STRUCTURE LEARNING OF BAYESIAN NETWORKS BY HYBRID GENETIC ALGORITHMS

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ABSTRACT

This paper demonstrates how Genetic Algorithms can be used to discover the structure of a Bayesian Network from a given database with cases. The results presented, were obtained by applying four different types of Genetic Algorithms – SSGA (Steady State Genetic Algorithm), GAeλ (Genetic Algorithm elistist of degree λ), hSSGA (hybrid Steady State Genetic Algorithm) and the hGAeλ (hybrid Genetic Algorithm elitist of degree λ) – to simulations of the ALARM Network. The behaviour of the mentioned algorithms is studied with respect to their parameters.

Keywords: Bayesian Network, Genetic Algorithms, Structure Learning.

1. INTRODUCTION

In recent years, the search for the structure of a Bayesian Network able to reflect all existing relations of interdependence in a database of cases has constituted a research topic of fundamental importance. Although the first algorithms were related to tree and polytree structures (see for instance Chow and Liu (1968), Rebane and Pearl (1989)), research has been concentrated upon multiple connected structures (Fung and Crawford (1990), Herskovits and Cooper (1990), Cooper and Herskovits (1992), Bouckaert (1993), Wedelin (1993), Lauritzen et al. (1993), Chickering et al. (1994), Bouckaert (1994)).

In this article we propose to obtain the Bayesian Network structure with the help of an intelligent search process, based on Genetic Algorithms.

2. GENETIC ALGORITHMS

Evolutionary Algorithms are probabilistic search algorithms which simulate natural evolution. They were proposed about 30 years ago. Their application to combinatorial optimization problems has, however, only recently become an actual research topic. Three different types of Evolutionary Algorithms exist: Genetic Algorithms (Holland (1975), Goldberg (1989), Davis (1991)), Evolution Strategies (Schwefel (1967)) and Evolutionary Programming (Fogel (1962)) . This paper, however, focusses upon Genetic Algorithms (GAs). GAs are search algorithms based on the mechanics of natural selection and genetics. They combine "survival of the fittest" among string structures with a structured yet randomized information exchange to form a search algorithm which, under certain conditions, evolves to the optimum with probability 1 (Eiben et al. (1990), Chakraborty and Dastidar (1993), Rudolph (1994)).

In GAs the search space of a problem is represented as a collection of individuals. The individuals are represented by character strings, which are often referred to as *chromosomes*. The purpose of a GA is to find the individual from the search space with the best "genetic material". The quality of an individual is measured with an objective function. The part of the search space to be examined in each iteration is called the *population*.

A Genetic Algorithm approximately works as follows. First, the initial population is chosen at random, and the quality of each of its individual is determined. Next, in every iteration parents are selected from the population. These parents produce children, which are added to the population. For all newly created individuals of the resulting population a probability near zero exits that they can "mutate", i.e. that they

change their hereditary distinctions. Later, some individuals are removed from the population according to a selection criterion in order to reduce the population to its initial size. One iteration of the algorithm is referred to as a *generation*.

The operators which define the child production process and the mutation process are called the *crossover operator* and the *mutation operator*, respectively. Mutation and crossover play different roles in the GA. Mutation is needed to explore new states and helps the algorithm to avoid being trapped on local optima. Crossover should increase the average quality of the population. By choosing adequate crossover and mutation operators, as well as a reduction mechanism, the probability that the GA results in a near-optimal solution in a reasonable number of iterations is enlarged.

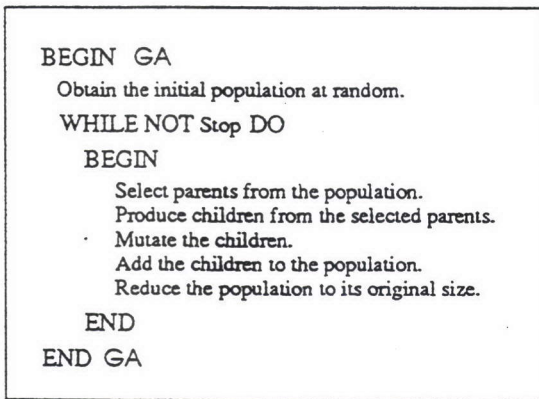In Figure 1 we show the basic structure of a Genetic Algorithm (GA).

```
BEGIN GA
    Obtain the initial population at random.
    WHILE NOT Stop DO
    BEGIN
        Select parents from the population.
        Produce children from the selected parents.
        Mutate the children.
        Add the children to the population.
        Reduce the population to its original size.
    END
END GA
```

Figure 1 : Basic Structure of the Genetic Algorithm (GA).

3. PROPOSED APPROACH

We represent a Bayesian Network structure by a *connectivity matrix* $C = (c_{ij})_{i,j=1,..,n}$, where

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

The inequality $i > j$ originates in the assumed ancestral order between the variables. Because of the inequality the crossover and mutation operators to be used are closed operators.

We consider four different Genetic Algorithms to which we refer as the SSGA (Steady State Genetic Algorithm), the GAeλ (Genetic Algorithm elitist of degree λ), the hSSGA (hybrid Steady State Genetic Algorithm) and the hGAeλ (hybrid Genetic Algorithm

elitist of degree λ).

In an iteration of the SSGA and the hSSGA only one new individual is created, while in the GAeλ and the hGAeλ the generation replacement has a global character. In all algorithms, the reduction criterion is elitist. In the SSGA and the hSSGA, the created individual is compared with the worst existing individual at the time of creation. In the GAeλ, and the hGAeλ, however, the population at time $t + 1$ consists of the λ best individuals of the set of the λ individuals which constitute the population at time t and their λ created children.

The behaviour of all algorithms is studied with the help of three different *population sizes* λ ($\lambda = 10$, $\lambda = 50$, $\lambda = 100$).

The *objective function* to be used to evaluate the quality of a structure, is based on the formula proposed by Cooper and Herskovits (1992), for a joint probability $P(B_S, D)$ of a Bayesian Network structure B, and a database D, expressed in terms of the natural logarithm. Therefore, our aim is to find the structure with the highest joint probability.

The *selection function* is based on the rank of the objective function. If we denote by I_t^j the j-th individual of the population at time t, and by $\text{rank}(g(I_t^j))$ the rank of its objective function, the probability $p_{j,t}$ that individual I_t^j is selected to be a parent is equal to

$$p_{j,t} = \frac{\text{rank}(g(I_t^j))}{\lambda(\lambda + 1)/2}.$$

The *reproduction function* to be used is the so-called 1-point crossover operator. Following the selection of two parents, the probability that these parents are crossed is 1. This probability makes it feasible to compare the algorithms.

The *mutation operator* consists of the probabilistic alteration of the bits, which represent the connectivity matrix. This alteration is performed with a probability near to zero. We consider two different mutation probabilities p_m, namely $p_m = 0.001$ and $p_m = 0.01$.

The algorithms *stop* when either, 10,000 structures have been evaluated or when in 1000 successive evaluations, the value of the objective function of the best structure corresponds with the average value of the objective function.

The initial population is generated at random, subject to the restriction that a node never has more than m parent nodes (in our case, $m = 4$).

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After applying the crossover and mutation operators, the created structures do not necessarily fulfil the restriction that the nodes all have at most m parents. To maintain this restriction, in a first approach (the algorithms SSGA and GAeλ), we select n parents at random, $(0 \leq n \leq m)$, for every node from the parent nodes resulting from crossover and mutation. This approach will give quite poor results. Therefore, we try a second approach in which the fundamental characteristic is the hybridization of the previously mentioned Genetic Algorithms, with the help of a *local optimizer*. This optimizer selects for every node in a child structure, the best subset of at most m elements from the set of its parents nodes. The process of generating child structures and the application of the local optimizer, is repeated in every iteration of the algorithm.

4. RESULTS

We describe the results of an experiment in which a database of cases generated by simulation of the ALARM Network is used to search for the structure which has a maximal joint probability. This joint probability is compared with the corresponding value of the structure of the ALARM Network. Also the Hamming distance between both structures, and the number of evaluations needed to obtain convergence are considered. All results were obtained with a SPARCserver 1000 under operating system Solaris 2.3.

We applied the algorithms to a database of 10,000 cases generated with the ALARM Network, which was constructed by Beilinch et al. (1989) as a prototype to model potential anesthesia problems in the operating room. The simulation of the 10,000 cases of this network has been achieved with the help of a Monte Carlo technique developed for Bayesian Networks by Henrion (1988). It corresponds with the first 10,000 cases generated by Herskovits (1991). We have considered different subsets consisting of the first 100, 200, 500, 1000, 2000, 3000, and 10,000 cases from the original database. The evaluations of the initial structures for the different databases can be seen in Table 1.

All algorithms are evaluated with respect to the population size and the mutation rate. For every possible combination of parameters 10 executions were carried out. Therefore, the total number of performed evaluations for every database of cases has been $2 \times 2 \times 3 \times 2 \times 10 = 240$.

Number of cases ALARM Network	$\log P(B_S, D)$
100	-6.3860e02
200	-1.1413e03
500	-2.6461e03
1000	-5.0345e03
2000	-9.7291e03
3000	-1.4412e04
10,000	-4.7086e04

Table 1: Evaluation of the ALARM Bayesian Network structure with different simulation sizes.

In Table 2 and Table 3 the results are presented. The legend BOF means the best value found of the objective function and AOF is the average value of the objective function. The legend HD refers to the Hamming distance between the ALARM Network structure and the one with the best objective function, while the number between parenthesis is the average Hamming distance.

By comparing Table 2 with Table 3, we see the importance of the local optimizer. While in Table 2 only for small population sizes (λ=10) the corresponding evaluation function of the ALARM Network was improved, all results of the hybrid algorithms hSSGA and hGAeλ (see Table 3) were better than the ones presented in Table 1.

Another remarkable point is the small variability in the results found by the hybrid algorithms (see Table 3) with respect to the ones obtained by the SSGA and the GAeλ (see Table 2).

Because of the mentioned considerations, we decided to analyze the algorithms SSGA and GAeλ separately from the hybrid algorithms.

The analysis of the 1680 (240 × 7) runs has been carried out using the Kruskal-Wallis test, which looks for differences statistically significants.

1.- Analysis of the results of the SSGA and the GAeλ

Objective Function

The average behaviour of the SSGA is similar to the GAeλ. There are no statistically significant differences in any of the 7 databases. However, statistically significant differences exist with respect to the population size, obtaining the best performance with

$\lambda=10$. The results found with the mutation rate $p_m=0.001$ are significantly better than the ones found with $p_m=0.01$.

Number of evaluations needed until convergence

For the population sizes $\lambda=50$ and $\lambda=100$, none of the algorithms was able to converge under the stop criterion earlier described. For $\lambda=10$, the convergence velocity, both of the SSGA as well as of the GAeλ, is significantly larger for $p_m=0.001$ than for $p_m=0.01$ for all databases considered.

The poor results found with this first approach we attribute to the "blind" parent selection process used for maintaining the restriction on the maximum number of parents.

2.- Analysis of the results of the hSSGA and the hGAeλ

Objective Function

For the small databases (100, 200 and 500 cases) we found statistically significant differences for the mutation rate, obtaining the best performance for $p_m=0.01$. The population size only resulted to be significant for the 500-case database, where the performance improved as the population size became larger. The large databases (1000, 2000, 3000 y 10,000 cases) did give statistically significant differences with respect to none of the three parameters considered (the type of the GA, the population s *Number of evaluations needed until convergence*

The stop criterion was sufficient for guaranteeing the convergence of the hybrid algorithms. We found, for all databases, that the hSSGA converges significantly faster than the hGAeλ. Moreover, the algorithms converged faster as the population size became smaller. Finally a mutation rate equal to 0.01 resulted in a faster convergence than a mutation rate of 0.001.

The best structure obtained by the hybrid algorithms coincided for both the algortihms and was found with both the 3000-case database as well as the 10,000-case database. If we compare this structure (see Figure 2(b)) with the ALARM Network (see Figure 2(a)), we see that the only difference between the two structures is the arc from node 12 to node 32, which is missing in the best structure found by the hybrid algorithms. The best structure found by the hybrid algorithms with the 2000-case database is shown in Figure 2(c). This structure has, in comparison with the ALARM Network, two additional arcs (the arc from node 24 to node 10, and the arc from node 30 to node 3) and one missing arc (the arc from node 12 to node 32).

The obtained improvements using the local optimizer, we interpret as an empirical demonstration of the validity of our hybrid approach. The local search related to every node involves that unimportant parts of the search space are not examined.

5. CONCLUSIONS AND FUTURE RESEARCH

We have illustrated how the genetic approach can be used in the Structure Learning of Bayesian Networks from a database of cases.

First, we have tried an approach in which a "blind" selection process was used to "repair" created structures with nodes which have too many parents. Second, we have followed a hybrid approach. The results of the latter approach are far better than the results of the former approach. In this case the results are independent of the generation gap and, in outline, also of the mutation rate and the population size.

In the future we plan to tackle the more general problem in which the assumption of the ancestral ordering between the variables is not assumed. Other potential research is related to the use of different evaluation functions, some of which appear in Bouckaert (1993, 1994) and Chickering et al. (1994).

We expect that our approach can also be applied to dynamical Bayesian Networks. Also, it would be interesting to investigate the use of other heuristical search methods, like i.e. Tabu Search.

Acknowledgements

		SSGA			GAeλ		
		$\lambda = 10$	$\lambda = 50$	$\lambda = 100$	$\lambda = 10$	$\lambda = 50$	$\lambda = 100$
100	BOF	-6.2014e02	-6.2363e02	-6.3223e02	-6.2090e02	-6.2650e02	-6.4073e02
	AOF	-6.3952e02	-6.4680e02	-6.5899e02	-6.3993e02	-6.5037e02	-6.6497e02
	HD	31(48.2)	32(51.7)	34(56.5)	37(49.4)	38(55)	51(65.7)
200	BOF	-1.1256e03	-1.1307e03	-1.1432e03	-1.1253e03	-1.1348e03	-1.1587e03
	AOF	-1.1556e03	-1.1673e03	-1.1911e03	-1.1543e03	-1.1755e03	-1.2038e03
	HD	19(38.5)	19(42.4)	34(52.9)	17(38.1)	22(45.5)	37(57.9)
500	BOF	-2.6350e03	-2.6438e03	-2.6741e03	-2.6354e03	-2.6492e03	-2.7069e03
	AOF	-2.6918e03	-2.7186e03	-2.7740e03	-2.6908e03	-2.7262e03	-2.7946e03
	HD	11(34.8)	18(41.2)	29(52.9)	12(33.2)	22(45.1)	41(58.8)
1000	BOF	-5.0279e03	-5.0404e03	-5.0799e03	-5.0286e03	-5.0611e03	-5.1533e03
	AOF	-5.1117e03	-5.1741e03	-5.2491e03	-5.1137e03	-5.2026e03	-5.3185e03
	HD	4(30.2)	15(40.8)	28(53.7)	2(30.2)	20(45.3)	38(60.5)
2000	BOF	-9.7200e03	-9.7440e03	-9.8159e03	-9.7200e03	-9.7538e03	-9.8769e03
	AOF	-9.8504e03	-9.8890e03	-9.9481e03	-9.8436e03	-9.9188e03	-10.0068e03
	HD	3(30.7)	11(41.4)	28(54.9)	3(30.1)	16(47.6)	43(66.1)
3000	BOF	-1.4404e04	-1.4425e04	-1.4485e04	-1.4405e04	-1.4450e04	-1.4649e04
	AOF	-1.4578e04	-1.4722e04	-1.4957e04	-1.4580e04	-1.4810e04	-1.5173e04
	HD	1(29)	12(41.4)	29(56.2)	2(30.3)	22(50.5)	48(68.8)
10,000	BOF	-4.7079e04	-4.7118e04	-4.7279e04	-4.7079e04	-4.7163e04	-4.7362e04
	AOF	-4.7462e04	-4.8019e04	-4.8506e04	-4.7531e04	-4.8264e04	-4.9083e04
	HD	2(31.1)	15(46.4)	34(61.2)	2(32.5)	26(55.6)	42(72.3)

Table 2: Results obtained with the SSGA and the GAeλ.

|		hSSGA			hGAeλ		
		$\lambda = 10$	$\lambda = 50$	$\lambda = 100$	$\lambda = 10$	$\lambda = 50$	$\lambda = 100$
100	BOF	-6.1901e02	-6.1901e02	-6.1901e02	-6.1901e02	-6.1901e02	-6.1901e02
	AOF	-6.1928e02	-6.1932e02	-6.1921e02	-6.1945e02	-6.1927e02	-6.1920e02
	HD	34(35.6)	34(35.6)	33(35.6)	34(35.7)	34(35.6)	32(35.3)
200	BOF	-1.1249e03	-1.1249e03	-1.1249e03	-1.1249e03	-1.1249e03	-1.1249e03
	AOF	-1.1249e03	-1.1253e03	-1.1249e03	-1.1249e03	-1.1249e03	-1.1250e03
	HD	19(19.9)	19(20)	20(20)	19(19.9)	18(19.6)	17(19.4)
500	BOF	-2.6350e03	-2.6350e03	-2.6350e03	-2.6350e03	-2.6350e03	-2.6350e03
	AOF	-2.6360e03	-2.6353e03	-2.6350e03	-2.6350e03	-2.6350e03	-2.6350e03
	HD	12(13)	11(12.5)	12(12.3)	12(12.6)	12(12.1)	11(12.1)
1000	BOF	-5.0279e03	-5.0279e03	-5.0279e03	-5.0279e03	-5.0279e03	-5.0279e03
	AOF	-5.0279e03	-5.0279e03	-5.0279e03	-5.0281e03	-5.0303e03	-5.0279e03
	HD	4(4)	4(4)	4(4)	4(4.1)	3(4.1)	4(4.1)
2000	BOF	-9.7200e03	-9.7200e03	-9.7200e03	-9.7200e03	-9.7200e03	-9.7200e03
	AOF	-9.7206e03	-9.7200e03	-9.7200e03	-9.7205e03	-9.7200e03	-9.7200e03
	HD	3(3.1)	3(3)	3(3)	3(3.1)	3(3)	3(3)
3000	BOF	-1.4404e04	-1.4404e04	-1.4404e04	-1.4404e04	-1.4404e04	-1.4404e04
	AOF	-1.4404e04	-1.4404e04	-1.4404e04	-1.4404e04	-1.4404e04	-1.4407e04
	HD	1(1)	1(1)	1(1)	1(1)	1(1)	1(1.2)
10,000	BOF	-4.7078e04	-4.7078e04	-4.7078e04	-4.7078e04	-4.7078e04	-4.7078e04
	AOF	-4.7078e04	-4.7082e04	-4.7078e04	-4.7078e04	-4.7083e04	-4.7078e04
	HD	1(1)	1(1.1)	1(1)	1(1)	1(1.1)	1(1)

Table 3: Results obtained with the hSSGA and the hGAeλ.

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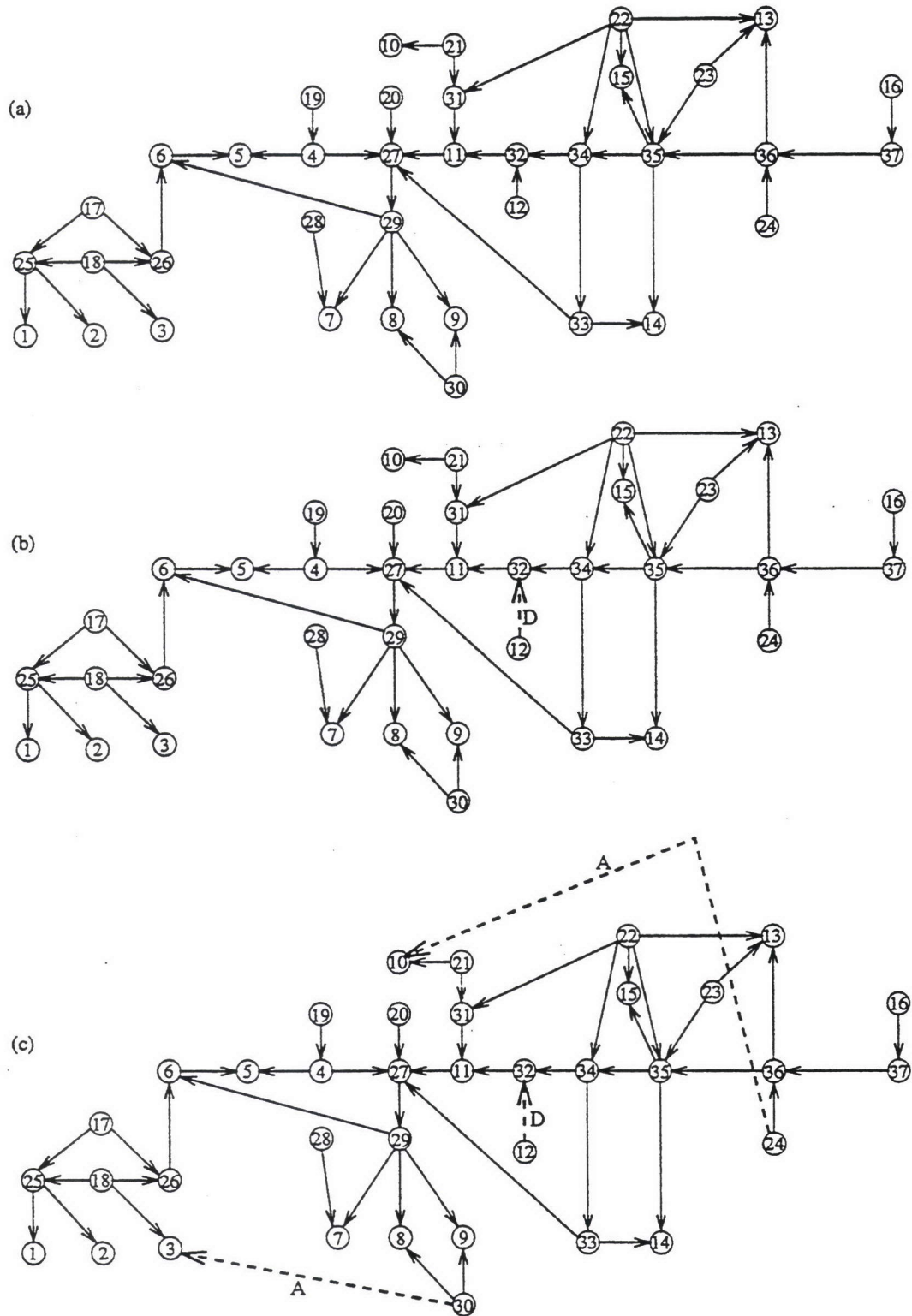
Figure 2: (a) The ALARM network structure. (b) The network structure learned by the hSSGA and the hGAeλ algorithms from a 10000-case and 3000-case database generated from the ALARM network. (c) The network structure learned by the hSSGA and the hGAeλ algorithms from a 2000-case database generated from the ALARM network. Arcs that are added or deleted with respect to the ALARM network are indicated with A and D respectively.

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