

Comparison of two methods for approximation of probability distributions with prescribed marginals

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Abstract

Let P be a discrete multidimensional probability distribution over a finite set of variables N which is only partially specified by the requirement that it has prescribed given marginals $\{P_A; A \in \mathcal{S}\}$, where \mathcal{S} is a class of subsets of N with $\bigcup \mathcal{S} = N$. The paper deals with the problem of approximating P on the basis of those given marginals. The divergence of an approximation \hat{P} from P is measured by the relative entropy $H(P|\hat{P})$. Two methods for approximating P are compared. One of them uses formerly introduced concept of *dependence structure simplification* [3]. The other one is based on an *explicit expression*, which has to be normalized. We give examples showing that neither of these two methods is universally better than the other. If one of the considered approximations \hat{P} really has the prescribed marginals then it appears to be the distribution P with minimal possible multiinformation. A simple condition on the class \mathcal{S} implying the existence of an approximation \hat{P} with prescribed marginals is recalled. If the condition holds then both methods for approximating P give the same result.

Keywords: marginal problem, relative entropy, explicit expression, dependence structure simplification, multiinformation, decomposable model, asteroid.

Preface - memories of the second author

This paper was written particularly for a special volume of *Kybernetika* in honour of Albert Perez. I had the opportunity to be the last doctoral student of his. In 1983 I joined the Institute of Information Theory and Automation to start my studies for CSc degree¹ under his supervision. I am indebted to him for directing me towards an interesting topic of probabilistic decision making. What I learned from him during my doctoral studies I also utilized in my later research on probabilistic conditional independence. For example, the basic idea to use information-theoretical tools in this field was inspired by his paper [3]. After defending my CSc thesis in 1987 I became a regular member of the department formerly led by Albert Perez. He tried to stimulate the activity of his colleagues in the department by organizing a weekly seminar (I also attended). Moreover, he himself continued in research activity until he retired in 1990.

We renewed our contacts in November 2001 when I invited him to a small celebration of my getting DrSc degree, in a restaurant. During the celebration, we agreed to have another meeting, this time in the institute, together with two other colleagues of mine and former co-workers of his, Radim Jiroušek and Otakar Kříž. Otakar, Radim and I expected an informal

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¹This is the official name of the scientific degree awarded in Czechoslovakia in the 1980s. Nowadays, doctoral students get PhD degree.

meeting over some refreshment but when Albert Perez came he wanted us to discuss with him on scientific theme. He wished to inform us about his latest research effort and, perhaps, to help him to prepare some paper(s) on that topic. Later, we organized one more seminar for four of us and agreed that Albert Perez would write something down and we would read it and give him critical comments in order to prevent obstacles during future reviewing process. In 2002, 82-year-old Albert Perez bought a personal computer and started, first time in his career, to work with it – of course, with substantial help and advice of Otakar Kříž. I myself, visited Albert Perez a few times in his flat. We mainly discussed former versions of the manuscript [6] and I also tried to invite him to participate in WUPES 2003 workshop. Note that he worked on several manuscripts that time and probably wanted to write a series of papers. During my last visit, Albert Perez offered me to become a co-author of his paper based on [6], mainly because I had helped him to find some counterexamples. Nevertheless, I had other commitments that time and did not want to delay submitting his paper. Thus, I told him I was pleased to help him anyway but preferred he would write the paper himself and would mention my name in an acknowledgement.

When I phoned him in December 2003 to arrange giving him my comments on the last version of [6] he did not answer the phone. My colleagues and I learned later that it was because he was already dead. After his funeral, Radim Jiroušek came with an idea to prepare a special volume of *Kybernetika* in honour of Albert Perez. I promised to write a paper based on [6] and submit it to the volume. Of course, the present paper differs from the source manuscript [6] very much: I changed the structure of the paper and omitted some points. Because the paper is substantially based on the results and ideas of Albert Perez he is the first author.

1 Introduction

The paper deals with the following problem. Let N be a finite non-empty set of variables, \mathcal{S} a class of subsets of N whose union is N and $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ a given system of marginals of a discrete probability distribution P over N .² In general, P is not uniquely determined by \mathcal{M} . Thus, we only know that P belongs to the class $\mathcal{K}_{\mathcal{M}}$ of discrete probability distributions over N that have the prescribed system of marginals \mathcal{M} . We are interested in the problem of approximating P on basis of \mathcal{M} . More specifically, we consider special approximations \hat{P} of P . These are probability distributions over N “constructed” from \mathcal{M} by means of “multiplication” in a special way. Actually, we deal with and compare two special methods for constructing approximations of this kind. The first approach leads to *dependence structure simplifications*, already introduced in [3]. In this paper, we introduce an alternative method which is based on certain *explicit expression*, which has to be normalized. To compare quality of approximations we use the relative entropy $H(P|\hat{P})$ as the measure of divergence of an approximation \hat{P} from P . The point is that the quality of an approximation \hat{P} of the considered kind actually does not depend on the choice of $P \in \mathcal{K}_{\mathcal{M}}$. This is because, for any $P \in \mathcal{K}_{\mathcal{M}}$ and any approximation \hat{P} of this kind, the following formula holds:

$$H(P|\hat{P}) = I(P) - I_{\mathcal{M}}(\hat{P}), \quad (1)$$

where $I(P)$ is the multiinformation of P and $I_{\mathcal{M}}(\hat{P})$ an expression, called the *information content* of \hat{P} , that does not depend on particular $P \in \mathcal{K}_{\mathcal{M}}$.

The motivation for this problem comes from probabilistic decision making. More specifically, the considered approximations can be utilized in multi-symptom diagnosis making. Let us

²Of course, P_A is a distribution over A where $A \subseteq N$.

assume that every variable $i \in N$ has assigned a non-empty finite set of possible values X_i . Let $d \in N$ be a *diagnostic variable*, that is, a variable whose value we would like to “determine” on basis of remaining variables. The variables in $S \equiv N \setminus \{d\}$ are, therefore, called *symptom variables*. Our decision should be based on an “observed” configuration of values $x_S \equiv [x_i]_{i \in S}$, where $x_i \in X_i$ for $i \in S$. On the basis of the configuration x_S , we would like to determine the most probable value of the diagnostic variable. That means, we would like to find $y \in X_d$ with maximal conditional probability $P_{d|S}(y|x_S)$.³ The complication is that we do not know the “actual” distribution P which describes the probabilistic relationships among variables in N . Therefore, we try to replace P by its approximation \hat{P} based on a given system of marginals $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ with $d \in A$ for every $A \in \mathcal{S}$.

There are two methodological procedures that can be applied in this situation. The first approach is based on *direct approximation* of P : we use an approximation \hat{P} instead of P which leads to the following estimator of the value y of the diagnostic variable:

$$\psi_1(x_S) = \operatorname{argmax} \{ \hat{P}([y, x_S]); y \in X_d \}.^4$$

The second approach is a Bayesian one. It is based on the idea that a prior distribution Q_d is given on X_d . In this case, we use $Q_d \cdot \hat{P}_{S|d}$ instead of P , where $\hat{P}_{S|d}$ is an estimate of the respective conditional probability. For fixed $y \in X_d$, we consider the system of probability distributions over subsets of $S \equiv N \setminus \{d\}$, namely $\mathcal{M}[y] = \{P_{A \setminus \{d\}|d}(\star|y); A \in \mathcal{S}\}$, which should be the system of marginals of the conditional probability $P_{S|d}(\star|y)$.⁵ Now, on basis of $\mathcal{M}[y]$, we can analogously construct an approximation $\hat{P}_{[y]}$ of $P_{S|d}(\star|y)$.⁶ This leads to the following estimator:

$$\psi_2(x_S) = \operatorname{argmax} \{ Q_d(y) \cdot \hat{P}_{[y]}(x_S); y \in X_d \}.$$

The structure of the paper is as follows. Section 2 is an overview of basic concepts and facts. We recall some information-theoretical concepts and describe the considered situation in detail in mathematical terms. In Section 3 we introduce the concept of \mathcal{M} -construct, which is the above mentioned approximation of $P \in \mathcal{K}_{\mathcal{M}}$ constructed from \mathcal{M} by “multiplication”. We also derive the formula (1) there. The concept of a dependence structure simplification (DSS) is dealt with in Section 4. We recall the definition from [7] and the respective formula for the information content. We also discuss the problem of finding an optimal DSS and a possible modification of the definition of a DSS. Section 5 is devoted to approximating P by means of an explicit expression. We explain the role of a normalizing constant, give the formula for the respective information content $I_{\mathcal{M}}(\hat{P})$ and discuss possible application of this type of approximation in probabilistic decision making. Section 6 is devoted to the case of fitting marginals. This is the fortunate case when \hat{P} falls within $\mathcal{K}_{\mathcal{M}}$. We show that then \hat{P} is the probability distribution from $\mathcal{K}_{\mathcal{M}}$ which has minimal multiinformation.⁷ We also discuss the barycenter principle of the choice of a representative of $\mathcal{K}_{\mathcal{M}}$ introduced in [4] and show that the choice of optimal DSS is in concordance with this principle. Section 7 contains examples showing that none of two

³Of course, this problem is equivalent to the problem of finding $y \in X_d$ which maximizes $P([y, x_S])$. This alternative formulation formally avoids assuming that the marginal probability $P^S(x_S)$ of the observed configuration is strictly positive, which assumption is needed to define the conditional probability $P_{d|S}(\star|x_S)$.

⁴The symbol $\operatorname{argmax} \{f(y); y \in Y\}$ denotes any $z \in Y$ such that $f(z) = \max \{f(y); y \in Y\}$.

⁵We implicitly assume that $P_d(y) > 0$ for every $y \in X_d$ for otherwise X_d can be reduced to $\{y \in X_d; P_d(y) > 0\}$.

⁶Indeed, the situation is completely analogous to the problem of approximating P on basis of \mathcal{M} – the only difference is that N is replaced by S and \mathcal{M} by $\mathcal{M}[y]$.

⁷This is equivalent to the requirement that it has minimal entropy within $\mathcal{K}_{\mathcal{M}}$.

described methods for approximating P is better than the other in the sense of information content. Section 9 gives a simple sufficient condition on \mathcal{S} which ensures that the approximation \hat{P} falls in $\mathcal{K}_{\mathcal{M}}$. The condition, named the *running intersection property*, is strongly related to well-known decomposable graphical models [2]. Section 10 contains conclusions and open problems.

2 Basic concepts

Throughout the paper we will assume the situation described in the following subsection.

2.1 The considered situation

Let N be a non-empty finite set of variables. Every $i \in N$ has assigned the respective *individual sample space* X_i , which is a non-empty finite set of its possible values. Given a set $A \subseteq N$, by a *configuration* of values for A we mean any list $[x_i]_{i \in A}$ such that $x_i \in X_i$ for any $i \in A$. Of course, if $A \neq \emptyset$ then a configuration for A is nothing but an element of the Cartesian product $\prod_{i \in A} X_i$. However, the above definition also formally introduces a configuration for the empty set; it is simply the empty list. We will denote the set of configurations for $A \subseteq N$ by X_A and call it the sample space for A . The *joint sample space* is then X_N .

Two basic operations with configurations are as follows. Given $A \subseteq B \subseteq N$ and $x = [x_i]_{i \in B} \in X_B$, the *marginal configuration* (of x) for A , denoted by x_A , is the restriction of the list x to the items that correspond the variables in A : $x_A = [x_i]_{i \in A}$. Given $A, C \subseteq N$, $A \cap C = \emptyset$, by *concatenation* of $x = [x_i]_{i \in A} \in X_A$ and $y = [y_i]_{i \in C} \in X_C$ we will understand the configuration $z = [z_i]_{i \in A \cup C}$ for $A \cup C$ obtained by merging the lists x and y : that is, $z_i = x_i$ for $i \in A$ and $z_i = y_i$ for $i \in C$. It will be denoted by $[x, y]$.

Further assumption is that a class \mathcal{S} of subsets of N is given whose union is N . The symbol \mathcal{S}^\downarrow will denote the class $\{B; B \subseteq A \text{ for } A \in \mathcal{S}\}$ of subsets of sets in \mathcal{S} . If $\mathcal{A} \subseteq \mathcal{S}$ is a non-empty subclass of \mathcal{S} then the symbol $\bigcup \mathcal{A}$, respectively $\bigcap \mathcal{A}$, will be used to denote the union, respectively the intersection, of sets in \mathcal{A} .

A basic concept is the concept of a probability measure on X_N . A probability measure of this kind is given by its *density*, which is a function $p : X_N \rightarrow [0, 1]$ such that $\sum \{p(x); x \in X_N\} = 1$. The respective probability measure is then a set function on subsets of X_N which ascribes $P(\mathbb{T}) = \sum \{p(x); x \in \mathbb{T}\}$ to every $\mathbb{T} \subseteq X_N$.⁸ By a discrete *probability distribution over N* we will understand a probability measure on any joint sample space X_N of the above-mentioned kind.

Given a probability measure P on X_N and $A \subseteq N$, the *marginal* of P for A is the probability measure P^A on X_A defined as follows:

$$P^A(\mathbb{Y}) = P(\{x \in X_N; x_A \in \mathbb{Y}\}) \quad \text{for } \mathbb{Y} \subseteq X_A.$$

It is easy to see that P^A is determined by the *marginal density* p^A for A , given by

$$p^A(y) = \sum \{p([x, y]); x \in X_{N \setminus A}\} \quad \text{for } y \in X_A.$$

In particular, $p^N = p$ and $p^\emptyset \equiv 1$. Observe that marginal densities comply with the following *vanishing principle*:

$$\text{if } A \subseteq B \subseteq N \text{ and } z \in X_B \text{ then } p^A(z_A) = 0 \text{ implies } p^B(z) = 0. \quad (2)$$

⁸Of course, then $P(\emptyset) = 0$ by a convention.

The last assumption is that a collection of marginals of a probability measure on X_N is given. More specifically, we assume that a collection of probability measures $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ is given, where P_A is a probability measure on X_A for $A \in \mathcal{S}$ and there exists at least one probability measure P on X_N such that

$$\forall A \in \mathcal{S} \quad P_A = P^A. \quad (3)$$

The last assumption on \mathcal{M} is the requirement of its *strong consistency*.⁹ We will use the symbol $\mathcal{K}_{\mathcal{M}}$ to denote the class of all probability measures P on X_N such that (3) holds. The assumption of strong consistency of \mathcal{M} means that $\mathcal{K}_{\mathcal{M}}$ is non-empty. Of course, $\mathcal{K}_{\mathcal{M}}$ may contain more than one probability measure in general.

An important question is how to verify the assumption of strong consistency of \mathcal{M} . In general, it is not an easy task. The only general method for its verification is to find $P \in \mathcal{K}_{\mathcal{M}}$ directly, but no universal instructions how to do it are available. To show that (3) is not fulfilled the following concept is suitable. We say that \mathcal{M} is *weakly consistent* if

$$\forall A, B \in \mathcal{S} \quad (P_A)^{A \cap B} = (P_B)^{A \cap B}. \quad (4)$$

Evidently, strong consistency of \mathcal{M} implies its weak consistency. As weak consistency is easy to verify the condition (4) can be used to disprove strong consistency. On the other hand, the weak consistency does not imply the strong one as the following example shows.

EXAMPLE 1 Put $N = \{a, b, c\}$ and $X_i = \{0, 1\}$ for every $i \in N$. Let $\mathcal{S} = \{A \subseteq N; |A| = 2\}$ be the class of two-element subsets of N and the density p_A of P_A for any $A \in \mathcal{S}$ is given as follows:

$$p_A(0, 0) = p_A(1, 1) = \frac{1}{10}, \quad p_A(0, 1) = p_A(1, 0) = \frac{2}{5}.$$

As $(p_A)^{\{i\}}(0) = (p_A)^{\{i\}}(1) = 1/2$ for both $i \in A$, the collection $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ is weakly consistent. However, (3) is not valid for any P on X_N . To see this assume for contradiction that $P \in \mathcal{K}_{\mathcal{M}}$ with density p exists and put $x \equiv p(1, 1, 1) \geq 0$. The fact $p_{\{b, c\}}(1, 1) = 1/10$ and (3) implies $p(0, 1, 1) = (1/10) - x$. Hence, by $p_{\{a, b\}}(0, 1) = 2/5$ observe $p(0, 1, 0) = 2/5 - [(1/10) - x] = (3/10) + x$. Finally, by $p_{\{a, c\}}(0, 0) = 1/10$ get $p(0, 0, 0) = 1/10 - [(3/10) + x] = -(2/10) - x$. The fact $p(0, 0, 0) \geq 0$ gives $x \leq -2/10$, which contradicts the assumption $x \geq 0$.

Fortunately, the condition (4) implies strong consistency under an additional assumption on the class \mathcal{S} , namely that \mathcal{S} satisfies so-called *running intersection property* – for detail see § 9. Moreover, even if that additional condition is not fulfilled strong consistency can sometimes be verified as follows. Provided that (4) holds, an approximation \hat{P} is constructed on basis of \mathcal{M} . Then one can check whether \hat{P} has \mathcal{M} as the collection of marginals. This happens whenever \mathcal{S} satisfies the running intersection property but it can also happen even if this is not the case – see Example 6 in § 6.

REMARK 1 One can assume without loss of generality that \mathcal{S} consists of incomparable sets, that is, $A \setminus B \neq \emptyset \neq B \setminus A$ for any pair of distinct sets $A, B \in \mathcal{S}$. This is because otherwise \mathcal{S} can be reduced to

$$\mathcal{S}^{\max} = \{A \in \mathcal{S}; \neg(\exists B \in \mathcal{S} \text{ with } A \subset B)\},^{10}$$

and \mathcal{M} to $\mathcal{M}^{\max} = \{P_A; A \in \mathcal{S}^{\max}\}$. Owing to strong consistency the collection \mathcal{M} can be reconstructed from \mathcal{M}^{\max} (and \mathcal{S}) and one has $\mathcal{K}_{\mathcal{M}} = \mathcal{K}_{\mathcal{M}^{\max}}$.

⁹As \mathcal{M} is supposed to be the class of marginals of a probability measure over N it is denoted by the letter \mathcal{M} .

¹⁰Here, \subset denotes strict inclusion of sets.

2.2 Some related concepts and notation

In this section we introduce some concepts used systematically in the rest of the paper.

2.2.1 The greatest supporter

Given probability measure P on X_N with density p , the set $N_P \equiv \{x \in \mathsf{X}_N; p(x) > 0\}$ will be called the *supporter* of P . It is the least subset $T \subseteq \mathsf{X}_N$ such that P is concentrated on T , that is, $P(\mathsf{X}_N \setminus T) = 0$. As $\mathcal{K}_{\mathcal{M}}$ is a convex set¹¹ and X_N has finitely many subsets there exists a probability measure $R \in \mathcal{K}_{\mathcal{M}}$ which has the greatest supporter in $\mathcal{K}_{\mathcal{M}}$.¹² It will be denoted by the symbol $N_{\mathcal{M}}$.

2.2.2 Relative entropy

Given two probability measures P, Q on X_N we say that P is *absolutely continuous* with respect to Q and write $P \ll Q$ if $Q(T) = 0$ implies $P(T) = 0$ for each $T \subseteq \mathsf{X}_N$.¹³ We also say that Q *dominates* P .

The well-known result is Radon-Nikodym theorem which says that $P \ll Q$ iff there exists a function $\frac{dP}{dQ} : \mathsf{X}_N \rightarrow [0, \infty)$, called the *Radon-Nikodym derivative* of P with respect to Q , such that

$$P(T) = \sum_{x \in T} \frac{dP}{dQ}(x) \cdot q(x) \quad \text{for any } T \subseteq \mathsf{X}_N,$$

where q is the density of Q . Of course, $\frac{dP}{dQ}$ is uniquely determined on N_Q , in particular, on N_P .

The *relative entropy* of P with respect to Q is defined by the formula

$$H(P|Q) \equiv \sum_{x \in \mathsf{X}_N, p(x) > 0} p(x) \cdot \ln \frac{dP}{dQ}(x) = \sum_{x \in \mathsf{X}_N} q(x) \cdot \frac{dP}{dQ}(x) \cdot \ln \frac{dP}{dQ}(x),$$

provided $P \ll Q$ and $H(P|Q) = \infty$ otherwise. A well-known fact is that $H(P|Q) \geq 0$ and $H(P|Q) = 0$ iff $P = Q$ – see § A.6.3 in [8]. Thus, it can be understood as a measure of distinction between P and Q .¹⁴ Observe that in the considered discrete case one has $H(P|Q) < \infty$ iff $P \ll Q$. In particular, it follows from the previous observations:

PROPOSITION 1 There exists $R \in \mathcal{K}_{\mathcal{M}}$ such that $\forall P \in \mathcal{K}_{\mathcal{M}} \quad H(P|R) < \infty$.

2.2.3 Dominating product measure

The first step is to realize that a given collection of marginals \mathcal{M} can uniquely be extended to a system of marginals $\mathcal{M}^\downarrow = \{P_B; B \in \mathcal{S}^\downarrow\}$. Indeed, given $B \in \mathcal{S}^\downarrow$ there exists $A \in \mathcal{S}$ with $B \subseteq A$ and we put $P_B = (P_A)^B$. The condition (4) implies that the definition does not depend on the choice of $A \in \mathcal{S}$, it only depends on \mathcal{M} . Actually, the fact that every $P \in \mathcal{K}_{\mathcal{M}}$ satisfies (3) implies $P_B = P^B$ for every $P \in \mathcal{K}_{\mathcal{M}}$ and $B \in \mathcal{S}^\downarrow$. Given \mathcal{M}^\downarrow and $B \in \mathcal{S}^\downarrow$ the symbol p_B will denote the density of P_B .

¹¹This means that it is closed under convex combinations: if $P, Q \in \mathcal{K}_{\mathcal{M}}$, $\alpha \in [0, 1]$ then $\alpha \cdot P + (1 - \alpha) \cdot Q \in \mathcal{K}_{\mathcal{M}}$.

¹²Realize that whenever $R = \alpha \cdot P + (1 - \alpha) \cdot Q$ with $\alpha \in (0, 1)$ then $N_R = N_P \cup N_Q$.

¹³Note that in the considered case of finite joint sample space X_N this is equivalent to the inclusion $N_P \subseteq N_Q$.

¹⁴However, because it may happen $H(P|Q) \neq H(Q|P)$ even if $P \ll Q \ll P$, it is not a distance.

Given $i \in N$, the assumption $\bigcup \mathcal{S} = N$ implies that $\{i\} \in \mathcal{S}^\downarrow$ for every $i \in N$. Let us put $P_i = P_{\{i\}}$ then. The product of these probability measures $\prod_{i \in N} P_i$ will be called the *dominating product measure* and denoted by L . It is a probability measure on \mathbf{X}_N with density l is given by

$$l(x) = \prod_{i \in N} p_{\{i\}}(x_i) \quad \text{for every } x = [x_i]_{i \in N} \in \mathbf{X}_N.$$

The terminology is justified because one can easily observe that $P \ll L$ for every $P \in \mathcal{K}_{\mathcal{M}}$.¹⁵ This allows one to derive $P_B \ll L^B$ for every $B \in \mathcal{S}^\downarrow$.¹⁶ In particular, the Radon-Nikodym derivative dP_B/dL^B exists for every $B \in \mathcal{S}^\downarrow$ and is uniquely determined on the supporter of L^B – it will be denoted by the symbol f_B in the sequel. Of course,

$$f_B(x_B) = p_B(x_B) \cdot \prod_{j \in B} p_{\{j\}}(x_j)^{-1} \quad \text{for any } x \in \mathbf{X}_N \text{ with } l(x) > 0 \text{ and } B \subseteq N.$$

REMARK 2 Note that we can assume without loss of generality that $l(x) > 0$ for every $x \in \mathbf{X}_N$. Indeed, otherwise replace every \mathbf{X}_i , $i \in N$ by $\mathbf{X}'_i = \{y \in \mathbf{X}_i; p_{\{i\}}(y) > 0\}$. Then every $P \in \mathcal{K}_{\mathcal{M}}$ is concentrated on $\mathbf{X}'_N = \prod_{i \in N} \mathbf{X}'_i$.

2.2.4 Multiinformation and entropy

Given a probability measure P on \mathbf{X}_N , the relative entropy $H(P | \prod_{i \in N} P^{\{i\}})$ will be called its *multiinformation* and denoted by $I(P)$. In the considered discrete case one always has $P \ll \prod_{i \in N} P^{\{i\}}$,¹⁷ which implies that $I(P) < \infty$. Of course, if $P \in \mathcal{K}_{\mathcal{M}}$ then $I(P) = H(P|L)$.

The *entropy* of a probability measure P on \mathbf{X}_N , denoted by $H(P)$, is given by the following formula:

$$H(P) = \sum_{x \in \mathbf{X}_N, p(x) > 0} p(x) \cdot \ln \frac{1}{p(x)}.$$
¹⁸

Note that entropy is a non-negative (finite) real number. The following lemma recalls basic facts on multiinformation and entropy in the considered situation.

LEMMA 2.1 There exists uniquely determined $P_* \in \mathcal{K}_{\mathcal{M}}$ such that

$$H(P_*) = \max \{ H(P); P \in \mathcal{K}_{\mathcal{M}} \}.$$

It coincides with unique $P_* \in \mathcal{K}_{\mathcal{M}}$ such that $I(P_*) = \min \{ I(P); P \in \mathcal{K}_{\mathcal{M}} \}$. Moreover, there exists (at least one) $P_\dagger \in \mathcal{K}_{\mathcal{M}}$ with $I(P_\dagger) = \max \{ I(P); P \in \mathcal{K}_{\mathcal{M}} \} < \infty$.

Proof: Let us introduce an auxiliary (continuous) real function $h : \mathbb{R} \rightarrow \mathbb{R}$ as follows:

$$h(y) = \begin{cases} y \cdot \ln y & \text{if } y > 0, \\ 0 & \text{otherwise.} \end{cases}$$

Observe that $-H(P) = \sum_{x \in \mathbf{X}_N} h(p(x))$ for every probability measure P on \mathbf{X}_N . As h is strictly convex on $[0, \infty)$ the function $P \mapsto -H(P)$ is a strictly convex continuous function on $\mathcal{K}_{\mathcal{M}}$. Moreover, $\mathcal{K}_{\mathcal{M}}$ is a convex bounded subset of $\mathbb{R}^{\mathbf{X}_N}$. Thus, the function achieves both the

¹⁵Observe that $p^{\{i\}}(x_{\{i\}}) = 0$ implies $p(x) = 0$ for $x \in \mathbf{X}_N$, $i \in N$ by the vanishing principle (2).

¹⁶Realize that $P_B = P^B$ and $P \ll L$ gives $P^B \ll L^B$.

¹⁷Use the vanishing principle (2).

¹⁸Of course, the definition only makes sense in the discrete case.

maximum and the minimum on $\mathcal{K}_{\mathcal{M}}$ and the $P_* \in \mathcal{K}_{\mathcal{M}}$ in which the minimum is achieved is uniquely determined. The second basic fact is that

$$I(P) = -H(P) + \sum_{i \in N} H(P^{\{i\}}) \quad \text{for every } P \in \mathcal{K}_{\mathcal{M}}. \quad (5)$$

Since one-dimensional marginals are shared within $\mathcal{K}_{\mathcal{M}}$, the second term in (5) is a constant. This observation implies the remaining claims of the lemma. \square

3 \mathcal{M} -construct

The following definition is modification of a concept introduced in [6].

DEFINITION 3.1 Let $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ be a strongly consistent collection of probability measures. By an \mathcal{M} -construct we will understand any probability measure Q on \mathbb{X}_N which is absolutely continuous with respect to the dominating product measure L and whose Radon-Nikodym derivative dQ/dL satisfies the condition

$$\forall x \in N_{\mathcal{M}} \quad \frac{dQ}{dL}(x) = k \cdot \prod_{B \in \mathcal{S}^\downarrow} f_B(x_B)^{\nu(B)}, \quad (6)$$

where $k \in (0, \infty)$ and $\nu(B) \in \mathbb{Z}$, $B \in \mathcal{S}^\downarrow$ are the respective parameters of Q .

The *multiinformation content* of the \mathcal{M} -construct Q given by (6) is the following number, denoted by $I_{\mathcal{M}}(Q)$,

$$I_{\mathcal{M}}(Q) = \ln k + \sum_{B \in \mathcal{S}^\downarrow} \nu(B) \cdot I(P_B). \quad (7)$$

An example of an \mathcal{M} -construct is the dominating product measure L – it suffices to put $k = 1$, $\nu(\{i\}) = 1$ for $i \in N$ and $\nu(B) = 0$ for remaining $B \in \mathcal{S}^\downarrow$.¹⁹ However, there are other examples of \mathcal{M} -constructs, namely the approximations of $P \in \mathcal{K}_{\mathcal{M}}$ mentioned in § 4 and § 5. The following lemma says that every \mathcal{M} -construct gives a lower estimate of minimal multiinformation in $\mathcal{K}_{\mathcal{M}}$.

LEMMA 3.1 Let $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ be a strongly consistent collection of probability measures and Q be an \mathcal{M} -construct. Then $P \ll Q \ll L$ for every $P \in \mathcal{K}_{\mathcal{M}}$. Moreover,

$$\min \{I(P); P \in \mathcal{K}_{\mathcal{M}}\} \geq I_{\mathcal{M}}(Q) \quad (8)$$

and the equality in (8) occurs iff $Q \in \mathcal{K}_{\mathcal{M}}$, in which case $I_{\mathcal{M}}(Q) = I(Q)$. Actually, one has $H(P|Q) = I(P) - I_{\mathcal{M}}(Q)$ for any $P \in \mathcal{K}_{\mathcal{M}}$ and an \mathcal{M} -construct Q .

Proof: The fact $Q \ll L$ follows directly from Definition 3.1. To show $P \ll Q$ it suffices to verify $p(x) > 0 \Rightarrow q(x) > 0$ for $x \in \mathbb{X}_N$. If $p(x) > 0$ then $l(x) > 0$ and to get $q(x) > 0$ one needs to show that $(dQ/dL)(x) > 0$.²⁰ However, then $x \in N_P \subseteq N_{\mathcal{M}}$ and the formula (6) for $dQ/dL(x)$ can be used. The vanishing principle for marginal densities (2) implies $p_B(x_B) > 0$ for every $B \subseteq N$ and this gives $f_B(x_B) > 0$ for any $B \in \mathcal{S}^\downarrow$.²¹ In particular, (6) implies $(dQ/dL)(x) > 0$, which was needed.

¹⁹Note that $f_B \equiv 1$ whenever $|B| = 1$.

²⁰Realize that $q(x) = dQ/dL(x) \cdot l(x)$.

²¹Recall that $p_B(x_B) = (dP_B/dL^B)(x_B) \cdot l^B(x_B) = f_B(x_B) \cdot l^B(x_B)$.

The next step is to observe that

$$\sum_{x \in \mathcal{X}_N, p(x) > 0} p(x) \cdot \ln \frac{dQ}{dL}(x) = I_{\mathcal{M}}(Q). \quad (9)$$

Indeed, whenever $x \in \mathcal{X}_N$, $p(x) > 0$ then $x \in N_P \subseteq N_{\mathcal{M}}$ and (6) can be used, which gives:

$$\sum_{x \in \mathcal{X}_N, p(x) > 0} p(x) \cdot \ln \frac{dQ}{dL}(x) = \sum_{p(x) > 0} p(x) \cdot \ln k + \sum_{B \in \mathcal{S}^\perp} \nu(S) \cdot \sum_{p(x) > 0} p(x) \cdot \ln f_B(x_B).$$

To get the expression in (7) write the last internal sum as follows:

$$\begin{aligned} \sum_{x \in \mathcal{X}_N, p(x) > 0} p(x) \cdot \ln f_B(x_B) &= \sum_{y \in \mathcal{X}_B, p_B(y) > 0} \sum_{z \in \mathcal{X}_{N \setminus B}, p([y, z]) > 0} p([y, z]) \cdot \ln f_B(y) \\ &= \sum_{y \in \mathcal{X}_B, p_B(y) > 0} \ln f_B(y) \cdot \sum_{z \in \mathcal{X}_{N \setminus B}, p([y, z]) > 0} p([y, z]) = \\ &= \sum_{y \in \mathcal{X}_B, p_B(y) > 0} \{\ln f_B(y)\} \cdot p_B(y), \end{aligned}$$

and realize that $f_B = dP_B/dL^B$.

Now, (9) can be used to derive (8). Consider $P \in \mathcal{K}_{\mathcal{M}}$. The fact $P \ll Q \ll L$ implies that $\frac{dP}{dQ}(x) = \frac{dP}{dL}(x)/\frac{dQ}{dL}(x)$ for every $x \in N_Q$.²² This allow one to write using (9):

$$\begin{aligned} 0 &\leq H(P|Q) = \sum_{x \in \mathcal{X}_N, p(x) > 0} p(x) \cdot \ln \frac{dP}{dQ}(x) \\ &= \sum_{p(x) > 0} p(x) \cdot \ln \frac{dP}{dL}(x) - \sum_{p(x) > 0} p(x) \cdot \ln \frac{dQ}{dL}(x) = I(P) - I_{\mathcal{M}}(Q). \end{aligned}$$

This gives $I(P) \geq I_{\mathcal{M}}(Q)$ and (8). Moreover, the equality $I(P) = I_{\mathcal{M}}(Q)$ means that $H(P|Q) = 0$ and this occurs iff $P = Q$. However, $P = Q$ implies $Q \in \mathcal{K}_{\mathcal{M}}$. Conversely, if $Q \in \mathcal{K}_{\mathcal{M}}$ then we put $P' = Q \in \mathcal{K}_{\mathcal{M}}$ and repeat the above consideration to get $0 = H(P'|Q) = I(P') - I_{\mathcal{M}}(Q)$. The formula (8) allows to write

$$I(P') \geq \min \{I(P); P \in \mathcal{K}_{\mathcal{M}}\} \geq I_{\mathcal{M}}(Q) = I(P'),$$

which implies that the equality in (8) occurs and $I(Q) = I(P') = I_{\mathcal{M}}(Q)$. The last equality mentioned in Lemma 3.1 was verified above. \square

4 Dependence structure simplifications

This is one of the ways to approximate measures from $\mathcal{K}_{\mathcal{M}}$, already proposed in the 1970s by the first author in [3]. Dependence structure simplifications were also dealt with in the CSc thesis of the second author [7]. The following is a minor modification of the definition from [7].

²²Observe that $\frac{dQ}{dL}(x) > 0$ for every $x \in N_Q$ and use the definition of the Radon-Nikodym derivative.

DEFINITION 4.1 Let $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ be a strongly consistent collection of probability measures. Let us choose a total ordering $\tau : S_1, \dots, S_n, n \geq 1$ of elements of \mathcal{S} and put $F_j \equiv S_j \cap (\bigcup_{k < j} S_k)$ and $G_j \equiv S_j \setminus F_j$ for $1 \leq j \leq n$.²³ By a *choice* for \mathcal{M} and τ we will understand a mapping ϑ which assigns a conditional density $p_{G_j|F_j}$ on X_{G_j} given X_{F_j} consistent with p_{S_j} to every $1 \leq j \leq n$.²⁴

By a *dependence structure simplification* (DSS) for \mathcal{M} determined by ordering τ and the choice ϑ will be understood a probability measure on X_N whose density $\bar{p}_{\tau, \vartheta}$ is given by

$$\bar{p}_{\tau, \vartheta}(x) = \prod_{j=1}^n p_{G_j|F_j}(x_{G_j}|x_{F_j}) \quad \text{for every } x \in \mathsf{X}_N. \quad (10)$$

The class of all DSSs for \mathcal{M} (determined by any possible τ and ϑ) will be denoted by $\mathcal{D}_{\mathcal{M}}$.

REMARK 3 The concept of a “choice for \mathcal{M} and τ ” is a technical concept which is needed to overcome some troubles one can come across if densities of given distributions from \mathcal{M} vanish for certain marginal configurations.

Of course, if $p_{F_j} > 0$ on X_{F_j} for some $j \in \{1, \dots, n\}$ ²⁶ then the conditional density $p_{G_j|F_j}$ consistent with p_{S_j} is uniquely determined as the ratio p_{S_j}/p_{F_j} . Therefore, if the ordering τ is such that $p_{F_j} > 0$ on X_{F_j} for any $j = 1, \dots, n$ ²⁷ then all terms in (10) are uniquely determined and it takes the form

$$\bar{p}_{\tau}(x) = \prod_{j=1}^n \frac{p_{S_j}(x_{S_j})}{p_{F_j}(x_{F_j})} \quad \text{for any } x \in \mathsf{X}_N. \quad (11)$$

In that special case the concept of choice for \mathcal{M} and τ is superfluous and can be omitted.

However, on the other hand, if $p_{F_j}(x_{F_j}) = 0$ for at least one $j \in \{1, \dots, n\}$ and $x \in \mathsf{X}_N$ then the respective term $p_{S_j}(x_{S_j})/p_{F_j}(x_{F_j})$ in (11) is an undefined ratio $0/0!$ It may even happen that no other term $p_{S_k}(x_{S_k})/p_{F_k}(x_{F_k})$ for $k \neq j$ vanishes for that particular configuration $x \in \mathsf{X}_N$, which means that $\bar{p}_{\tau}(x)$ is not defined then – see Example 4. Therefore, some additional “conventions” are needed to ensure that the formula (11) defines a density on X_N . One of the methods to settle the matter is to choose and fix versions of conditional densities. Surprisingly, this choice appears not to influence the quality of the resulting approximation from the point of view we consider – see Lemma 4.1. Another possible approach to deal with the above problem is mentioned in Remark 4.

Another interesting observation is that whenever $S_j \subseteq \bigcup_{k < j} S_k$ for some $j \in \{1, \dots, n\}$ then p_{S_j} does not influence the value of $\bar{p}_{\tau, \vartheta}$.²⁸ The following is a basic fact concerning DSSs.

LEMMA 4.1 Assume that $l(x) > 0$ for every $x \in \mathsf{X}_N$.²⁹ Then every $Q \in \mathcal{D}_{\mathcal{M}}$ is an \mathcal{M} -construct

²³In particular, $F_1 = \emptyset$ and $G_1 = S_1$.

²⁴By a *conditional density* on X_A given X_C is meant a function of two variables $[y, z] \mapsto p_{A|C}(y|z)$, $y \in \mathsf{X}_A$, $z \in \mathsf{X}_C$ such that $\forall z \in \mathsf{X}_C$ its restriction $y \mapsto p_{A|C}(y|z)$, $y \in \mathsf{X}_A$ is a density of a probability measure on X_A . It is called *consistent* with a density q on X_{AC} if $p_{A|C}(y|z) = q([y, z])/q^C(z)$ whenever $q^C(z) > 0$.

²⁵It can be shown by induction on n that (10) indeed defines a density of a probability measure on X_N .

²⁶Observe that p_{F_j} belongs to the extended system \mathcal{M}^\downarrow mentioned in § 2.2.3 and that if $F_j = \emptyset$ the $p_{F_j} > 0$ on $\mathsf{X}_{F_j} = \mathsf{X}_\emptyset$ owing to our convention from § 2.1.

²⁷This happens whenever $p_S > 0$ on X_S for every $S \in \mathcal{S}$, by vanishing principle.

²⁸This is because then $G_j = \emptyset$ and $p_{G_j|F_j}(x_{G_j}|x_{F_j}) = p_{\emptyset|S_j}(x_\emptyset|x_{S_j}) = 1$ for any $x \in \mathsf{X}_N$.

²⁹This unrestrictive assumption – see Remark 2 – is needed to ensure $Q \ll L$ for every $Q \in \mathcal{D}_{\mathcal{M}}$. Alternatively, we can modify Definition 4.1 and restrict our choices to conditional densities $p_{G_j|F_j}$ on X'_{G_j} given X'_{F_j} .

and, provided that its density $\bar{p}_{\tau, \vartheta}$ is given by (10), its multiinformation content is

$$I_{\mathcal{M}}(Q) = \sum_{A \in \mathcal{S}} I(P_A) - \sum_{j=2}^n I(P_{F_j}) = \prod_{B \in \mathcal{S}^\downarrow} \nu(B) \cdot I(P_B), \quad (12)$$

where

$$\nu(B) = |\{j; S_j = B\}| - |\{j; F_j = B\}| \quad \text{for any } B \in \mathcal{S}^\downarrow. \quad (13)$$

In particular, the multiinformation content of Q does not depend on the choice ϑ for \mathcal{M} and τ .

Proof: As $l(x) > 0$ for every $x \in \mathbf{X}_N$, the claim $Q \ll L$ is evident. We can express the Radon-Nikodym derivative dQ/dL as the ratio of respective densities $\bar{p}_{\tau, \vartheta}$ and l . To verify (6) let us choose $P \in \mathcal{K}_{\mathcal{M}}$ such that $N_P = N_{\mathcal{M}}$. Thus, given $x \in N_{\mathcal{M}}$ one has $p(x) > 0$ and this implies by the vanishing principle $p_{F_j}(x_{F_j}) > 0$ for every $j = 1, \dots, n$. Another point is that the density l of the dominating product measure L can formally be written as follows:

$$l(x) = \prod_{i \in N} l_i(x_i) = \prod_{j=1}^n l_{G_j}(x_{G_j}) = \prod_{j=1}^n \frac{l_{S_j}(x_{S_j})}{l_{F_j}(x_{F_j})} \quad \text{for } x \in \mathbf{X}_N.$$

Therefore, we can write for $x \in N_{\mathcal{M}}$ by (10) and the above formula:

$$\frac{dQ}{dL}(x) = \frac{\bar{p}_{\tau, \vartheta}(x)}{l(x)} = \prod_{j=1}^n \frac{p_{S_j}(x_{S_j}) \cdot l_{F_j}(x_{F_j})}{l_{S_j}(x_{S_j}) \cdot p_{F_j}(x_{F_j})} = \prod_{j=1}^n \frac{f_{S_j}(x_{S_j})}{f_{F_j}(x_{F_j})} = \prod_{B \in \mathcal{S}^\downarrow} f_B(x_B)^{\nu(B)},$$

where $\nu(B)$ is given by (13). Thus, (6) holds with $k = 1$. By substituting $\nu(B)$, $B \in \mathcal{S}^\downarrow$ to (7) and realizing that $I(P_{F_1}) = I(P_\emptyset) = 0$ we get (12). \square

The following example shows that the multiinformation content of a DSS Q need not equal to its multiinformation.

EXAMPLE 2 Put $N = \{a, b, c, d\}$, $\mathbf{X}_i = \{0, 1\}$ for every $i \in N$ and consider a class of sets $\mathcal{S} = \{S_1, S_2, S_3\}$, where $S_1 = \{a, b\}$, $S_2 = \{a, c\}$ and $S_3 = \{b, c, d\}$. The collection of probability measures $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ is introduced by means of densities:

$$p_A(0, 0) = p_A(1, 1) = \frac{1}{5}, \quad p_A(0, 1) = p_A(1, 0) = \frac{3}{10} \quad \text{for } A = S_1 \text{ and } A = S_2,$$

while for $B = S_3 = \{b, c, d\}$

$$p_B(0, 0, 0) = p_B(1, 1, 0) = \frac{1}{5}, \quad p_B(0, 1, 1) = p_B(1, 0, 1) = \frac{3}{10}.$$

To see that \mathcal{M} is strongly consistent consider a density $p : \mathbf{X}_N \rightarrow [0, 1]$, where $p(0, 0, 0, 0) = p(1, 1, 1, 0) = 1/20$ and $p(x) = 3/20$ for any of the following six configurations: $(0, 0, 1, 1)$, $(0, 1, 0, 1)$, $(0, 1, 1, 0)$, $(1, 0, 0, 0)$, $(1, 0, 1, 1)$ and $(1, 1, 0, 1)$. Take an ordering $\tau : S_1, S_2, S_3$ and observe that $p_{F_j} > 0$ for $j = 2, 3$. Therefore, the density $q = \bar{p}_\tau$ of the respective DSS Q is unambiguously defined. It has the same supporter as the above mentioned joint density p . More specifically, $q(0, 0, 0, 0) = q(1, 1, 1, 0) = 2/25$, $q(0, 1, 1, 0) = q(1, 0, 0, 0) = 9/50$ and $q(x) = 3/25$ for the following four configurations: $(0, 0, 1, 1)$, $(0, 1, 0, 1)$, $(1, 0, 1, 1)$ and $(1, 1, 0, 1)$. Hence, one has for $B = \{b, c, d\}$:

$$q_B(0, 0, 0) = q_B(1, 1, 0) = \frac{13}{50}, \quad q_B(0, 1, 1) = q_B(1, 0, 1) = \frac{6}{25}.$$

To express the difference $I(Q) - I_{\mathcal{M}}(Q)$ we first write the multiinformation of Q as follows:

$$I(Q) = I(Q_{ab}) + I(Q_{ac}) + I(Q_{bcd}) - I(Q_a) - I(Q_{bc}).^{30}$$

Now, by (12), $I_{\mathcal{M}}(Q)$ has the same form, but Q_A is replaced by P_A for respective sets $A \subseteq N$ there. As $Q_{ab} = P_{ab}$ and $Q_{ac} = P_{ac}$ one has

$$I(Q) - I_{\mathcal{M}}(Q) = [I(Q_{bcd}) - I(Q_{bc})] - [I(P_{bcd}) - I(P_{bc})],$$

and the reader can obtain by direct computation³¹ $I(Q_{bcd}) - I(Q_{bc}) = \frac{13}{25} \cdot \ln \frac{25}{13} + \frac{12}{25} \cdot \ln \frac{25}{12}$ and $I(P_{bcd}) - I(P_{bc}) = \frac{2}{5} \cdot \ln \frac{5}{2} + \frac{3}{5} \cdot \ln \frac{5}{3}$. Hence, $I(Q) - I_{\mathcal{M}}(Q) = -\frac{14}{25} \cdot \ln 2 + \frac{3}{25} \cdot \ln 3 + \ln 5 - \frac{13}{25} \cdot \ln 13 \neq 0$.

Thus, Lemmas 4.1 and 3.1 allow one to derive the following corollary, already given in [7].

COROLLARY 4.1 Provided $l(x) > 0$ for every $x \in \mathbf{X}_N$, $Q \in \mathcal{D}_{\mathcal{M}}$ and $P \in \mathcal{K}_{\mathcal{M}}$ and one has

$$H(P|Q) = I(P) - I_{\mathcal{M}}(Q) = I(P) - \sum_{A \in \mathcal{S}} I(P_A) + \sum_{j=2}^n I(P_{F_j}).$$

The previous corollary substantially simplifies the task of finding an optimal DSS.

DEFINITION 4.2 Let $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ be a strongly consistent collection of probability measures. A DSS $Q \in \mathcal{D}_{\mathcal{M}}$ will be called *optimal* relative to $P \in \mathcal{K}_{\mathcal{M}}$ if

$$H(P|Q) = \min \{H(P|Q'); Q' \in \mathcal{D}_{\mathcal{M}}\}.$$

It follows from the formula in Corollary 4.1 that $Q = \overline{P}_{\tau, \vartheta} \in \mathcal{D}_{\mathcal{M}}$ is optimal iff it maximizes the multiinformation content $I_{\mathcal{M}}(Q)$ given by (12). Of course, this occurs if τ minimizes the value of the function $\tau \mapsto \iota(\tau) \equiv \sum_{j=2}^n I(P_{F_j})$. In particular, the fact that $Q \in \mathcal{D}_{\mathcal{M}}$ is optimal relative to a particular $P \in \mathcal{K}_{\mathcal{M}}$ actually does not depend on P ! Note that the problem of finding an ordering yielding an optimal DSS was dealt with in more detail in [7]. The following example illustrates the procedure. In this case, an optimal DSS is unique.³²

EXAMPLE 3 Put $N = \{a, b, c\}$, $\mathbf{X}_i = \{0, 1\}$ for every $i \in N$ and $\mathcal{S} = \{A \subseteq N; |A| = 2\}$. These are the densities of probability measures from $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$:

$$p_{\{a,b\}}(0,0) = p_{\{a,b\}}(0,1) = \frac{1}{4}, \quad p_{\{a,b\}}(1,0) = \frac{1}{8}, \quad p_{\{a,b\}}(1,1) = \frac{3}{8},$$

$p_{\{a,c\}}(x) = 1/4$ for every $x \in \mathbf{X}_{\{a,c\}}$, and

$$p_{\{b,c\}}(0,0) = p_{\{b,c\}}(1,0) = \frac{1}{4}, \quad p_{\{b,c\}}(0,1) = \frac{1}{8}, \quad p_{\{b,c\}}(1,1) = \frac{3}{8}.$$

To show that \mathcal{M} is strongly consistent consider a density p on $\mathbf{X}_{\{a,b,c\}}$ given as follows: $p(0,0,0) = p(0,1,1) = p(1,1,0) = 1/4$ and $p(1,0,1) = p(1,1,1) = 1/8$.

³⁰To see this one can utilize the concept of conditional independence and the formula (2.17) in [8]. Indeed, by construction one has $d \perp\!\!\!\perp a \mid bc [Q]$ and $b \perp\!\!\!\perp c \mid a [Q]$.

³¹Actually, $I(Q_{bcd}) - I(Q_{bc}) = H(Q_{bcd}|Q_{bc} \times Q_d)$ and $I(P_{bcd}) - I(P_{bc}) = H(P_{bcd}|P_{bc} \times P_d)$ and one use the above formulas for q_B and p_B with $B = \{b, c, d\}$.

³²On the other hand, in Example 2, each of three possible DSSs is optimal.

For example, the ordering $\tau_1 : S_1 = \{a, b\}, S_2 = \{a, c\}, S_3 = \{b, c\}$ gives $F_2 = \{a\}$ and $F_3 = \{b, c\}$ and this leads to the value $\iota(\tau_1) = I(P_a) + I(P_{bc}) = I(P_{bc})$. Clearly, the value of $\iota(\tau)$ is the multiinformation of the last marginal in the ordering τ . As $I(P_{ac}) = 0$ and $I(P_{ab}) = I(P_{bc}) = \frac{3}{2} \cdot \ln 2 - \frac{5}{8} \cdot \ln 5 > 0$ there are two “optimal” orderings, namely $\{a, b\}, \{b, c\}, \{a, c\}$ and $\{b, c\}, \{a, b\}, \{a, c\}$. They both lead to the same DSS, given by this density q :

$$\begin{aligned} q(0, 0, 0) &= \frac{1}{6}, & q(0, 0, 1) &= \frac{1}{12}, & q(0, 1, 0) &= \frac{1}{10}, & q(0, 1, 1) &= \frac{3}{20}, \\ q(1, 0, 0) &= \frac{1}{12}, & q(1, 0, 1) &= \frac{1}{24}, & q(1, 1, 0) &= \frac{3}{20}, & q(1, 1, 1) &= \frac{9}{40}. \end{aligned}$$

The last example in this section illustrates what was mentioned in Remark 3, namely that an undefined expression can occur in the formula (11).

EXAMPLE 4 Put $N = \{a, b, c, d\}$ and $\mathbf{X}_i = \{0, 1\}$ for every $i \in N$. Consider a class of sets $\mathcal{S} = \{S_1, S_2, S_3\}$, where $S_1 = \{a, b\}$, $S_2 = \{a, c\}$ and $S_3 = \{b, c, d\}$. The densities of probability measures from $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ are given as follows: $p_{\{a,b\}}(x) = 1/4$ for any $x \in \mathbf{X}_{\{a,b\}}$, $p_{\{a,c\}}(x) = 1/4$ for any $x \in \mathbf{X}_{\{a,c\}}$ and $p_{\{b,c,d\}}$ has the value $1/4$ for any of the following four configurations: $(0, 0, 0)$, $(0, 0, 1)$, $(1, 1, 0)$ and $(1, 1, 1)$. To see that \mathcal{M} is strongly consistent consider a density p on $\mathbf{X}_{\{a,b,c,d\}}$ such that $p(x) = 1/8$ for any configuration x of the following eight ones: $(0, 0, 0, 0)$, $(0, 0, 0, 1)$, $(0, 1, 1, 0)$, $(0, 1, 1, 1)$, $(1, 0, 0, 0)$, $(1, 0, 0, 1)$, $(1, 1, 1, 0)$ and $(1, 1, 1, 1)$.

If we consider the ordering $\tau : S_1, S_2, S_3$ then $F_2 = \{a\}$ and $F_3 = \{b, c\}$. The point is that $p_{\{b,c\}}(0, 1) = p_{\{b,c\}}(1, 0) = 0$. Therefore, one has:

$$\bar{p}_\tau(0, 0, 1, 0) = \frac{p_{\{a,b\}}(0, 0) \cdot p_{\{a,c\}}(0, 1) \cdot p_{\{b,c,d\}}(0, 1, 0)}{p_{\{a\}}(0) \cdot p_{\{b,c\}}(0, 1)} = \frac{\frac{1}{4} \cdot \frac{1}{4} \cdot 0}{\frac{1}{2} \cdot 0},$$

which is an undefined expression. Actually, the sum of the defined terms in (11), that is, $\bar{p}_\tau(x)$ with $x_{\{b,c\}} = (0, 0)$ or $x_{\{b,c\}} = (1, 1)$, is $1/2$. This indicates that the idea to put $\bar{p}_\tau(x) = 0$ whenever the expression is not defined does not solve the problem.

REMARK 4 An alternative formal definition of a DSS, mentioned implicitly in the manuscript [6], is as follows. The convention $(0/0) \equiv 0$ is accepted. Then (11) defines “density” of a non-negative measure on \mathbf{X}_N . However, in general, $0 < d \equiv \sum_{x \in \mathbf{X}_N} \bar{p}_\tau(x) \leq 1$.³³ One can introduce a density q by the formula $q(x) = d^{-1} \cdot \bar{p}_\tau(x)$ for $x \in \mathbf{X}_N$. The point is that this alternative definition of a DSS³⁴ leads to a different formula for the multiinformation content, namely $\ln d^{-1} + \sum_{A \in \mathcal{S}} I(P_A) - \sum_{j=2}^n I(P_{F_j})$; see (7). Paradoxically, this can give better approximation of $P \in \mathcal{K}_{\mathcal{M}}$ than the DSS introduced in Definition 4.1 – because the multiinformation content is enlarged by the factor $\ln d^{-1}$. Nevertheless, this only can happen in “non-standard” situations. For example, as mentioned in Remark 3, if $p_S > 0$ for any $S \in \mathcal{S}$ then all terms in (11) are defined and there is no difference between those two formal definitions of a DSS.

5 Explicit expression

This is a method for approximating measures from $\mathcal{K}_{\mathcal{M}}$ proposed newly in [6]. The motivation for this proposal was to utilize maximally the information given by \mathcal{M} and, moreover, impose

³³The fact $d > 0$ can be derived from strong consistency of \mathcal{M} . Indeed, consider the density p of $P \in \mathcal{K}_{\mathcal{M}}$, $x \in \mathbf{X}_N$ with $p(x) > 0$. Then, by (2), all nominators and denominators in (11) are positive and $\bar{p}_\tau(x) > 0$.

³⁴It is also an \mathcal{M} -construct – one can modify the arguments from the proof of Lemma 4.1.

the minimal possible amount of dependencies between variables. The idea was elicited by the first author when he tried to solve the approximation problem described in §1 by the method of Lagrange multipliers.

DEFINITION 5.1 Given $n \in \mathbb{N}$, the symbol $sg(n)$ will denote $(-1)^n$; that is, $sg(n) = +1$ for even n and $sg(n) = -1$ for odd n . Let $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ be a strongly consistent collection of probability measures. Let us put

$$\text{Exe}(x) = \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} p_{\cap \mathcal{A}}(x_{\cap \mathcal{A}})^{-sg(|\mathcal{A}|)} \quad \text{for every } x \in \mathbf{X}_N,^{35} \quad (14)$$

where we accept the convention that $0^{-1} \equiv 0$. Then we put $c = \sum_{x \in \mathbf{X}_N} \text{Exe}(x)^{36}$ and define

$$\overline{\text{Exe}}(x) = c^{-1} \cdot \text{Exe}(x) \equiv c^{-1} \cdot \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} p_{\cap \mathcal{A}}(x_{\cap \mathcal{A}})^{-sg(|\mathcal{A}|)} \quad \text{for every } x \in \mathbf{X}_N. \quad (15)$$

Of course, $\overline{\text{Exe}}$ is a density of a probability measure on \mathbf{X}_N , denote by P_{exe} . The number c will be called the *norm* (of the explicit expression Exe) and denoted by $|\text{Exe}|$.

Note that the norm $|\text{Exe}|$ could be both higher and lower than 1 – examples are given in §7. Nevertheless, even if $|\text{Exe}| = 1$ then the respective explicit expression approximation P_{exe} need not belong to $\mathcal{K}_{\mathcal{M}}$ as the following example shows.

EXAMPLE 5 Consider the system of marginals \mathcal{M} from Example 3. Then $p_{\{a\}}(0) = p_{\{a\}}(1) = 1/2 = p_{\{c\}}(0) = p_{\{c\}}(1)$ and $p_{\{b\}}(0) = 3/8$, $p_{\{b\}}(1) = 5/8$; this allows one to write by (14):

$$\text{Exe}(0, 0, 0) = \frac{p_{\{a,b\}}(0, 0) \cdot p_{\{a,c\}}(0, 0) \cdot p_{\{b,c\}}(0, 0) \cdot p_{\emptyset}(-)}{p_{\{a\}}(0) \cdot p_{\{b\}}(0) \cdot p_{\{c\}}(0)} = \frac{\frac{1}{4} \cdot \frac{1}{4} \cdot \frac{1}{4} \cdot 1}{\frac{1}{2} \cdot \frac{3}{8} \cdot \frac{1}{2}} = \frac{2 \cdot 8 \cdot 2}{4 \cdot 4 \cdot 4 \cdot 3} = \frac{1}{6}.$$

Actually, the result of detailed calculation of Exe is the density q of the optimal DSS mentioned in Example 3. In particular, $|\text{Exe}| = 1$ and P_{exe} has density q . However, $q_{\{a,c\}}(0, 0) = (1/6) + (1/10) = 8/30 \neq 1/4 = p_{\{a,c\}}(0, 0)$, which means $P_{exe} \notin \mathcal{K}_{\mathcal{M}}$. On the other hand, the example also shows that P_{exe} can coincide with an optimal DSS.

LEMMA 5.1 Let $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ be a strongly consistent collection of probability measures. Then the probability measure P_{exe} is an \mathcal{M} -construct. Its multiinformation content is

$$I_{\mathcal{M}}(P_{exe}) = -\ln |\text{Exe}| + \sum_{B \in \mathcal{S}^\downarrow} \nu(B) \cdot I(P_B), \quad (16)$$

where

$$\nu(B) = \sum \{-sg(|\mathcal{A}|); \emptyset \neq \mathcal{A} \subseteq \mathcal{S}, \bigcap \mathcal{A} = B\} \quad \text{for any } B \in \mathcal{S}^\downarrow. \quad (17)$$

Proof: The first observation is that

$$\forall i \in N \quad \sum \{sg(|\mathcal{A}|); \emptyset \neq \mathcal{A} \subseteq \mathcal{S}, i \in \bigcap \mathcal{A}\} = -1. \quad (18)$$

³⁵Observe that Exe defines a “density” of a measure EXE on \mathbf{X}_N such that $P \ll \text{EXE}$ for every $P \in \mathcal{K}_{\mathcal{M}}$. Indeed, (2) implies that whenever $p(x) > 0$ for $x \in \mathbf{X}_N$ then $p_{\cap \mathcal{A}}(x_{\cap \mathcal{A}}) > 0$ for every $\emptyset \neq \mathcal{A} \subseteq \mathcal{S}$.

³⁶The assumption of strong consistency of \mathcal{M} implies that $c > 0$ – use what it says in the preceding footnote.

Indeed, consider a fixed $i \in N$, denote by \mathcal{H} the class of $A \in \mathcal{S}$ with $i \in A$ and write using the definition of $sg(n)$ and binominal formula:

$$\begin{aligned}
\sum_{\emptyset \neq \mathcal{A} \subseteq \mathcal{H}} sg(|\mathcal{A}|) &= \sum_{\emptyset \neq \mathcal{A} \subseteq \mathcal{H}} (-1)^{|\mathcal{A}|} = \sum_{\ell=1}^{|\mathcal{H}|} \sum_{\mathcal{A} \subseteq \mathcal{H}, |\mathcal{A}|=\ell} (-1)^\ell = \sum_{\ell=1}^{|\mathcal{H}|} (-1)^\ell \cdot |\{\mathcal{A} \subseteq \mathcal{H}; |\mathcal{A}| = \ell\}| \\
&= \sum_{\ell=1}^{|\mathcal{H}|} (-1)^\ell \cdot \binom{|\mathcal{H}|}{\ell} = -1 + \sum_{\ell=0}^{|\mathcal{H}|} (-1)^\ell \cdot 1^{|\mathcal{H}|-\ell} \cdot \binom{|\mathcal{H}|}{\ell} \\
&= -1 + (-1+1)^{|\mathcal{H}|} = -1 + 0^{|\mathcal{H}|} = -1.
\end{aligned}$$

The main step is to introduce a measure Q on \mathbf{X}_N such that $Q \ll L$ and its Radon-Nikodym derivative $\frac{dQ}{dL}$ has the following form:

$$\frac{dQ}{dL}(x) = \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} f_{\cap \mathcal{A}}(x_{\cap \mathcal{A}})^{-sg(|\mathcal{A}|)} \quad \text{for any } x \in \mathbf{X}_N. \quad (19)$$

To show that P_{exe} is an \mathcal{M} -construct it suffices to show that the density q of Q coincides with Exe . This is easy to see for $x \in \mathbf{X}_N$ with $l(x) = 0$. Then $p_{\{i\}}(x_i) = 0$ for some $i \in N$ and the assumption $\bigcup \mathcal{S} = N$ forces the existence of $A \subseteq \mathcal{S}$ with $i \in A$. Therefore, the vanishing principle (2) implies that at least one factor in (14) vanishes and $\text{Exe}(x) = 0$.

To verify $q(x) = \text{Exe}(x)$ for $x \in \mathbf{X}_N$ with $l(x) > 0$ we first observe that

$$\prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} \prod_{j \in \cap \mathcal{A}} p_{\{j\}}(x_j)^{sg(|\mathcal{A}|)} = \prod_{i \in N} p_{\{i\}}(x_i)^{-1}. \quad (20)$$

Indeed, one can write it with the help of (18) as follows:

$$\begin{aligned}
\prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} \prod_{j \in \cap \mathcal{A}} p_{\{j\}}(x_j)^{sg(|\mathcal{A}|)} &= \prod_{i \in N} \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}, i \in \cap \mathcal{A}} p_{\{i\}}(x_i)^{sg(|\mathcal{A}|)} \\
&= \prod_{i \in N} p_{\{i\}}(x_i)^{\sum \{sg(|\mathcal{A}|); \emptyset \neq \mathcal{A} \subseteq \mathcal{S}, i \in \cap \mathcal{A}\}} = \prod_{i \in N} p_{\{i\}}(x_i)^{-1}.
\end{aligned}$$

The formulas (19), $f_B = p_B \cdot \prod_{j \in B} p_{\{j\}}^{-1}$ for $B \subseteq N$ (see § 2.2.3) and (20) now allows one to write $q(x)$ as follows:

$$\begin{aligned}
q(x) &= \frac{dQ}{dL}(x) \cdot l(x) = \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} f_{\cap \mathcal{A}}(x_{\cap \mathcal{A}})^{-sg(|\mathcal{A}|)} \cdot \prod_{i \in N} p_{\{i\}}(x_i) \\
&= \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} \{ p_{\cap \mathcal{A}}(x_{\cap \mathcal{A}})^{-sg(|\mathcal{A}|)} \cdot \prod_{j \in \cap \mathcal{A}} p_{\{j\}}(x_j)^{sg(|\mathcal{A}|)} \} \cdot \prod_{i \in N} p_{\{i\}}(x_i) \\
&= \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} p_{\cap \mathcal{A}}(x_{\cap \mathcal{A}})^{-sg(|\mathcal{A}|)} \cdot \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} \prod_{j \in \cap \mathcal{A}} p_{\{j\}}(x_j)^{sg(|\mathcal{A}|)} \cdot \prod_{i \in N} p_{\{i\}}(x_i) \\
&= \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} p_{\cap \mathcal{A}}(x_{\cap \mathcal{A}})^{-sg(|\mathcal{A}|)} \cdot \prod_{i \in N} p_{\{i\}}(x_i)^{-1} \cdot \prod_{i \in N} p_{\{i\}}(x_i) \\
&= \prod_{\emptyset \neq \mathcal{A} \subseteq \mathcal{S}} p_{\cap \mathcal{A}}(x_{\cap \mathcal{A}})^{-sg(|\mathcal{A}|)} \cdot 1 = \text{Exe}(x).
\end{aligned}$$

The observation $q = \text{Exe}$ means that P_{exe} is c^{-1} -multiple of Q where $c = |\text{Exe}|$. In particular, by (19), $P_{exe} \ll L$ and

$$\frac{dP_{exe}}{dL}(x) = c^{-1} \cdot \prod_{\emptyset \neq A \subseteq S} f_{\cap A}(x_{\cap A})^{-sg(|A|)} = c^{-1} \cdot \prod_{B \in \mathcal{S}^\downarrow} f_B(x_B)^{\sum \{-sg(|A|); \emptyset \neq A \subseteq B, \cap A = B\}}.$$

Then, by Definition 3.1, P_{exe} is an \mathcal{M} -construct with $k = c^{-1}$ and $\nu(B)$, $B \subseteq N$ given by (17). The formula (16) follows from (7). \square

COROLLARY 5.1 Given $P \in \mathcal{K}_{\mathcal{M}}$ one has

$$H(P|P_{exe}) = I(P) - I_{\mathcal{M}}(P_{exe}) = I(P) + \ln |\text{Exe}| - \sum_{B \in \mathcal{S}^\downarrow} \nu(B) \cdot I(P_B),$$

where $\nu(B)$, $B \in \mathcal{S}^\downarrow$ is given by (17). In particular, $\min_{P \in \mathcal{K}_{\mathcal{M}}} I(P) \geq I_{\mathcal{M}}(P_{exe})$ and the equality occurs iff $P_{exe} \in \mathcal{K}_{\mathcal{M}}$, in which case $I_{\mathcal{M}}(P_{exe}) = I(P_{exe})$.

Proof: This follows from Lemma 3.1: we put $Q = P_{exe}$ and use the formula (16). \square

REMARK 5 An useful observation concerning explicit expression approximation was made in [6]. If we consider the multi-symptom diagnostic problem mentioned in § 1 and base our estimator on direct approximation of P by means of the explicit expression $\hat{P} = P_{exe}$, then it is *not necessary* to compute the norm $|\text{Exe}|$. This is because $\bar{\text{Exe}}$ and Exe only differ in multiplicative positive factor and always achieve their maxima in same configurations. Thus, in this particular case, one has

$$\psi_1(x_S) = \text{argmax} \{ \text{Exe}([y, x_S]); y \in X_d \}.$$

6 The case of fitting marginals

It may happen that an approximation \hat{P} of measures from $\mathcal{K}_{\mathcal{M}}$ fits the prescribed marginals, that is, \hat{P} really has the measures from \mathcal{M} as marginals and, therefore, it belongs to $\mathcal{K}_{\mathcal{M}}$. The following example shows that both methods for approximation mentioned in this paper may result in a distribution from $\mathcal{K}_{\mathcal{M}}$.

EXAMPLE 6 Put $N = \{a, b, c\}$, $X_a = X_c = \{0, 1\}$, $X_b = \{0, 1, 2\}$ and $\mathcal{S} = \{A \subseteq N; |A| = 2\}$. The densities of measures from $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ are given as follows:

$$\begin{aligned} p_{\{a,b\}}(0,0) &= \frac{2}{9}, & p_{\{a,b\}}(0,1) &= \frac{1}{9}, & p_{\{a,b\}}(1,1) &= p_{\{a,b\}}(1,2) = \frac{1}{3}, \\ p_{\{a,c\}}(0,0) &= p_{\{a,c\}}(1,1) = \frac{2}{9}, & p_{\{a,c\}}(0,1) &= \frac{1}{9}, & p_{\{a,c\}}(1,0) &= \frac{4}{9}, \end{aligned}$$

and, finally

$$p_{\{b,c\}}(0,0) = p_{\{b,c\}}(0,1) = p_{\{b,c\}}(2,0) = \frac{1}{9}, \quad p_{\{b,c\}}(1,0) = \frac{4}{9}, \quad p_{\{b,c\}}(2,1) = \frac{2}{9}.$$

Detailed calculation of Exe gives this

$$\text{Exe}(0,0,0) = \text{Exe}(0,0,1) = \text{Exe}(0,1,0) = \text{Exe}(1,2,0) = \frac{1}{9}, \quad \text{Exe}(1,1,0) = \frac{1}{3}, \quad \text{Exe}(1,2,1) = \frac{2}{9},$$

and $\text{Exe}(x) = 0$ for remaining configurations $x \in X_N$. In particular, $|\text{Exe}| = 1$ and the density p of P_{exe} coincides with Exe . It is easy to see that $p^A = p_A$ for $A \in \mathcal{S}$. Moreover, the calculation of DSS for $\tau: S_1 = \{a, b\}$, $S_2 = \{b, c\}$, $S_3 = \{a, c\}$ gives the same result.

Note that the fact a DSS has the prescribed marginals implies that it is optimal.

COROLLARY 6.1 Assume $l(x) > 0$ for every $x \in X_N$. If $Q^* \in \mathcal{D}_{\mathcal{M}} \cap \mathcal{K}_{\mathcal{M}}$ then Q^* is an optimal DSS (relative to any $P \in \mathcal{K}_{\mathcal{M}}$).

Proof: By Lemma 4.1, Q^* is an \mathcal{M} -construct and Lemma 3.1 says that $Q^* \in \mathcal{K}_{\mathcal{M}}$ implies $\min \{I(P); P \in \mathcal{K}_{\mathcal{M}}\} = I_{\mathcal{M}}(Q^*)$. Given arbitrary $Q \in \mathcal{D}_{\mathcal{M}}$, again by Lemmas 4.1 and 3.1, observe that

$$I_{\mathcal{M}}(Q^*) = \min \{I(P); P \in \mathcal{K}_{\mathcal{M}}\} \geq I_{\mathcal{M}}(Q).$$

Therefore, $I_{\mathcal{M}}(Q^*) = \max \{I_{\mathcal{M}}(Q); Q \in \mathcal{D}_{\mathcal{M}}\}$. However, this means Q^* is optimal – see the explanation after Definition 4.2. \square

The approximations should be reasonable in the sense that if an estimate \hat{P} incidentally has the prescribed marginals from \mathcal{M} then it is a distinguished representative of the class $\mathcal{K}_{\mathcal{M}}$. There are more principles for the choice of a representative of a class of distributions suitable from the point of view of probabilistic decision-making. One of them is the *maximum entropy principle*. The idea is to choose $P \in \mathcal{K}_{\mathcal{M}}$ which maximizes the entropy $H(P)$. By Lemma 2.1, this distribution is uniquely determined. The results from §4 and §5 imply that both approximation methods dealt with in this paper are in concordance with this principle.

COROLLARY 6.2 Let $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ be a strongly consistent collection of probability measures. If $P_{exe} \in \mathcal{K}_{\mathcal{M}}$ then $\hat{P} = P_{exe}$ is the measure maximizing entropy in $\mathcal{K}_{\mathcal{M}}$. Assuming $l(x) > 0$ for all $x \in X_N$ and $Q \in \mathcal{D}_{\mathcal{M}} \cap \mathcal{K}_{\mathcal{M}}$ the distribution $\hat{P} = Q$ maximizes entropy in $\mathcal{K}_{\mathcal{M}}$.

Proof: Lemmas 5.1 and 4.1 imply that the considered approximation \hat{P} in an \mathcal{M} -construct. Then, Lemma 3.1 says that $\hat{P} \in \mathcal{K}_{\mathcal{M}}$ implies the equality in (8); that is, $\min \{I(P); P \in \mathcal{K}_{\mathcal{M}}\} = I_{\mathcal{M}}(\hat{P})$ and, moreover, $I_{\mathcal{M}}(\hat{P}) = I(\hat{P})$. Thus, \hat{P} minimizes the multiinformation in $\mathcal{K}_{\mathcal{M}}$ and, by Lemma 2.1, it maximizes the entropy. \square

7 Examples

In general, it is not possible to claim that one of the above-mentioned methods for approximation of a distribution P with prescribed marginals is better than the other, if one takes the relative entropy $H(P|\hat{P})$ as the measure of divergence of an approximation \hat{P} from P .

The following example shows that the optimal DSS approximation could be better than the explicit expression approximation. Actually, in this particular example, the optimal DSS approximation has fitting marginals. The example also shows that it can be the case that $|\text{Exe}| > 1$.

EXAMPLE 7 Put $N = \{a, b, c\}$, $X_i = \{0, 1\}$ for every $i \in N$ and $\mathcal{S} = \{A \subseteq N; |A| = 2\}$. Densities of measures from $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ are given as follows:

$$p_A(0, 0) = p_A(0, 1) = p_A(1, 1) = \frac{1}{3} \quad \text{for } A = \{a, c\} \text{ and } A = \{b, c\},$$

while $p_{\{a,b\}}(0, 0) = 2/3$, $p_{\{a,b\}}(1, 1) = 1/3$. Clearly, \mathcal{M} is strongly consistent; consider the density p which ascribes $1/3$ to any of the following three configurations of $x_{\{a,b,c\}}$: $(0, 0, 0)$, $(0, 0, 1)$ and $(1, 1, 1)$. Actually, if one takes the ordering $\tau_* : S_1 = \{a, b\}, S_2 = \{b, c\}, S_3 = \{a, c\}$ then the respective DSS has just the density p . In particular, $\mathcal{D}_{\mathcal{M}} \cap \mathcal{K}_{\mathcal{M}} \neq \emptyset$ and p defines an optimal

DSS. As described in §4, one can come to the same conclusion by minimizing the function $\tau \mapsto \iota(\tau)$; in this case one has $\ln 3 - \frac{4}{3} \cdot \ln 2 = I(\{a, c\}) = I(\{b, c\}) < I(\{a, b\}) = \ln 3 - \frac{2}{3} \cdot \ln 2$.

Direct calculation of Exe gives this result:

$$\text{Exe}(0, 0, 0) = \frac{1}{2}, \quad \text{Exe}(0, 0, 1) = \frac{1}{4}, \quad \text{Exe}(1, 1, 1) = \frac{1}{2},$$

and $\text{Exe}(x) = 0$ for remaining configurations $x \in \mathbf{X}_N$. Therefore, $|\text{Exe}| = 5/4 > 1$ and the respective explicit expression approximation has the form

$$\overline{\text{Exe}}(0, 0, 0) = \frac{2}{5}, \quad \overline{\text{Exe}}(0, 0, 1) = \frac{1}{5}, \quad \overline{\text{Exe}}(1, 1, 1) = \frac{2}{5},$$

and $\overline{\text{Exe}}(x) = 0$ for other configurations $x \in \mathbf{X}_N$. Hence, $\overline{\text{Exe}}_{\{a,b\}}(0, 0) = \frac{3}{5} \neq \frac{2}{3} = p_{\{a,b\}}(0, 0)$ implies that $P_{\text{exe}} \notin \mathcal{K}_{\mathcal{M}}$. The formulas (12) and (16) allow one to compare multiinformation contents of the optimal DSS Q and the explicit expression P_{exe} directly:

$$I_{\mathcal{M}}(Q) - I_{\mathcal{M}}(P_{\text{exe}}) = -I(\{a, c\}) + \ln |\text{Exe}| = -(\ln 3 - \frac{4}{3} \cdot \ln 2) + \ln \frac{5}{4} = \ln 5 - \ln 3 - \frac{2}{3} \cdot \ln 2 > 0.$$

On the other hand, the next example shows that the explicit expression approximation could be better than the optimal DSS approximation. Moreover, it also shows that it may happen $|\text{Exe}| < 1$.

EXAMPLE 8 Put $N = \{a, b, c\}$, $\mathbf{X}_i = \{0, 1\}$ for every $i \in N$ and $\mathcal{S} = \{A \subseteq N; |A| = 2\}$. The density p_A of P_A for any $A \in \mathcal{S}$ is given as follows:

$$p_A(0, 0) = \frac{2}{3}, \quad p_A(0, 1) = p_A(1, 0) = \frac{1}{3}, \quad p_A(1, 1) = 0.$$

To see that $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ is strongly consistent consider the density p given as follows:

$$p(0, 0, 0) = \frac{1}{2}, \quad p(0, 0, 1) = p(0, 1, 0) = p(1, 0, 0) = \frac{1}{6},$$

and $p(x) = 0$ for remaining $x \in \mathbf{X}_N$. Since $I(P_A) = \frac{7}{3} \cdot \ln 2 + \ln 3 - \frac{5}{3} \cdot \ln 5 \equiv k > 0$ for any $A \in \mathcal{S}$, every ordering τ gives an optimal DSS. For example, the ordering $S_1 = \{a, b\}$, $S_2 = \{b, c\}$, $S_3 = \{a, c\}$ leads to the following density q of an optimal DSS:

$$q(0, 0, 0) = \frac{8}{15}, \quad q(0, 0, 1) = q(1, 0, 0) = \frac{2}{15}, \quad q(0, 1, 0) = \frac{1}{6}, \quad q(1, 0, 1) = \frac{1}{30},$$

and $q(x) = 0$ for remaining $x \in \mathbf{X}_N$. Direct computation of Exe gives this result:

$$\text{Exe}(0, 0, 0) = \frac{64}{125}, \quad \text{Exe}(0, 0, 1) = \text{Exe}(0, 1, 0) = \text{Exe}(1, 0, 0) = \frac{20}{125},$$

and $\text{Exe}(x) = 0$ for remaining configurations $x \in \mathbf{X}_N$. In particular, $|\text{Exe}| = 124/125 < 1$. Therefore,

$$\overline{\text{Exe}}(0, 0, 0) = \frac{16}{31}, \quad \overline{\text{Exe}}(0, 0, 1) = \overline{\text{Exe}}(0, 1, 0) = \overline{\text{Exe}}(1, 0, 0) = \frac{5}{31},$$

and $\overline{\text{Exe}}(x) = 0$ for other $x \in \mathbf{X}_N$. Of course, $P_{\text{exe}} \notin \mathcal{K}_{\mathcal{M}}$ as $\overline{\text{Exe}}_{\{a,b\}}(0, 0) = \frac{21}{31} \neq \frac{2}{3} = p_{\{a,b\}}(0, 0)$. Formulas (16) and (12) allow one to compare multiinformation contents of both (types) of approximation:

$$I_{\mathcal{M}}(P_{\text{exe}}) - I_{\mathcal{M}}(Q) = (-\ln |\text{Exe}| + 3k) - (3k - k) = k - \ln |\text{Exe}| = k + \ln \frac{125}{124} > 0,$$

which means that P_{exe} is better.

Note that so far no example was found that $P_{\text{exe}} \in \mathcal{K}_{\mathcal{M}}$ and $\mathcal{K}_{\mathcal{M}} \cap \mathcal{D}_{\mathcal{M}} = \emptyset$.

8 Barycenter principle

Another principle for the choice of a representative of a class of probability distributions, different from the maximum entropy principle, is the *barycenter principle*. It was proposed by the first author in the 1980s [4, 5]. The following restricted definition is suitable for the purpose of this paper.

DEFINITION 8.1 Let \mathcal{K} and \mathcal{T} are two classes of probability measures on the same sample space, say, on X_N . The *barycenter* of \mathcal{K} (taken) in \mathcal{T} is any probability measure $R_* \in \mathcal{T}$ which minimizes the function

$$R \mapsto \mu(R) \equiv \max_{P \in \mathcal{K}} H(P|R), \quad R \in \mathcal{T}, \quad (21)$$

that is, in other words, it is obtained by the following “mini-max” procedure:

$$\max_{P \in \mathcal{K}} H(P|R_*) = \min_{R \in \mathcal{T}} \max_{P \in \mathcal{K}} H(P|R).$$

An implicit technical requirement is that the classes \mathcal{K} and \mathcal{T} are such that the maxima in (21) exist and the function μ is finite for at least one $R \in \mathcal{T}$.

The interpretation is that \mathcal{T} is the class of approximations of distributions from \mathcal{K} . Thus, we typically have in mind the set $\mathcal{K}_{\mathcal{M}}$ in place of \mathcal{K} . If we put $\mathcal{T} = \mathcal{D}_{\mathcal{M}}$ the the concept of barycenter reduces to the concept of an optimal DSS.

PROPOSITION 2 Let \mathcal{M} be a strongly consistent collection of probability measures. Assume $l(x) > 0$ for every $x \in X_N$. Then every optimal DSS for \mathcal{M} is a barycenter of $\mathcal{K}_{\mathcal{M}}$ in $\mathcal{D}_{\mathcal{M}}$.

Proof: It follows from Lemma 2.1 that $\max_{P \in \mathcal{K}_{\mathcal{M}}} I(P) < \infty$ and that at least one P_{\dagger} in $\mathcal{K}_{\mathcal{M}}$ exists with $I(P_{\dagger}) = \max_{P \in \mathcal{K}_{\mathcal{M}}} I(P)$. Moreover, it follows from Lemmas 4.1 and 3.1 that $H(P|Q) = I(P) - I_{\mathcal{M}}(Q)$ for any $P \in \mathcal{K}_{\mathcal{M}}$ and $Q \in \mathcal{D}_{\mathcal{M}}$. In particular, given $Q \in \mathcal{D}_{\mathcal{M}}$, one has

$$\max_{P \in \mathcal{K}_{\mathcal{M}}} H(P|Q) = \max_{P \in \mathcal{K}_{\mathcal{M}}} \{I(P) - I_{\mathcal{M}}(Q)\} = \{ \max_{P \in \mathcal{K}_{\mathcal{M}}} I(P) \} - I_{\mathcal{M}}(Q) = I(P_{\dagger}) - I_{\mathcal{M}}(Q),$$

and the task to minimize $Q \mapsto \max_{P \in \mathcal{K}_{\mathcal{M}}} H(P|Q)$, $Q \in \mathcal{D}_{\mathcal{M}}$ is equivalent to the task to maximize $I_{\mathcal{M}}(Q)$ on $\mathcal{D}_{\mathcal{M}}$. However, as explained after Definition 4.2, Q is an optimal DSS iff it maximizes the multiinformation content $I_{\mathcal{M}}(Q)$ on $\mathcal{D}_{\mathcal{M}}$. \square

The above definition of barycenter is general enough: one can even put $\mathcal{T} \equiv \mathcal{K}$, which means that one is looking for a barycenter of a class of distributions \mathcal{K} in itself. Actually, this is an alternative to the maximum entropy principle proposed already in [5]. It was shown there that in several common situations, the maximum entropy principle and (this special) barycenter principle yield the same result. However, this is not always the case. The following example shows that, if we consider the case of $\mathcal{K} = \mathcal{K}_{\mathcal{M}}$, then the barycenter principle and the maximum entropy principle may result in a different approximation.

EXAMPLE 9 Put $N = \{a, b\}$, $X_a = X_b = \{0, 1\}$ and $\mathcal{S} = \{A \subseteq N; |A| = 1\}$. The collection $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ is given by respective marginal densities:

$$p_{\{a\}}(0) = \frac{1}{3}, \quad p_{\{a\}}(1) = \frac{2}{3}, \quad p_{\{b\}}(0) = \frac{1}{4}, \quad p_{\{b\}}(1) = \frac{3}{4}.$$

We omit the proof of the fact that $\mathcal{K}_{\mathcal{M}}$ consists of convex combinations of two probability measures, namely the measure R^1 given by the density

$$r^1(0,0) = 0, \quad r^1(0,1) = \frac{1}{3}, \quad r^1(1,0) = \frac{1}{4}, \quad r^1(1,1) = \frac{5}{12},$$

and the measure R^2 given by the density

$$r^2(0,0) = \frac{1}{4}, \quad r^2(0,1) = \frac{1}{12}, \quad r^2(1,0) = 0, \quad r^2(1,1) = \frac{2}{3}.$$

In particular, the product measure $Q = P_{\{a\}} \times P_{\{b\}}$ with density

$$q(0,0) = \frac{1}{12}, \quad q(0,1) = \frac{1}{4}, \quad q(1,0) = \frac{1}{6}, \quad q(1,1) = \frac{1}{2}$$

has the form $Q = \frac{2}{3} \cdot R^1 + \frac{1}{3} \cdot R^2$. Note that this measure minimizes the multiinformation in $\mathcal{K}_{\mathcal{M}}$ and, therefore, it maximizes the entropy – see Lemma 2.1. To show that Q differs from the measure chosen by the barycenter principle it suffices to find at least one $R \in \mathcal{K}_{\mathcal{M}}$ such that

$$\mu(Q) \equiv \max_{P \in \mathcal{K}_{\mathcal{M}}} H(P|Q) > \max_{P \in \mathcal{K}_{\mathcal{M}}} H(P|R) \equiv \mu(R).$$

A basic observation is that, given $Q' \in \mathcal{K}_{\mathcal{M}}$ with strictly positive density, the function $P \mapsto H(P|Q')$, $P \in \mathcal{K}_{\mathcal{M}}$ is convex on $\mathcal{K}_{\mathcal{M}}$ and achieves its minimum 0 at $P = Q'$. Moreover, in the considered case, $\mathcal{K}_{\mathcal{M}}$ is an “interval” between R^1 and R^2 , for which reason the maximum of the function $P \mapsto H(P|Q')$ is achieved in one of the “extreme” measures R^1 and R^2 . In particular,

$$\max_{P \in \mathcal{K}_{\mathcal{M}}} H(P|Q') = \max \{ H(R^1|Q'), H(R^2|Q') \}.$$

Now, direct computation gives

$$H(R^2|Q) = \frac{4}{3} \cdot \ln 2 - \frac{1}{2} \cdot \ln 3 > \frac{-1}{2} \cdot \ln 3 + \frac{5}{12} \cdot \ln 5 = H(R^1|Q),$$

which means that $\mu(Q) = H(R^2|Q) = \frac{4}{3} \cdot \ln 2 - \frac{1}{2} \cdot \ln 3$. We put $R = \frac{1}{3} \cdot R^1 + \frac{2}{3} \cdot R^2$ and observe it has the following density:

$$r(0,0) = r(0,1) = \frac{1}{6}, \quad r(1,0) = \frac{1}{12}, \quad r(1,1) = \frac{7}{12}.$$

Thus, we can analogously get

$$H(R^1|R) = \frac{1}{3} \cdot \ln 2 + \frac{1}{4} \cdot \ln 3 + \frac{5}{12} \cdot \ln 5 - \frac{5}{12} \cdot \ln 7 > \frac{5}{3} \cdot \ln 2 + \frac{1}{4} \cdot \ln 3 - \frac{2}{3} \cdot \ln 7 = H(R^2|R),$$

which means that $\mu(R) = H(R^1|R) = \frac{1}{3} \cdot \ln 2 + \frac{1}{4} \cdot \ln 3 + \frac{5}{12} \cdot \ln 5 - \frac{5}{12} \cdot \ln 7$. It is straightforward to observe by detailed computation that $\mu(Q) > \mu(R)$.

9 Simple sufficient condition

Of course, as mentioned in §6, the ideal case is if the approximation has prescribed marginals from \mathcal{M} . The problem is often to ensure this situation. There exists simple strong sufficient condition for this in terms of the class \mathcal{S} . The condition has close connection to graphical models [2], more precisely, to so-called *decomposable graphical models*. Even more special and simpler case is the case of so-called *asteroid*, which is the concept introduced in the manuscript [6].

DEFINITION 9.1 Let \mathcal{S} be a class of subsets of N such that $\bigcup \mathcal{S} = N$. We say that it is *decomposable* if there exists an ordering $\tau : S_1, \dots, S_n$, $n \geq 1$ of sets in \mathcal{S} that satisfies the *running intersection property*:

$$\forall j > 2 \quad \exists \ell < j \quad F_j \equiv S_j \cap \left(\bigcup_{k < j} S_k \right) \subseteq S_\ell. \quad (22)$$

Given a partitioning $\{E_1, \dots, E_r\}$, $r \geq 2$ of the set N , an *asteroid* with core $C = E_1$ (generated by that partitioning) is the class of sets

$$\mathcal{S} = \{E_1 \cup E_i; i = 2, \dots, r\}.$$

It is evident that every asteroid is a decomposable class; actually, any ordering of sets of an asteroid satisfies the running intersection property.³⁷ The point is that the decomposability condition is a necessary and sufficient condition for the equivalence of weak and strong consistency of any system \mathcal{M} of probability measures which has \mathcal{S} as the class of “indexing” sets – see [7] and [1]. However, in the context of this paper, the following observation is crucial.

PROPOSITION 3 Let \mathcal{S} be a decomposable class of subsets of N with $\bigcup \mathcal{S} = N$ and $\mathcal{M} = \{P_A; A \in \mathcal{S}\}$ be a (strongly) consistent collection of probability measures. Then any total ordering $\tau : S_1, \dots, S_n$, $n \geq 1$ of sets in \mathcal{S} satisfying the running intersection property (22) yields an optimal DSS. The respective optimal DSS coincides with P_{exe} and has fitting prescribed marginals from \mathcal{M} . Moreover, it coincides with the distribution chosen from $\mathcal{K}_{\mathcal{M}}$ by the maximum entropy principle.

Proof: To show the first claim it suffices to verify that the respective DSS has prescribed marginals from \mathcal{M} and apply Corollary 6.1. The statement that if τ satisfies (22) then the density $\bar{p}_{\tau, \vartheta}$ given by (10) has p_{S_1}, \dots, p_{S_n} as marginal densities can be proved by induction on n .³⁸ It is evident for $n = 1$. If $n > 1$ then we denote $H = \bigcup_{j < n} S_j$, consider a shortened ordering $\tau' : S_1, \dots, S_{n-1}$, a restricted choice ϑ' and derive from (10):

$$\bar{p}_{\tau, \vartheta}(x) = \bar{p}_{\tau', \vartheta'}(x_H) \cdot p_{G_n | F_n}(x_{G_n} | x_{F_n}) \quad \text{for } x \in \mathbf{X}_N. \quad (23)$$

Hence, $(\bar{p}_{\tau, \vartheta})^H = \bar{p}_{\tau', \vartheta'}$,³⁹ which allows one to observe by the induction assumption that $\bar{p}_{\tau, \vartheta}$ has $p_{S_1}, \dots, p_{S_{n-1}}$ as marginal densities:

$$\forall j < n \quad (\bar{p}_{\tau, \vartheta})^{S_j} = ((\bar{p}_{\tau, \vartheta})^H)^{S_j} = (\bar{p}_{\tau', \vartheta'})^{S_j} = p_{S_j}.$$

To show that it has p_{S_n} as marginal density find $\ell < n$ with $F_n \subseteq S_\ell$. Now, the induction assumption says $(\bar{p}_{\tau', \vartheta'})^{S_\ell} = p_{S_\ell}$ which allows one to observe that $\bar{p}_{\tau', \vartheta'}$ has p_{F_n} as a marginal density:

$$(\bar{p}_{\tau', \vartheta'})^{F_n} = ((\bar{p}_{\tau', \vartheta'})^{S_\ell})^{F_n} = (p_{S_\ell})^{F_n} = p_{F_n}.$$

Therefore, by (23), the marginal density of $\bar{p}_{\tau, \vartheta}$ for S_n can be written as follows:

$$(\bar{p}_{\tau, \vartheta})^{S_n} = (\bar{p}_{\tau', \vartheta'})^{F_n} \cdot p_{G_n | F_n} = p_{F_n} \cdot p_{G_n | F_n} = p_{S_n},$$

because the conditional density $p_{G_n | F_n}$ is consistent with p_{S_n} . This completes the induction step.

³⁷This is because the core C is the set $S_j \cap (\bigcup_{k < j} S_k)$ for any $j > 2$.

³⁸This holds irrespective of what choice ϑ for \mathcal{M} and τ is considered.

³⁹Use the definition of conditional density.

To show that the respective optimal DSS coincides with P_{exe} we first observe that if $\tau : S_1, \dots, S_n, n \geq 1$ satisfies (22) then the concept of choice for \mathcal{M} and τ is not needed because the density $\bar{p}_{\tau, \vartheta}$ given by (10) does not depend on ϑ . Actually, the density of the respective DSS is then given by (11) where we accept the convention $0^{-1} \equiv 0$.⁴⁰ Thus, (11) implies that the density \bar{p}_τ has the form:

$$\bar{p}_\tau(x) = \prod_{B \in \mathcal{S}^\downarrow} p_B(x_B)^{\nu(B)} \quad \text{for } x \in \mathbf{X}_N,$$

where $\nu(B), B \in \mathcal{S}^\downarrow$ is given by (13) and the convention $0^{-1} = 0$ is accepted. Now, the formula (14) implies

$$\text{Exe}(x) = \prod_{B \in \mathcal{S}^\downarrow} p_B(x_B)^{\nu(B)} \quad \text{for } x \in \mathbf{X}_N,$$

where $\nu(B), B \in \mathcal{S}^\downarrow$ is given by (17) and the same convention holds. The point is that if τ satisfies the running intersection property (22) then the formulas (13) and (17) give the same result – this is what is proved in Lemma 7.2 in [8].⁴¹ In particular, $\bar{p}_\tau = \text{Exe}$. As \bar{p}_τ is a density of a probability measure $|\text{Exe}| = 1$ and one has $\bar{p}_\tau = \overline{\text{Exe}}$. Thus, the respective DSS Q coincides with P_{exe} . We have already shown that Q has prescribed marginals.

The last claim of Proposition 3 follows from Corollary 6.2. □

10 Conclusions and open problems

Let us summarize the results of the paper. We have compared two methods for approximation of probability distributions with prescribed marginals: the optimal DSS approximation and the explicit expression approximation. Both these methods can be applied to multi-symptom diagnosis making as explained in §1. The conclusion is that none of these two methods is universally better than the other – we gave the respective examples in §7. As mentioned in [6], the formal advantage of the explicit expression approximation is that if we use this approach then we automatically avoid the optimization procedure needed in the case of DSS approximations.

Moreover, in the case of fitting marginals, both methods result in the distribution chosen by the maximum entropy principle – see §6. A simple sufficient condition for this in terms of \mathcal{S} was recalled in §9. Finally, in §8, we compared the barycenter principle and the maximum entropy principle and showed that they differ in the considered special case; actually, this disproves one of the conjectures from [6].

Of course, some questions remain open. One of them is as follows. It is true that if $|\text{Exe}| = 1$ then P_{exe} coincides with an optimal DSS approximation? Thus was also mentioned in [6] as a conjecture. The second author tried to verify or disprove that conjecture but he has not succeeded so far. The conjecture was verified in the case $|\mathbf{X}_i| = 2$ for $i \in N$ and $|\mathcal{S}| \leq 3$ – this was done with the essential help of a computer program Mathematica. Another open question was mentioned in the end of §7: is it true that if $P_{exe} \in \mathcal{K}_\mathcal{M}$ then $\mathcal{K}_\mathcal{M} \cap \mathcal{D}_\mathcal{M} \neq \emptyset$?⁴²

⁴⁰Given $x \in \mathbf{X}_N$ consider the first (possible) $j \geq 2$ with $p_{F_j}(x_{F_j}) = 0$ and, by (22), find $1 \leq \ell < j$ with $F_j \subseteq S_\ell$. As \mathcal{M} is strongly consistent, by (2), $p_{S_\ell}(x_{S_\ell}) = 0$. However, as $p_{F_\ell}(x_{F_\ell}) > 0$ one certainly has $p_{G_\ell|F_\ell}(x_{G_\ell}|x_{F_\ell}) = 0$ and $\bar{p}_{\tau, \vartheta}(x) = 0$, no matter what choice ϑ was considered.

⁴¹It can be verified by the induction on n .

⁴²Note that if $P_{exe} \in \mathcal{K}_\mathcal{M}$ then $\mathcal{K}_\mathcal{M} \cap \mathcal{D}_\mathcal{M} \neq \emptyset$ is equivalent to $P_{exe} \in \mathcal{D}_\mathcal{M}$ – use Corollary 6.2.

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