a_x \in \{1, \dots, n + 1\}$$

$$\text{for } x = 1, \dots, n + 1$$

$$a_j \neq a_k \text{ iff } j \neq k$$

$$c_{i,j} = \begin{cases} 1 & \text{if } a_i \text{ is a parent of } a_j \\ 0 & \text{otherwise} \end{cases} \quad (12)$$

which fully represents G' . If the deleted root is denoted as a_{n+1} and the ordering among the $n + 1$ variables are selected as

$$O' = a_{n+1} a_1 a_2 \cdots a_n \quad (13)$$

then the original DAG with $n + 1$ nodes can be represented by an upper triangular connectivity matrix,

$$C' = \begin{pmatrix} 0 & c_{n+1,1} & c_{n+1,2} & c_{n+1,3} & \cdots & c_{n+1,n-1} & c_{n+1,n} \\ 0 & 0 & c_{1,2} & c_{1,3} & \cdots & c_{1,n-1} & c_{1,n} \\ 0 & 0 & 0 & c_{2,3} & \cdots & c_{2,n-1} & c_{2,n} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & c_{n-1,n} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & C'_{12} \\ 0 & C \end{pmatrix} \quad (14)$$

with respect to the ordering $O' = a_{n+1}a_1a_2 \cdots a_n$ where

$$c_{i,j} = \begin{cases} 1 & \text{if } a_i \text{ is a parent of } a_j \\ 0 & \text{otherwise} \end{cases}$$

and C is $n \times n$ upper triangular matrix
and C'_{12} is $1 \times n$ matrix (15)

Similarly, if G is decomposed as a connection of a leaf and a small DAG G'' , the leaf and the connected arcs can be removed. Then, by the assumption, a proper ordering O among n variables and upper triangular connectivity matrix C of (11) can be found, which fully represents the small DAG G'' . If the deleted leaf is denoted as a_{n+1} and the ordering among the $n+1$ variables are selected as

$$O'' = a_1a_2 \cdots a_na_{n+1} \quad (16)$$

then the original DAG with $n+1$ nodes can be represented by an upper triangular connectivity matrix,

$$C'' = \begin{pmatrix} 0 & c_{1,2} & c_{1,3} & c_{1,4} & \cdots & c_{1,n} & c_{1,n+1} \\ 0 & 0 & c_{2,3} & c_{2,4} & \cdots & c_{2,n} & c_{2,n+1} \\ 0 & 0 & 0 & c_{3,4} & \cdots & c_{3,n} & c_{3,n+1} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & c_{n,n+1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} C & C''_{12} \\ 0 & 0 \end{pmatrix} \quad (17)$$

where

$$c_{i,j} = \begin{cases} 1 & \text{if } a_i \text{ is a parent of } a_j \\ 0 & \text{otherwise} \end{cases}$$

and C is $n \times n$ upper triangular matrix
and C''_{12} is $n \times 1$ matrix (18)

This means that if the property is true for n , the property is also true for $n+1$ and the proof is completed. $\square$

3.2.2 Crossover

Consider the genetic operations (crossover and mutation) for the dual chromosome. First, let us consider the crossover. In the case of connectivity matrix, any upper triangular matrix is valid as a BN structure. Thus, the plain crossover is enough and is closed in the domain of the connectivity chromosomes as in [7]. However, in the case of the ordering chromosome, the crossover is not straightforward. In order

to explain the genetic crossover for the ordering chromosomes, let X_o and Y_o be two n dimensional ordering chromosomes represented by

$$X_o = x_1x_2 \cdots x_n$$

$$Y_o = y_1y_2 \cdots y_n \quad (19)$$

The proposed crossover generates a random number r from a uniform distribution from 1 to n and creates two new chromosomes X'_o and Y'_o according to following equations.

$$X'_o = x'_1x'_2 \cdots x'_n$$

$$Y'_o = y'_1y'_2 \cdots y'_n \quad (20)$$

$$x'_i = \begin{cases} x_i & \text{if } i < r \\ y_{\alpha_{i-r}} & \text{otherwise} \end{cases}$$

$$y'_i = \begin{cases} y_i & \text{if } i < r \\ x_{\beta_{i-r}} & \text{otherwise} \end{cases} \quad (21)$$

where

$$\alpha_0, \alpha_1, \dots, \alpha_{n-r} \in \{1, 2, \dots, n\}$$

$$\alpha_0 < \alpha_1 < \cdots < \alpha_{n-r}$$

$$y_{\alpha_j} \neq x_1, x_2, \dots, x_{r-1} \text{ for } j = 0, 1, 2, \dots, n-r$$

$$\beta_0, \beta_1, \dots, \beta_{n-r} \in \{1, 2, \dots, n\}$$

$$\beta_0 < \beta_1 < \cdots < \beta_{n-r}$$

$$x_{\beta_j} \neq y_1, y_2, \dots, y_{r-1} \text{ for } j = 0, 1, 2, \dots, n-r \quad (22)$$

Example 2 (Crossover for ordering chromosome):

Consider the two BNs in Example 1. Assume that the crossover operation is applied to the ordering chromosomes at the point between the second and the third genes, which means $r = 3$ and $n = 6$ in this example. The offspring start with

$$X'_{1o} = 12xxxx$$

$$X'_{2o} = 54xxxx \quad (23)$$

Since X'_{1o} contains "1" and "2", the two digits in X'_{2o} are deleted. Then the remaining sub-chromosome of X'_{2o} is "5436." The concatenation of the two parts yields an offspring ordering chromosome $X'_{1o} = 125436$. In the same way, "54" and "1263" are concatenated and the another offspring ordering chromosome becomes $X'_{2o} = 541263$.

$$X'_{1o} = 125436$$

$$X'_{1c} = 110000100010010$$

$$X'_{2o} = 541263$$

$$X'_{2c} = 110001100010011 \quad (24)$$

$$C'_1 = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, C'_2 = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (25)$$

If the connectivity chromosomes are the same as the parents, then the offspring BNs are depicted as in Fig. 3. $\square$

Fig. 3 Offspring BNs after crossover (Example 2).

The following shows the pseudo code of crossover for the ordering chromosome:

procedure OrderCrossover(Population)

Size=crossover_rate*Population_Size;

While (Size>0) **Do**

select p1 and p2 from Population;

select the crossover point value randomly from 1 to chromosome length;

generate two children chromosomes c1,c2;

i=0;

j=0;

While (i<crossover point) **Do**

put ith gene of p1 into that of c1;

put ith gene of p2 into that of c2;

i=i+1;

end

While (i<chromosome length) **Do**

While (j<chromosome length) **Do**

If jth gene of p2 is not in c1 **Then**

put jth gene of p2 into ith gene of c1;

i=i+1;

Else

j=j+1;

end

end

i=(crossover point);

j=0;

While (i<chromosome length) **Do**

While (j<chromosome length) **Do**

If jth gene of p1 is not in c2 **Then**

put jth gene of p1 into ith gene of c2;

i=i+1;

Else

j=j+1;

end

end

end

Size=Size-2;

chromosome[p1]=chromosome[c1];

chromosome[p2]=chromosome[c2];

end

end

Fig. 4 Two BNs before and after mutation (Example 3).

3.2.3 Mutation

For the connectivity chromosome, the plain mutation produces only the upper triangular matrix as in case of the crossover operation. Thus, the plain mutation is enough and is closed in the domain of the connectivity chromosomes as in [7]. The ordering chromosome is not the case. The following discussion explains the genetic mutation for the ordering chromosome. Let X_o be the n dimensional ordering chromosome,

$$X_o = x_1 x_2 \cdots x_n \quad (26)$$

The proposed mutation operator generates a random number r_1 and r_2 from a uniform distribution from 1 to n and creates the new chromosomes X'_o according to following equations:

$$X'_o = x'_1 x'_2 \cdots x'_n \quad (27)$$

$$x'_i = \begin{cases} x_{r_2} & \text{if } i = r_1 \\ x_{r_1} & \text{else if } i = r_2 \\ x_i & \text{otherwise} \end{cases} \quad (28)$$

Example 3 (Mutation for ordering chromosome):

Consider a BN structure with three variables as shown in Fig. 4 (a).

Using the proposed dual genetic encoding, the ordering and the connectivity chromosomes are represented as:

$$X_o = 123$$

$$X_c = 110 \quad (29)$$

respectively, and the connectivity matrix is as follows.

$$C = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (30)$$

Suppose that the first and the second genes of the ordering chromosome are exchanged, which means $r_1 = 1$, $r_2 = 2$, and $n = 3$ in this example, and the connectivity chromosome does not change. The resulting dual chromosome and the connectivity matrix become:

$$X'_o = 213$$

$$X'_c = 110 \quad (31)$$

$$C' = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (32)$$

Fig. 4 (b) depicts the mutated BN. $\square$

The following shows the pseudo code of mutation operation for the ordering chromosome:

```

procedure OrderMutation(Population)
  Size=mutation_rate*Population_Size;
  While (Size>0) Do
    select a chromosome from Population
    randomly;
    select two mutation point values i,j
    randomly from 1 to chromosome length;
    exchange ith and jth gene of the
    chromosome;
    Size=Size-1;
  end
end

```

4. Simulation

In this section, the proposed method is applied to three real-world problems and the validity of this method is demonstrated through computer simulation. In all the simulations, we restrict the maximum number of parents of each node to five. The restriction is not necessary but we place it for simple implementation. Without the restrictions, the number of possible configurations would increase exponentially with the number of parents [21]. It is a trade off between the performance and the computational cost.

4.1 Home Network System

In this section, the proposed method is applied to the home network system. The home network system is a typical test bed of the ubiquitous computing and sensor network, while it is expected to upgrade the quality of living over approximately the next decade. The implementation of context-aware computing is the key issue in the home network and has received attention from engineers and scientists. Context-aware computing is jargon coined by computer scientists and it is aimed at

1. gathering information about the users from various sensors distributed in a smart home,
2. recognizing the intention of the users, and
3. providing them with human friendly services.

In context-aware computing, it is assumed that

1. the home appliances and devices are equipped with wired/wireless sensors,
2. they gather information about the circumstances under which they operate,
3. they presume the intention or action of the users, and
4. they react according to the intention of the users.

Literature provides that the contexts of user activities can be presumed from the state of the environment [19]. However, context-awareness is not fully understood and the tools and techniques for developing context-aware applications

Fig. 5 An example of the BN structure for a Home network system.

are still in their infancy. BNs are one of the possible tools for the context-aware computing. In this example, the proposed method is applied and a BN is developed that presumes the intention or action of a single user, who lives in the home network system. Figure 5 shows the example of BN structure of the context-aware system for the home network.

A web-based virtual action simulator was developed in FLASH and a database of 672 cases for a context-aware system was built, for the purpose of training the BN [13]. Forty two random variables are used to implement the context-awareness of the BN. Twenty one variables represent the state of the home appliances such as the TV, lights in the living room, the refrigerator, etc. The other twenty one variables represent the activities of a single user, for example whether he/she is studying, sleeping, or dressing. Using the proposed method, the Bayesian network is trained such that the action of the user is presumed from the measurements of the sensors distributed in the context-aware home.

4.2 Car Diagnosis Problems

The car diagnosis problem introduced by Norsys is a simple example of belief network. The reason why a car does not move is presumed, based on spark plugs, headlights, main fuse, etc [14]. Eighteen nodes are used in this BN and all nodes of the network take discrete values. Some of them can take on three discrete states and the others can take on two states. A database of two thousand cases is utilized to train the BN. The database was generated from Netica tool [14]. Figure 6 shows the structure of the car diagnosis problem depicted by Netica from which the sample cases were collected. Note that, Fig. 6 depicts the desired BN structure and the goal of the structure learning for BN is to obtain the structures which are close to this desired one.

4.3 ALARM Network

ALARM (A Logical Alarm Reduction Mechanism) is a medical diagnostic system for patient monitoring. It is a complex belief network with eight diagnoses, sixteen findings, and thirteen intermediate variables [20]. A database of two thousand cases is utilized to train the BN. As in the previous example, the database is generated from Netica tool [14]. Figure 7 shows the structure of the ALARM network depicted by Netica from which the sample cases are collected. Note that, Fig. 10 depicts the desired BN structure

Fig. 6 The structure of the Car diagnosis problem network.

Fig. 7 The structure of the ALARM network.

and the goal of the structure learning for BN is to obtain the structures which are close to this desired one.

4.4 Simulation Results

Using the three databases, the BNs were built to represent the probabilistic relationships between the variables. Theorem 4 was utilized to apply the proposed dual genetic algorithms and evaluate the validity of the structure of the given BN [10].

Theorem 4:

Let Z be a set of n discrete variables, where a variable A_i , in Z has r_i possible value assignments: $(v_{i1}, \dots, v_{ir_i})$. Let D be a database of m cases, where each case contains a value assignment for each variable in Z . Let B_s denote a belief network structure containing just the variables in Z . Each variable A_i , in B_s has a set of parents, which are represented with a list of variables $pa(A_i)$. Let w_{ij} denote the j th unique instantiation of $pa(A_i)$ relative to D . Suppose there are q_i such unique instantiations of $pa(A_i)$. Define N_{ijk} to be the

number of cases in D in which variable A_i has the value v_{ik} and $pa(A_i)$ is instantiated as w_{ij} . Let $N_{ij} = \sum_{k=1}^{r_i} N_{ijk}$. If the cases occur independently and the probability density function $f(B_p|B_s)$ is uniform, where B_p is a vector whose values denote the conditional probability assignments associated with belief network structure B_s , then it follows that

$$P(B_s, D) = P(B_s) \prod_{i=1}^n \prod_{j=1}^{q_i} \frac{(r_i - 1)!}{(N_{ij} + r_i - 1)!} \prod_{k=1}^{r_i} N_{ijk}! \quad (33)$$

Since $P(B_s, D) = P(B_s)P(D|B_s)$ and $P(B_s)$ is uniformly distributed, the fittest BN structure B_s is determined by maximizing

$$P(D|B_s) = \prod_{i=1}^n \prod_{j=1}^{q_i} \frac{(r_i - 1)!}{(N_{ij} + r_i - 1)!} \prod_{k=1}^{r_i} N_{ijk}! \quad (34)$$

The simulation was run ten times for each problem and the parameters of the simulations were as follows: the population size of GA was 50, the crossover rate was 0.65 and

Fig. 8 Performance of the conventional and proposed methods (Home network system).

Fig. 9 Performance of the conventional and proposed methods (Car diagnosis problem).

Fig. 10 Performance of the conventional and proposed methods (ALARM network).

the mutation rate was 0.05. The formula in Theorem 4 was used, as an objective function to be maximized. The algorithms were stopped when 5,000 structures had been evaluated, which means that 100 generations have been evaluated. In this simulation, we assume that there is no prior knowledge about the node ordering or the casual relationship between the nodes. Therefore, we randomly select the order of the nodes in the conventional method. Figures 8, 9, and

Table 1 Comparison of the proposed and the previous methods (Home network problem).

Application	Trial time	Conventional method	Proposed method
Home network System	1	23895.26	17823.24
	2	27617.36	20605.52
	3	20809.5	19482.32
	4	19119.23	20047.76
	5	20850.03	21245.77
	6	21808.97	19360.47
	7	18104.05	21817.03
	8	21760.08	22136.7
	9	24102.79	21767.96
	10	24806.22	20328.63
	Average	22287.35	20461.54
	Variance	8103187	1811859
	Best	18104.05	17823.24
	Worst	27617.36	22136.7

Table 2 Comparison of the proposed and the previous methods (Car diagnosis problem).

Application	Trial time	Conventional method	Proposed method
Car diagnosis problem	1	39687.91	37821.28
	2	41628.53	38468.16
	3	43565.91	39754.24
	4	42368.24	37821.28
	5	38214.65	37821.28
	6	39658.21	37923.45
	7	39462.29	38165.23
	8	40216.35	37821.28
	9	39845.23	37821.28
	10	41268.24	38321.46
	Average	40591.56	38173.89
	Variance	2538557.87	365593.57
	Best	38214.65	37821.28
	Worst	43565.91	39754.24

10 show the learning result of the first run for the home network, car diagnosis, and ALARM problems, respectively. In the figures, the dashed lines represent the result of the conventional method and the solid lines represent the result of the proposed method. The vertical axis is the negative logarithm of (34) and the horizontal axis is the number of generations. As BN attempts to approximate the entire database, the vertical axis approaches zero, since the probability of one corresponds to zero on the negative logarithm axis. In the home network and car diagnostic systems, it can be seen that the proposed method initially outperforms the conventional method and continues to outperform the conventional method for the next one hundred generations, as shown in Figs. 8 and 9, respectively.

Although the proposed method does not show good performance for less than thirty generations, it outperforms the conventional method after thirty generations in the ALARM network, as shown in Fig. 10.

The reason for the excellence of the proposed method could be attributed to the fact that the search space was fully explored by the dual encoding of GA. Tables 1, 2, and 3 compare the performances of the conventional method and the proposed method in terms of (34). The simulation was

Table 3 Comparison of the proposed and the previous methods (Home network problem).

Application	Trial time	Conventional method	Proposed method
ALARM network	1	86548.32	73401.54
	2	84231.24	75860.24
	3	79324.23	73401.54
	4	86954.94	73401.54
	5	84321.12	78203.38
	6	81423.24	73401.54
	7	75165.21	73401.54
	8	84246.73	74632.21
	9	81234.23	75352.21
	10	87549.65	73401.54
	Average	83099.891	74445.73
	Variance	14905182.13	2613249.931
	Best	75165.21	73401.54
	Worst	87549.65	78203.38

Fig. 11 Network structure of the proposed learning result (Car diagnosis problem). **Fig. 12** structure of the proposed learning result (ALARM network).

run until 5,000 structures had been evaluated. This was repeated ten times. For all three problems, the proposed method outperforms the conventional method in not only the average case but also in the best and worst cases.

Figures. 11 and 12 show the network structures for the learning results of the first run in case of Car diagnosis prob-

Table 4 Index and name of the nodes (Car diagnosis problem).

Node index	Node name	Node index	Node name
1	Starter system	10	Spark plugs
2	Headlights	11	Fuel system
3	Charging system	12	Car cranks
4	Alternator	13	Air filter
5	Battery voltage	14	Air system
6	Distributor	15	Car starts
7	Spark timing	16	Battery age
8	Voltage at plug	17	Starter motor
9	Spark quality	18	Main fuse

Table 5 Index and name of the nodes (ALARM network).

Node index	Node name	Node index	Node name
1	Catechol	20	SaO2
2	HR	21	PAP
3	LVFailure	22	PulmEmbolus
4	LVEDVolume	23	ErrCauter
5	Hypovolemia	24	VentAlv
6	CVP	25	Intubation
7	HRBP	26	VentLung
8	HREKG	27	KinkedTube
9	HRSat	28	Disconnect
10	ErrLowOutput	29	VentTube
11	TPR	30	Press
12	Anaphylaxis	31	ArtCO2
13	BP	32	ExpCO2
14	PCWP	33	MinVol
15	StrokeVolume	34	MinVolSet
16	CO	35	VentMach
17	PVSat	36	FiO2
18	InsuffAnesth	37	History
19	Shunt		

Table 6 Statistical results of the conventional and proposed method.

Application	Algorithm	Best	Mean	Variance
Car diagnosis problem	Conventional	38214.65	40591.56	2538557.87
	Proposed	37821.28	38173.89	365593.57
	Target		37821.28	
ALARM network	Conventional	75165.21	83099.89	14905182.13
	Proposed	73401.54	74445.73	2613249.93
	Target		73401.54	
Home network system	Conventional	18104.05	22287.35	8103187
	Proposed	17823.24	20461.54	1811859
	Target		N/A	

lem and ALARM network, respectively. It can be shown that the resulting structures are same as the target network structures in Figs. 6 and 7, respectively. Tables 4 and 5 represent the indices and names of the node which are shown in Figs. 11 and 12, respectively.

Statistical results are summarized in Table 6. In the table, the learned structures are compared with the target structure from which the sample data are taken. In case of the Home network system, there is no target structure since the data are collected not from the target structure but from the virtual simulator.

For further evaluation, we compare the proposed method with the conventional method in terms of number of arcs correctly added between the same nodes as those in the target network, the number of missed arcs of the target network, or the number of extra arcs added wrongly. In Tables 7

Table 7 Comparison with the target structure (Car diagnosis problem).

Application	Trial time	Conventional method		Proposed method	
		missed arcs	wrongly added arcs	missed arcs	wrongly added arcs
Car diagnosis problem	1	2	2	0	0
	2	4	2	1	2
	3	5	1	2	1
	4	3	3	0	0
	5	1	0	0	0
	6	1	1	0	1
	7	2	0	1	1
	8	3	0	0	0
	9	3	0	0	0
	10	4	0	1	0

Table 8 Comparison with the target structure (ALARM network).

Application	Trial time	Conventional method		Proposed method	
		missed arcs	wrongly added arcs	missed arcs	wrongly added arcs
Car diagnosis problem	1	5	2	0	0
	2	4	1	2	0
	3	4	2	0	0
	4	6	1	0	0
	5	4	0	3	1
	6	3	0	0	0
	7	3	0	0	0
	8	4	1	1	1
	9	3	2	1	2
	10	7	2	0	0

and 8, the two methods are compared. It can be seen that the proposed method finds the target network much better than the conventional method and the reason might be that the proposed method fully explore the entire search space for the fittest structure.

5. Conclusions

In this paper, a new structure learning approach for BNs has been proposed. In this method, the BN is encoded as a dual chromosome that is composed of an ordering chromosome and a connectivity chromosome. It is rigorously shown that the proposed dual genetic encoding fully represents the possible BN structure. A wider solution space is explored than in previous method. The proposed method is applied to three real-world and benchmark problems, while simulation reveals improved performance over the previous method for all three case studies. In this experimentation, it should be noted that the cost function (34) taken from [10] does not consider the computation complexity and the cases that there are some unobserved nodes. If we can devise more reasonable cost function which overcomes these problems, we can obtain better BN structure. Finally, this is recommended as a future work.

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