Approximating Discrete Probability Distributions
with Decomposable Models

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Abstract—A heuristic procedure is presented to approximate an n-dimensional discrete probability distribution with a decomposable model of a given complexity. It is shown that, without loss of generality, the search space can be restricted to a suitable subclass of decomposable models, whose members are called elementary models. The selected elementary model is constructed in an incremental manner according to a local-optimality criterion that consists in minimizing a suitable cost function. It is further shown with an example that the solution computed by the procedure is sometimes optimal.

I. INTRODUCTION

It is generally acknowledged that, when designing information systems such as communication, pattern recognition, knowledge and data base systems, the problem that typically arises is that of approximating (or estimating) an n-dimensional discrete probability distribution from a finite number of given marginals (or samples), and storing the distributions in a certain limited amount of machine memory.

In [16] the problem of approximating an n-dimensional discrete probability distribution with a product form was considered. In [5], a method for optimally approximating an n-dimensional discrete probability distribution with a set of n - 1 first-order dependence relationships among the n variables (i.e., bidimensional marginal distributions) was presented. The procedure in [5], which is inspired by a hill-climbing search strategy, involves an optimization process to construct a dependence tree of maximum weight. As a matter of fact, in many applications unidimensional and bidimensional marginal distributions are inappropriate to extract features that distinguish different patterns.

Better approximations can be obtained by considering interaction models [2], [7] (also called dependency models [23]) made up of arbitrary sets of marginal distributions. Decomposable models [2], [7], [10], [11] are special interaction models that possess a number of desirable properties. The two following properties stress the desirability of decomposable models both from a semantic and formal point of view:

(semantic property) a decomposable model can be represented by a "Markovian belief network" [23],
(formal property) the approximation generated by a decomposable model has a "product form" [2], [10], [11], [19].

In this paper, we address the problem of finding the model that generates the best approximation to a given discrete probability distribution, selected among the decomposable models of a given complexity.

Apart from special cases, this problem can be solved exactly only by exhaustive search [23]. Now, when the number of variables involved is high, exhaustive search is impractical since the number of models that must be examined is enormous. Therefore, one is forced to relax the optimality requirement and settle for finding a good solution using only a reasonable amount of search effort.

II. BACKGROUND

Let X = {A_1, · · ·, A_n} be a set of discrete random variables, whose value sets will be denoted by range(A_1), · · · , range(A_n). Given a joint probability distribution p(x), an approximation to p(x) can be obtained by hypothesizing a structural model [2] over X, that is, a specific stochastic relation among the variables in X. In what follows, by domain of a structural model μ we mean the set of all probability distributions over X that are perfectly fitted by the model μ.

The simplest example of structural model over X is given by an independence model, which consists in viewing the variables in X partitioned into (stochastically) independent sets. Let M = {X_1, · · ·, X_m} be such a partition of X and μ the independence model generated by M. The domain of μ contains all the probability distributions p(x) that can be factorized as

\[ p(x) = p_1(x_1) · · · p_m(x_m) \]

where \( p_h(x_h) \) is the marginal of \( p(x) \) relative to \( X_h (h = 1, · · · , m) \).

In information-theoretic terms, independence of \( X_1, · · ·, X_m \) is expressed by the condition that the (mutual) information [26] of \( X_1, · · ·, X_m, \) defined as

\[ I(X_1, · · · , X_m) = H(X_1) + · · · + H(X_m) - H(X) \]

is zero. Here, \( H(X_h) \) and \( H(X) \) stand for the entropies [26] of the probability distributions \( p_h(x_h) \) and \( p(x) \), that is,

\[ H(X_h) = - \sum_{x_h} p_h(x_h) \log p_h(x_h) \]

and

\[ H(X) = - \sum_{x} p(x) \log p(x) \]

A widely used structural model, which is a natural extension of an independence model, is a conditional-independence model [8], [12] (or zero-partial-association model [29]), which consists in viewing the variables in X partitioned into nonempty sets \( Y_0, Y_1, · · ·, Y_m \) such that \( Y_1, · · ·, Y_m \) are conditionally independent given \( Y_0 \). The domain of such a model contains all the probability distributions \( p(x) \) that can be factorized as follows

\[ p(x) = p_0(y_0) p_1(y_0, y_1) · · · p_m(y_0, y_m) / p_0(y_0)^{m-1} \]

In information-theoretic terms, the conditional independence of \( Y_1, · · ·, Y_m \), given \( Y_0 \) is expressed by the condition that the average conditional information [26] of \( Y_1, · · ·, Y_m \) given \( Y_0 \), defined as

\[ I(Y_1, · · · , Y_m / Y_0) = H(Y_1 / Y_0) + · · · + H(Y_m / Y_0) - H(Y_1 · · · Y_m / Y_0) \]

is zero. Here, \( H(Z / Y) \) denotes the average conditional entropy [26] of the variable set \( Z \) given the variable set \( Y \), defined as

\[ H(Y \cup Z) - H(Y) \]
The most general form of independence is taken into account by an interaction model over $X$, which groups the variables in $X$ into (possibly overlapping) sets (to be called the generators of the model) having "interaction zero" [13], [18]. If $X_1, \ldots, X_m$ denote the generators of such an interaction model $\mu$, as usual we assume that 1) $X = (X_1, \ldots, X_m$ and that 2) no generator of $\mu$ is a subset of any other. According to the terminology used in graph theory [1], [15], the set $M = \{X_1, \ldots, X_m\}$ will be called the generating hypergraph (also called "generating class") [2], [7], [8], [9], [10] of $\mu$. The domain $P_\mu$ of the interaction model $\mu$ generated by the hypergraph $M$ contains all the probability distributions $p(x)$ that can be expressed in the following multiplicative form

$$p(x) = f_1(x_1) \cdots f_m(x_m)$$

(1)

where $f_1(x_1) \cdots f_m(x_m)$ are implicit functions uniquely determined by the condition that the multiplicative form (1) represent an extension of the marginals $p_1(x_1), \ldots, p_m(x_m)$ of $p(x)$, that is, for all $h = 1, \ldots, m$

$$p_h(x_h) = \sum_{x \in M - X_h} \sum_{x_{\in M-h} \in \text{graph}(M)} p(x)$$

$$= f_h(x_h) \left[ \sum_{x \in M - X_h} \sum_{x_{\in M-h} \in \text{graph}(M)} \prod_{i \neq h} f_i(x_i) \right]$$

An interaction model $\mu$ over $X$ can be represented by an ordinary graph, to be called a dependence graph denoted by $G_\mu$, which has $X$ as its node set and an edge between every pair of variables that are contained in a single generator of $\mu$. An expressive property of $G_\mu$ is that if $Y_0$ is a cutset and $Y_1, Y_2, \ldots, Y_m$ are the connected components of the graph obtained from $G_\mu$ by deleting $Y_0$, then $Y_1, Y_2, \ldots, Y_m$ are conditionally independent given $Y_0$ [8].

Consider now the problem of approximating a given probability distribution $p(x)$ using interaction models. Let $\mu$ be the interaction model generated by the hypergraph $M = \{X_1, \ldots, X_m\}$, the approximation $p_\mu(x)$ to $p(x)$ based on $\mu$ is defined as the extension of the marginals $p_1(x_1), \ldots, p_m(x_m)$ of $p(x)$, which is uniquely determined by the membership in $P_\mu$, that is, by the multiplicative form (1) [14]. It is well-known [4], [16] that $p_\mu(x)$ is the maximum-entropy extension of the marginals $p_1(x_1), \ldots, p_m(x_m)$ of $p(x)$. Moreover, $p_\mu(x)$ can be computed using an iterative proportional fitting procedure [4], [21].

Now, let us consider the problem of selecting the "best" approximation to an $n$-dimensional probability distribution $p(x)$ among the approximations based on interaction models of a given complexity. The aspects of this problem with regards to complexity will be discussed in the next section, while the remainder of this section will be devoted to the criterion for evaluating the accuracy of the approximation $p_\mu(x)$ to $p(x)$ based on an arbitrary interaction model $\mu$. As usual [4], [5], [14], [16], this will be measured by the information divergence [6] (or discrimination information [13], [14] or cross-entropy [28] or Kullback-Leibler distance [3])

$$D(p, p_\mu) = \sum_x p(x) \log \frac{p(x)}{p_\mu(x)}$$

$$= -H(X) - \sum_x p(x) \log p_\mu(x)$$

(2)

which can be interpreted as the difference of the information contained in $p(x)$ and that contained in $p_\mu(x)$ about $p(x)$ [16]. The information divergence $D(p, p_\mu)$ is a non-negative quantity that vanishes if and only if $p_\mu(x)$ coincides with $p(x)$, that is, if and only if $p(x)$ belongs to the domain of the interaction model $\mu$.

According to the choice of measuring the accuracy of approximation with the information divergence, given any two models $\mu$ and $\mu'$ over $X$, $\mu'$ provides a better solution than $\mu$ to the problem of approximating $p(x)$ if $D(p, p_{\mu'}) < D(p, p_\mu)$. Of course, the information divergence is not the only way of measuring the closeness of $p_\mu(x)$ to $p(x)$; an alternative might be the so-called $\chi^2$ distance [3] defined as

$$\chi^2(p, p_\mu) = \sum_x [p(x) - p_\mu(x)]^2/p(x)$$

but, the $\chi^2$ distance has not some desirable properties (e.g., additive property) that are possessed by the information divergence. On the other hand, it is well-known [3] that $D(p, p_\mu) \approx (1/2)\chi^2(p, p_\mu)$, so that minimizing $\chi^2(p, p_\mu)$ would lead to the same results that are obtained by minimizing $D(p, p_\mu)$.

Furthermore, recently it has been proved that under certain assumptions the minimization of the information divergence can be derived by minimizing an upper bound of the Bayes error rate [30]. Other properties of the minimum information divergence principle are studied from an axiomatic point of view in [28].

III. THE SEARCH SPACE

In this section, we will specify the complexity of the interaction models among which the solution to the approximation problem will be searched for. We shall do this by introducing the notion of a decomposable model of rank $k$, which can be regarded as a natural extension of a first-order dependence tree used by Chow and Liu in [5].

We begin by considering the set of all possible interaction models over a given set $X$ of $n$ random variables. This set can be partially ordered according to the relationship of "refinement": $\mu$ is finer than $\mu'$ (or, equivalently, $\mu'$ is coarser than $\mu$) if each generator of $\mu'$ is a subset of some generator of $\mu$. It is obvious that if $\mu$ is finer than $\mu'$, then the domain of $\mu'$ is a subset of the domain of $\mu$.

The infimum $\nu$ and the supremum $\tau$ of the partial ordering induced by refinement are generated respectively by the point hypergraph $X$ and the trivial hypergraph $\{X\}$. The model $\nu$ assumes independence among the $n$ variables in $X$ and the model $\tau$ makes no assumptions.

The search space, in which we set out in pursuit of the solution to the problem of approximating $p(x)$, is the class of all decomposable models of rank $k$, which are defined as interaction models over $X$ satisfying the two following constraints.

A. Decomposable Models

An interaction model $\mu$ is decomposable [7] (also called multiplicative in [29]) if an ordering $\{X_1, \ldots, X_m\}$ of its generators exists such that for each $h > 1$ either

1) $(X_1 \cup \cdots \cup X_{h-1}) \cap X_h = \emptyset$ or

2) $(X_1 \cup \cdots \cup X_{h-1}) \cap X_h \neq \emptyset$ and there is an integer $j(h) < h$ such that $(X_1 \cup \cdots \cup X_{j(h)}) \cap X_h = X_{j(h)} \cap X_h$.

Such an ordering, to be called a running intersection ordering (RIO), can be pictured by a collection $T$ of arborescences (directed trees) [1] having as its vertex set the generating hypergraph of $\mu$; the roots of the arborescences in $T$ are $X_1$ and all the generators of type 1), and every arc in $T$ is of the form $(X_{j(h)} \cup X_h, X_j \cup X_{j(h)})$ being a generator of type 2). The undirected graph underlying $T$ is called a join forest [17], [23], and each traversal of such a join forest starting at any node determines an appropriate RIO of the generators of $\mu$.

In what follows, given a decomposable model and an RIO $\{X_1, \ldots, X_m\}$ of $X_1$ as well as the generators of type 1) will be called root generators, and the generators of type 2) will be called descending generators.
Example: Let us consider the model generated by the hypergraph $M = \{ABC, CDE, FG\}$. $M$ is decomposable for $(ABC, CDE, FG)$ is an RIO, with respect to which $ABC$ and $FG$ are root generators, and $CDE$ is a descending generator (see Fig. 1).

Notice that the model $\epsilon$ generated by the trivial hypergraph is decomposable.

The constraint of decomposability is here introduced because decomposable models possess a number of desirable properties [2], [9], [10], [11], [17], [19]. In particular, one has that does the following

1) Decomposable models are characterized by chordal, conformal dependence graphs [8], [17], [23].

We require some preliminary notions of graph theory. A clique in a dependence graph $G_{\mu}$ is a set of nodes (variables) such that every pair forms an edge of $G_{\mu}$. A dependence graph $G_{\mu}$ is conformal if every clique is contained in some generator of $\mu$. A dependence graph $G_{\mu}$ is chordal (or triangulated) if every cycle with at most four distinct nodes has a chord, that is, an edge connecting two non-consecutive nodes of the cycle. Notice that by the dependence graph associated to a decomposable model of rank 2 is a forest of trees, called first-order dependence trees in [5].

2) A decomposable model can be interpreted in terms of conditional independence [8].

Since the relations of conditional independence can be treated in an axiomatic way [22], [23] and the associated formal system can be used as the inference engine of a common sense logic for reasoning about relevance relations [24], [25], decomposability is a desirable quality of belief networks [23].

3) The approximation based on a decomposable model has a closed product-form expression [2], [19], [21].

Let $\mu$ be a decomposable model and $(X_{1}, \ldots, X_{m})$ an RIO of its generators. Let us partition the index vertex $J = \{1, 2, \ldots, m\}$ into the two subsets $J' = \{h \in J : X_{h}$ is a root generator$\}$ and $J'' = \{h \in J : X_{h}$ is a descending generator$\}$. Moreover, if $X_{h}$ is a root generator and $X_{j(h)}$ is its parent, let us denote by $Y_{h}$ the nonempty intersection of $X_{h}$ and $X_{j(h)}$, that is, $Y_{h} = X_{h} \cap X_{j(h)}$. Then, the approximation $p_{\mu}(x)$ to a given distribution $p(x)$ can be written as follows

$$p_{\mu}(x) = \prod_{h \in J'} p_{h}(x_{h}) \prod_{h \in J''} p_{h}(x_{h}/y_{h})$$

(3)

or, equivalently,

$$p_{\mu}(x) = \prod_{h \in J'} p_{h}(x_{h})/\prod_{h \in J''} p_{h}(y_{h})$$

(4)

As a consequence of (4), the entropy $H_{\mu}(X)$ of $p_{\mu}(x)$ amounts to

$$H_{\mu}(X) = -\sum_{x} p_{\mu}(x) \log p_{\mu}(x)$$

$$= -\sum_{x} p_{\mu}(x) \left[\sum_{h \in J'} \log p_{h}(x_{h}) + \sum_{h \in J''} \log p_{h}(x_{h}/y_{h})\right]$$

$$= -\sum_{h \in J'} \log p_{h}(y_{h})$$

Notice that both the numerator's and the denominator's factors are independent; $\mu$ is equivalent to the assumption of the two following relations of independence:

1) $ABC$ and $FG$ are independent;
2) $AB$ and $DE$ are conditionally independent given $C$.

The approximation $p_{\mu}(abcd|defg)$ to a given probability distribution $p(abcd|defg)$ based on $\mu$, by (4) is

$$p_{\mu}(abcd|defg) = p(abcd)p(defg)/p(c).$$

Notice that both the numerator's and the denominator's factors are in a one-to-one correspondence with the nodes and edges of the join forest, shown in Fig. 1(b), respectively. Moreover, by (5) the entropy of $p_{\mu}(abcd|defg)$ is

$$H_{\mu}(ABCDEFG) = H(ABC) + H(CDE) + H(FG) - H(C).$$

Bounded-Rank Models

A model $\mu$ is of rank $k$ if $1 < k < n$ if $k$ is the maximum cardinality of the generators of $\mu$.

It should be noted that such a constraint must be introduced to avoid the trivial solution represented by the model $\epsilon$ generated by the trivial hypergraph.

At this point, our approximation problem can be stated as follows.

1) A Minimization Problem: Given a probability distribution $p(x)$ over a set of $n$ discrete random variables, find the approximation $p_{\mu}(x)$ to $p(x)$ such that

$$D(p, p_{\mu}) = \min$$

where $D(p, p_{\mu})$ is the Kullback-Leibler divergence.
over all decomposable models of rank $k$ over $X$. The requirement of decomposability for the interaction models in the search space entails some important simplifications to the approximation problem.

From property (3) the following lemma follows.

**Lemma:** For every approximation $p_* (x)$ to $p(x)$ based on a decomposable model $\mu$, the information divergence $D(p; p_*)$ equals the difference between the entropy $H_\mu(X)$ of $p_*(x)$ and the entropy $H(X)$ of $p(x)$.

**Proof:** The term $- \sum x p(x) \log p_*(x)$ in (2) can be expanded as follows

\[ - \sum x p(x) \log p_*(x) = - \sum x p(x) \left( \sum h \in J(x) \log p_*(x_h) \right) \]

\[ = \sum h \in J(x) \left( - \sum x p(x) \log p_*(x_h) \right) \]

\[ = \sum h \in J(x) \left( \sum x p(x) \log p(x_h) - \sum x p(x) \log p_*(x_h) \right) \]

\[ = \sum h \in J(x) \left( - \sum x p(x) \log p_*(x_h) \right) \]

\[ = \sum h \in J(x) \left( \sum x p(x) \log p(x_h) - \sum x p(x) \log p_*(x_h) \right) \]

\[ = \sum h \in J(x) \left( H(X_h) - H_*(X_h) \right) \]

which, by (5), is nothing more than the entropy $H_\mu(X)$ of $p_*(x)$. Q.E.D.

As a consequence of this lemma, one has that, since the entropy $H(X)$ is independent of the decomposable model $\mu$, minimizing the information divergence $D(p; p_*)$ over decomposable models of rank $k$ is equivalent to minimizing the entropy $H_\mu(X)$. By virtue of the following property, this result can be stated.

**Theorem 1:** Let $\mu$ and $\mu'$ be two decomposable models over $X$. If $\mu'$ is coarser than $\mu$, then $\mu'$ provides a better solution than $\mu$ to the problem of approximating any probability distribution over $X$.

**Proof:** Let $\mu$ and $\mu'$ be two decomposable models over $X$. If $\mu'$ is coarser than $\mu$, then $p_\mu \supseteq p_{\mu'}$ and, consequently, $H_\mu(X) \geq H_{\mu'}(X)$. Then, regardless of the probability distribution $p(x)$, from Lemma it follows that $D(p; p_\mu) \geq D(p; p_{\mu'})$. Q.E.D.

Furthermore, since for every decomposable model $\mu$ of rank $k$, $H_\mu(X)$ depends on $p(x)$ only through its marginals $p_1 (x_1), p_2 (x_2), \ldots, p_m (x_m)$, the solution of our minimization problem does not require knowledge of the entire distribution $p(x)$; the $k$-dimensional marginals are sufficient for this purpose. This property proves to be useful in the analysis of contingency tables [2] and for the management of statistical databases [20].

Generally speaking, our minimization problem can be solved in an exact way only by exhaustive search [23]. However, it was proved by Chow and Liu [5] that, if the model search is carried out among dependence trees (i.e., decomposable models of rank 2 generated by connected hypergraphs), the exact solution can be found by using a Kruskal-like step-by-step search procedure. Similarly, optimal decomposable models of rank $k = n - 1$ can be found directly, by ranking the $n(n-1)/2$ average conditional informations of the form

\[ I(A, B|X - (A, B)) \]

\[ = H(X - \{A\}) + H(X - \{B\}) - H(X) - H(X - \{A, B\}) \]

for each pair $A$ and $B$ of variables in $X$. Greedy algorithms, which for a given value of $k$ compute a good solution to our minimization problem, are described in Section V.

**IV. UNIFORM AND ELEMENTARY MODELS**

In this section, we will introduce a special class of decomposable models of rank $k$, to be called **elementary models of rank $k$**, and will show that, without loss of generality, the search space of our minimization problem can be restricted to such models. This will be done in two steps. First, we shall prove that, without loss of generality, the search space can be restricted to the class of uniform decomposable models of rank $k$, i.e., decomposable models whose generators are $k$-sets in the sense that each generator contains exactly $k$ variables. Subsequently, we shall prove that the search space can be further restricted to the class of elementary decomposable models of rank $k$ (whose definition will be introduced later on).

**Theorem 2:** For every decomposable model $\mu$ of rank $k$, a uniform model of rank $k$ that is coarser than $\mu$ always exists.

**Proof:** We prove the theorem by indicating a constructive method for obtaining a uniform model of rank $k$ from an arbitrary decomposable model $\mu$ of rank $k$. Let $(X_1, X_2, \ldots, X_h)$ be an RIO associated to $\mu$ such that $|X_i| = k$. Since at least one generator of $\mu$ contains $k$ variables, such an RIO always exists and can be obtained by visiting the nodes of a join tree associated to $\mu$ starting at $X_1$. For $h = 2, 3, \ldots, m$, apply the following procedure to all generators $X_h$ of $\mu$ containing less than $k$ variables.

**Procedure:** Let $X_h$ be a generator containing $k'(k' < k)$ variables. Two cases are to be distinguished depending on whether $X_h$ is a descending generator or a root generator. In the former case, let $X_{j(h)}$ be the parent of $X_h$ and, consequently, $X_{j(h)} = X_h \cup y$ where $y$ is such that:

1) $X_{j(h)} \supseteq y \supseteq X_h \cap X_{j(h)}$;

2) $|y| = k - r$.

(A set such as $y$ always exists because $j(h) < h$ and, therefore, $X_{j(h)} \neq k$). In the latter case, replace $X_h$ by $Y_h = X_h \cup Y$ where $Y$ is any subset of $X_{h-1}$ with exactly $k - k' - 1$ variables.

The result of the replacement of $X_h$ by $Y_h$ in the original RIO is again an RIO because:

1) if $X_h$ is a descending generator with parent $X_{j(h)}$, then

$\{X_1 \cup \cdots \cup X_{h-1}\} \cap Y_h = X_{j(h)} \cap X_h$

(Notice that $Y_h$ has the same parent that $X_h$ had in the original RIO).

2) if $X_h$ is a root generator, then

$\{X_1 \cup \cdots \cup X_{h-1}\} \cap Y_h = X_{h-1} \cap Y_h$

(Notice that in the new RIO $Y_h$ is a descending generator and $X_{h-1}$ is its parent).

Therefore, after applying this procedure to all generators of $\mu$ containing less than $k$ variables, one obtains a uniform model of rank $k$, that is coarser than the decomposable model $\mu$. Q.E.D.

**Example (continued):** The decomposable model generated by

$M = \{ABC, CDE, FG\}$

is of rank 3 but is not uniform. $N = \{ABC, CDE, EFG\}$ is an example of a uniform decomposable model of rank 3 that can be obtained by applying the previous procedure.

A further restriction of the search space without loss of generality can be achieved after introducing the notion of an elementary model, which can be viewed as a generalization of a dependence tree.

Let $\mu$ be a uniform decomposable model of rank $k$ and $(X_1, \ldots, X_m)$ is an RIO. Generator $X_h$ ($h > 1$) is said to be **elementary** if the set $X_h - (X_1, \ldots, X_{h-1})$ is a singleton; otherwise, it is said to be **multiple**.

A uniform decomposable model of rank $k$ is an **elementary model of rank $k$** if an RIO exists in which each $X_h$ ($h > 1$) is elementary. Thus, an elementary model of rank $k$ has exactly
$m = n - k + 1$ generators and every join forest associated to its generating hypergraph is a tree. On account of this, formula (5) becomes

$$H_{\mu}(X) = H(X_1) + \sum_{h=2,\ldots,n-k+1} [H(X_h) - H(Y_h)]$$

(6)

It should be noted that for $k = n - 1$, an elementary model consists of a pair of conditionally independent variables given the $(n - 2)$ remaining variables. For this reason, such models are called "elementary conditional-independence models" [29] (or "elementary zero-partial-association models") [29].

Elementary models of rank $k$ are important because of the following property.

**Theorem 3:** For every uniform decomposable model $\mu$ of rank $k$, an elementary model of rank $k$ that is coarser than $\mu$ always exists.

**Proof:** We prove the theorem by indicating a constructive method for obtaining such a model starting from an arbitrary RIO $(X_1, X_2, \ldots, X_n)$ of the generators of $\mu$. For $h = 2, 3, \ldots, m$, apply the following procedure to all multiple generators $X_h$ of $\mu$.

**Procedure**: Insert between $X_{h-1}$ and $X_h$ in the RIO a sequence of $k$-sets obtained as follows. Two cases are to be distinguished depending on whether $X_h$ is a descending root or a root generator.

In the former case, if $X_{j(h)}$ is the parent of $X_h$ and $X_h - X_{j(h)} = \{A_1, A_2, \ldots, A_r \}$, then set $Z_i = Y_i \cup \{A_1, A_2, \ldots, A_r \}$ where $Y_i = Y_i \cup \{A_r, A_{r-1}, \ldots, A_1 \}$ is a sequence of subsets of $X_{j(h)}$ such that:

1) $X_{j(h)} \supseteq Y_1 \supseteq Y_2 \supseteq \cdots \supseteq Y_{r-1} \supseteq X_h \cap X_{j(h)}$;
2) $|Y_i| = i (i = 1, \ldots, r - 1)$.

Finally, insert between $X_{h-1}$ and $X_h$ in the RIO the sequence $(Z_1, Z_2, \ldots, Z_r, X_h)$. In the latter case, if $X_h = \{A_1, A_2, \ldots, A_k \}$, then set $Z_i = Y_i \cup \{A_k, A_{k-1}, \ldots, A_1 \}$ is a sequence of nonempty subsets of $X_{j(h)}$ such that:

1) $X_{j(h)} \supseteq Y_1 \supseteq Y_2 \supseteq \cdots \supseteq Y_{k-1} \supseteq X_h \cap X_{j(h)}$;
2) $|Y_j| = j (j = 1, \ldots, r - 1)$.

Finally, insert between $X_{h-1}$ and $X_h$ in the RIO the sequence $(Z_1, Z_2, \ldots, Z_k, X_h)$. One can immediately see that in both cases the result of the insertion of the $k$-sets $Z_i$ between $X_{h-1}$ and $X_h$ is again an RIO. Therefore, after applying this procedure to all multiple generators of $m$, one obtains an elementary model of rank $k$ that is coarser than the decomposable model $\mu$. Q.E.D.

**Example (continued):** The hypergraph $N = \{ABC, CDE, EFG\}$ generates a uniform decomposable model of rank 3, which is not elementary. $Q = \{ABC, BCD, CDE, DEF, EFG\}$ is an example of an elementary model of rank 3 that can be obtained by applying the previous procedure.

As a consequence of Theorems 1–3, one has that, without loss of generality, the search space of our minimization problem can be restricted to elementary models of rank $k$.

V. GREEDY ALGORITHMS

In this section we describe a hill-climbing procedure for computing solutions that are, in some sense, locally optimal. When, in Section VI, we shall apply this procedure to a sample distribution, we shall find that the computed solutions are close to optimal, and, in one case, that the solution is actually optimal.

The heuristic technique that will be employed consists in viewing the construction of the generating hypergraph of the goal model as a sequence of $n - k + 1$ decisions, which extend partial solutions (i.e., \{X_1, \ldots, X_h\}) by including a single generator, selected in such a way as to preserve decomposability. Each decision is made according to a local-optimality criterion consisting in minimizing a suitable cost function.

Bearing in mind the expression (6) of the objective function $H_{\mu}(X)$, we define the cost for a partial solution \{X_1, \ldots, X_h\} ($h = 1, \ldots, n - k + 1$) as follows:

- For $h = 1$ cost $\{X_1\} = H(X_1)$
- For $h = 2, \ldots, m$ cost \{X_1, \ldots, X_h\} = $H(X_1) + \sum_{i=2,\ldots,n-k+1} [H(X_i) - H(Y_i)]$

Now, for a cost function to work correctly, for all partial solutions \{X_1, \ldots, X_h\} and all extensions \{X_1, \ldots, X_h, X_{h+1}\} we must have [27]:

$$\text{cost } \{X_1, \ldots, X_h\} \leq \text{cost } \{X_1, \ldots, X_h, X_{h+1}\}$$

In fact, only if the cost function has this property, can a partial solution \{X_1, \ldots, X_h\} be discarded when its cost is greater than or equal to the cost of a previously computed solution.

However, in our case, when a partial solution \{X_1, \ldots, X_h\} is extended to \{X_1, \ldots, X_{h+1}\}, it might happen that the parents of $X_{h+1}$ change, and this would cause an undesirable, non-monotonic behavior in the cost function. The following example illustrates this anomaly.

If, after choosing $X_1 = ABC$ and $X_2 = CDE$, one attempted to enter the set $X_3 = BCD$ as the third generator of the model, one would find that cost $\{X_1, \ldots, X_3\} \geq \text{cost } \{X_1, X_2, X_3\}$. In fact one has

$$\text{cost } \{ABC, CDE\} = H(ABC) + [H(CDE) - H(C)]$$
$$\text{cost } \{ABC, CDE, BCD\} = H(ABC) + [H(CDE) - H(C)] + [H(BCD) - H(BC)]$$

and the quantity

$$\text{cost } \{ABC, CDE\} - \text{cost } \{ABC, CDE, ACD\}$$
$$= H(BC) + H(CD) - H(C) - H(BCD)$$

is non-negative for it is nothing more than $I(B, D/C)$, i.e., the average conditional information of $B$ and $D$ given $C$.

To overcome this difficulty, the generators of the goal model will be selected according to the search scheme that binds each partial solution to be itself an elementary model of rank $k$. In other terms, the generator $X_{h+1}$ will be added to the partial solution $\{X_1, \ldots, X_h\}$ ($h = 1, \ldots, n - k + 1$) will be selected from among the $k$-sets that are elementary with respect to $\{X_1, \ldots, X_h, X_{h+1}\}$. At this point, we can state our first greedy algorithm, referred to as Algorithm G in what follows.

**Algorithm G**

**Step 1:** Among all the $k$-sets, select $X_1$ so that the entropy $H(X_1)$ be as little as possible.

**Step 2:** If, after choosing $X_1, \ldots, X_h$, one selects $X_{h+1}$ among all the possible elementary $k$-sets so that, if $X_{j(h+1)}$ is the parent of $X_{h+1}$ and $Y_{h+1} = X_{h+1} \cap X_{j(h+1)}$, then the quantity $H(X_{h+1}) - H(Y_{h+1})$ be as little as possible.

**Step 3:** Exit when $n - k + 1$ $k$-sets have been selected.

The search effort $e$ of Algorithm G can be measured by the number of $k$-sets that have to be evaluated.

In what follows, $S_k(Y)$ denotes the family of the subsets of $Y$ having cardinality $k$. If $|Y| = s$, then $S_k(Y) = \{C_k\}$, where $C_k = \{s!/[k!(s - k)!]\}$ is the number of combinations of $s$ variables taken $k$ at a time.

Since $X_1$ is taken from $S_1(X)$ and $|X| = n$, the degrees of freedom in the choice of $X_1$ are $e_1 = s!/[k!(s - k)!]$.
As to \( X_h + 1 \) \((h = 1, \ldots, n - k)\), it is obtained by adding one variable (entering variable) to a \((k - 1)\)-set taken from the following family
\[
S_{k-1}(X_1) \cup S_{k-1}(X_2) \cup \cdots \cup S_{k-1}(X_h).
\]

In order to evaluate the degrees of freedom in the choice of \( X_{h+1} \), let us begin by noting that, if \( X_{j(i)} \) is the parent of \( X_i \) \((i = 2, \ldots, h)\), then
\[
S_{k-1}(X_1) \cap (S_{k-1}(X_2) \cup \cdots \cup S_{k-1}(X_i - 1)) = S_{k-1}(X_1) \cap S_{k-1}(X_{j(i)}).
\]
Therefore, one has
\[
|S_{k-1}(X_1) \cup \cdots \cup S_{k-1}(X_{h-1}) \cup S_{k-1}(X_h)| = |S_{k-1}(X_1)| + \cdots + |S_{k-1}(X_{h-1})| + |S_{k-1}(X_{h})|,
\]
and
\[
|S_{k-1}(X_1) \cap S_{k-1}(X_{j(i) - 1})| = |S_{k-1}(X_1)| - |S_{k-1}(X_{j(i) - 1})|.
\]
Furthermore, \( S_{k-1}(X_1) \cap S_{k-1}(X_{j(i)}) \) contains exactly one set, i.e., \( X_{j(i)} \cap X_i \), so that one has
\[
|S_{k-1}(X_1) \cup \cdots \cup S_{k-1}(X_{h-1}) \cup S_{k-1}(X_h)| = k + (h - 1)(k - 1) = h(k - 1) + 1.
\]
Now, since the possible entering variables are \((n - k + h + 1)\), the degrees of freedom in the choice of \( X_{h+1} \) are
\[
e_k = [h(k - 1) + 1](n - k - h + 1).
\]
In conclusion, on account of the formulas:
\[
\sum_{k=1, \ldots, n} h = m(n + 1)/2
\]
\[
\sum_{k=1, \ldots, n} h^2 = m(n + 1)(2m + 1)/6
\]
we can conclude that the search effort \( e_k = \Sigma h = k \in \epsilon_k \) of Algorithm \( G \) amounts to
\[
e_k = \Sigma C_k + \Pi (n-k)(n-k+1)(k-1)(n-k+2) + 3)/6.
\]

In order to appreciate the convenience of our heuristic approach, one must compare \( e \) with the effort of an exhaustive search, which can be measured by the number of all possible elementary models of rank \( k \). Since an evaluation of this number is difficult, we shall use the following lower bound \( E \):
\[
E = \left( \prod_{h=1, \ldots, n-k+1} f_h \right) / (n-k+1)!
= \prod_{h=1, \ldots, n-k} [1 + h(k - 1)!(n-k+1)]
\]

obtained by dividing the number of all possible ROI's by the number of permutations of \( n - k + 1 \) objects (generators). Notice that for \( k = n - 1 \), one has \( E = \Sigma C_k \), which is exactly the number of elementary conditional-independence models.

One can easily see that, if \( n \) is high, then \( E \) is far greater than \( e \). A cheaper algorithm than Algorithm \( G \) can be worked out if the ranges of the variables in \( X \) do not have the same cardinality. To this end, we need the notion of a minimal-range \( k \)-set.

The range of a set \( Y \) of random discrete variables is defined by the Cartesian product of the ranges of the variables in \( Y \). Minimal-range \( k \)-sets are \( k \)-sets whose ranges have the least cardinality. Now, if \( Y \) is a \( k \)-set whose range has cardinality \( t \), then \( H(Y) \leq H_0(Y) = \log t \) and, therefore, the minimum-entropy \( k \)-set is likely to be a \( k \)-set minimizing \( H_0(Y) \), that is, a minimal-range \( k \)-sets. In this way, the search effort made to select the \( h \)th generator \( X_1 \) is reduced by a quantity equal to \( e_k - C_k \), if \( e_k \) is the number of the minimal-range \( k \)-sets, among which \( Y_h \) is selected. This leads us to state a second greedy algorithm, called Algorithm \( G^* \), which is more efficient than Algorithm \( G \) and usually gives the same results, as shown in the example discussed in Section VI.

Algorithm \( G^* \)

**Step 1:** Among all the minimal-range \( k \)-sets, select \( X_1 \) so that the entropy \( H(X_1) \) be as little as possible.

**Step 2:** After choosing \( X_1, \ldots, X_h \), select \( X_{h+1} \) among all the minimal-range elementary \( k \)-sets so that, if \( X_{j(h+1)} \) is the parent of \( X_{h+1} \) and \( Y_{h+1} = X_{h+1} \cap X_{j(h+1)} \), then the quantity \( H(X_{h+1}) - H(Y_{h+1}) \) be as little as possible.

**Step 3:** Exit when \( n - k + 1 \) \( k \)-sets have been selected.

**VI. EXPERIMENTAL RESULTS**

We present experimental results on the application of the proposed procedure to the probability distribution obtained from sample data reported in Table I containing information on the structural habitat of *grahami* and *opalinus* lizards from Whitehouse, Jamaica, taken from Bishop et al. [2]. The data consists of observed counts for perch height, perch diameter, insolation, and time-of-day categories for both *grahami* and *opalinus* lizards. The four habitat variables are referred to as variables \( A, B, C \) and \( D \), respectively, and species is variable \( E \). The table is of dimension \( 2 \times 2 \times 2 \times 2 \times 2 \times 2 \).

The following are the values of the entropy for the marginal probability distributions. Moreover \( H(ABCDE) = 3.21732 \).

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<th>2-sets</th>
<th>3-sets</th>
<th>4-sets</th>
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<td>ABCD</td>
<td>2.73327</td>
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<td>AC</td>
<td>AE</td>
<td>1.19777</td>
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<td>C</td>
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<td>AD</td>
<td>CD</td>
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<td>D</td>
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<td>CD</td>
<td>1.55183</td>
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<tr>
<td>E</td>
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<td>BC</td>
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</table>

Fig. 3. Dependence graph associated to the model generated by the hypergraph \( \{AE, BE, CD, CE\} \).
We applied both Algorithms $G$ and $G^*$ for $k = 2, 3, 4$, and obtained the following results.

Case ($k = 2$). Both Algorithm $G$ and Algorithm $G^*$ select the same model $\mu$, which is generated by the hypergraph $\{ABE, ACE, CDE\}$. Algorithm $G$ does so after selecting

1) $X_1 = CE$ among the ten possible 2-sets;
2) $X_2 = AE$ among the six following 2-sets: $AC, AE, BC, BE, CD, DE$;
3) $X_3 = BE$ among the following 2-sets: $AB, AD, BC, BE, CD, DE$;
4) $X_4 = CD$ among the four following 2-sets: $AD, BD, CD, DE$.

Algorithm $G^*$ does so after selecting

1) $X_1 = CE$ among the six following 2-sets: $AB, AC, AE, BC, BE, CE$;
2) $X_2 = AE$ among the four following 2-sets: $AC, AE, BC, BE$;
3) $X_3 = BE$ among the three following 2-sets: $AB, BC, BE$;
4) $X_4 = CD$ among the four following 2-sets: $AD, BD, CD, DE$.

The corresponding value of the cost function amounts to $H_{\mu}(ABC) = 1.293$. The dependence graph of $\mu$ is shown in Fig. 4.

By inspecting this dependence graph, it is easy to recognize that $\mu$ is equivalent to the assumption of the two relations of independence:

1) $ABE$ and $D$ are conditionally independent given $C$;
2) $A, B$ and $C$ are conditionally independent given $E$.

The exhaustive examination of the 70 possible elementary models of rank 3 shows that there are three models better than $\mu$, namely,

$\mu_1 = \{ABE, BDE, CDE\}$ with $H_{\mu_1}(ABC) = 3.24115$ (the optimal model)

$\mu_2 = \{ABE, ADE, CDE\}$ with $H_{\mu_2}(ABC) = 3.24197$

$\mu_3 = \{ABE, BCE, CDE\}$ with $H_{\mu_3}(ABC) = 3.24327$

Case ($k = 4$). Both Algorithm $G$ and Algorithm $G^*$ select the same model $\mu$, which is generated by the hypergraph $\{ABE, ACE, CDE\}$. Algorithm $G$ does so after selecting

1) $X_1 = ABCE$ among the five possible 4-sets;
2) $X_1 = ACDE$ among the four remaining 4-sets.

Algorithm $G^*$ does so after selecting

1) $X_1 = ABCE$ as the minimal-range 4-set;
2) $X_1 = ACDE$ among the four remaining 4-sets.

The corresponding value of the cost function amounts to $H_{\mu}(ABC) = 3.23282$. The dependence graph $\mu$ is shown in Fig. 5.

By inspecting this dependence graph, it is easy to recognize that $\mu$ is equivalent to the assumption of the hypothesis of conditional independence of $D$ and $E$ given $ACE$.

The exhaustive examination of the ten possible elementary models of rank 4 shows that there are three models better than $\mu$, namely,

$\mu_1 = \{ABCD, ACDE\}$ with $H_{\mu_1}(ABC) = 3.22640$ (the optimal model)

$\mu_2 = \{ABDE, BCDE\}$ with $H_{\mu_2}(ABC) = 3.22869$

$\mu_3 = \{ABCD, ABDE\}$ with $H_{\mu_3}(ABC) = 3.23030$.

---

**Table I**

<table>
<thead>
<tr>
<th>Cell (ABCDE)</th>
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<th>Cell (ABCDE)</th>
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</tbody>
</table>

*From Whitehouse, Jamaica. The sample size is 561.
At the end, the two following decomposable models of rank 2 were selected, using a backward-selection procedure. After evaluating all of the elementary conditional-independence models, of which only six ("baseline models") were accepted, his procedure backwards steps by examining all the decomposable models that are finer than the baseline models. At the end, the two following decomposable models of rank 3 were selected:

\[
\{ABE, CE, D\} \text{ and } \{ABE, BDE, CD\}.
\]

Both of them are finer than the model selected by our greedy algorithms, which therefore turns out to be better than both.

VII. CONCLUSION

We have treated the problem of approximating a given multidimensional probability distribution with interaction models as a minimization problem, which uses information divergence as its cost function and the class of decomposable models of a certain rank as its search space. The optimal solution to this problem is known to require an exhaustive examination of all models in the search space, except for the case rank=2, which can be solved by using a greedy selection procedure.

We have presented two greedy algorithms, which show that, if one relaxes the optimality requirement and is content with a suboptimal solution, even in the general case (rank\(\geq 2\)) the search effort is bearable. Both of the proposed algorithms restrict the search space to elementary models, which are a subclass of decomposable models. Such a restriction is made on account of the two following facts:

1) the optimal solution to the minimization problem is an elementary model;
2) in the search space of elementary models, the cost function has an additive, closed form.

The additivity of the cost function has been exploited to select a suboptimal solution, which is built up in an incremental manner by using a greedy selection procedure, based on the minimization of the single additive components of the cost function. Such a selection procedure, when compared with other procedures existing in literature, has two unquestionable advantages:

1) the selected solution is found directly (that is, without passing through intermediate solutions) and, hence, faster;
2) the solution does not require knowledge of the entire distribution to be approximated, but only of its \(k\)-dimensional marginals.

ACKNOWLEDGMENT

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REFERENCES