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# <sup>14</sup> Unifying parameter learning and modelling complex <sup>15</sup> systems with epistemic uncertainty using probability <sup>16</sup> interval

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# 22 Abstract

17

Modeling complex dynamical systems from heterogeneous pieces of knowledge varying in precision and reliability is a challenging task. We propose the combination of dynamical Bayesian networks and of imprecise probabilities to solve it. In order to limit the computational burden and to make interpretation easier, we also propose to encode pieces of (numerical) knowledge as probability intervals, which are then used in an imprecise Dirichlet model to update our knowledge. The idea is to obtain a model flexible enough so that it can easily cope with different uncertainties (i.e., stochastic and epistemic), integrate new pieces of knowledge as they arrive and be of limited computational complexity.

23 Keywords: Dynamic credal networks, imprecise probability, Dirichlet

<sup>24</sup> model, knowledge integration, uncertainty, modelling.

# 25 1. Introduction

Firms and industrials of all sectors have to face up new challenging situations. On the one hand, citizens as well as public authorities have stronger demands in terms of quality, safety, ... and on the other hand, they must adapt to the increase of population, global warming and the depletion of fossil resources. This means, among other things, that industrial projects have to integrate sustainability from local to world scale in their conception. Possessing adequate tools to model their systems is likely to make the task easier.

In order to provide relevant conclusions and recommendations, such tools should be able to integrate as much available knowledge as possible, however heterogeneous it is, both in terms of nature (e.g., qualitative expert knowledge vs statistical data) and quality (different precision or degrees of reliability). Such systems are also complex, meaning that the modeling tool

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<sup>39</sup> must be able to cope with different scales (e.g., molecular to macroscopic) <sup>40</sup> and with dynamic, time-varying processes. Current researches rely on the <sup>41</sup> development of mathematical tools [53, 6] capable of helping decision-makers <sup>42</sup> to deal with uncertainties, linked for instance to meteorological variations, <sup>43</sup> to expert reliability, *etc.* To summarize, ideal modeling tools should be able <sup>44</sup> to deal with:

- heterogeneous sources of knowledge (Web, data warehouse, experts,
   ...)
- mathematical formalisms used by different disciplines (differential equations, graphs, cognitive maps, ...)
- various manipulated scales (molecular, cellular, population, ...)
- different forms of uncertainty [32, 36, 40] (natural randomness, imprecision in expert opinions, data scarcity, vagueness, ...)

In this paper, we propose dynamic credal networks as a possible answer 52 to these challenging tasks to describe complex dynamical systems tainted 53 with stochastic and epistemic uncertainty. As an extension of dynamic 54 Bayesian networks (DBNs) [51], their network structure provides an intu-55 itively appealing interface for human experts to model highly-interacting sets 56 of variables, resulting in a qualitative representation of knowledge. Stochas-57 tic and epistemic uncertainties pertaining to the system are then taken into 58 account by quantifying dependence between variables by means of convex 59 sets of conditional probability distributions. The concept of DCNs makes it 60 possible to combine different sources of information, from qualitative expert 61 knowledge to experimental data. 62

In this paper, we are specifically interested in the problem of param-63 eter learning for a given network structure (assumed to be known), when 64 faced with heterogeneous knowledge. Indeed, while DCN are very attractive 65 modeling tools, they also come with a number of challenges, such as how to 66 control their computational tractability, or how to combine efficiently and 67 easily various pieces of information. For example, how to combine simu-68 lations coming from stochastic differential equations with an experimental 69 database, both offering information for the same parameters? We propose 70 to use an imprecise Dirichlet model [7] as a model of the conditional prob-71 abilities, and probability intervals as a common uncertainty model to treat different pieces of knowledge. Once transformed, these information pieces 73 gradually increment the set of prior distributions according to the received 74 knowledge, using the Generalized Bayes rule each time additional informa-75 tion arrives. Lower and upper expected a posteriori (EAP) are then used as 76 probability bounds to draw inferences from the network. The combination 77 of information is done through a weighted average, allowing us to weigh the 78 importance of the different sources of knowledge. 79

Section 2 details the material regarding imprecise probabilities as well as the proposed updating scheme of a given parameter set. We then describe in Section 3 how various common sources of information can be transformed into probability intervals. Section 4 presents how we extend Dynamic Bayesian Networks to sets of conditional probabilities, while Section 5 illustrates the whole approach on a real-case scenario involving cheese ripening.

# <sup>87</sup> 2. Imprecise probabilities and Dirichlet model

Let X be a variable <sup>1</sup> taking its values on the finite set  $\mathcal{X} = \{x_1, \ldots, x_n\}$ , and  $p : \mathcal{X} \mapsto [0, 1], \sum_{x \in \mathcal{X}} p(x) = 1$  be a probability mass function over  $\mathcal{X}$ . p(X) will denote the vector mass function, while p(x) will denote the value taken by p for X = x. Such a mass function defines a measure  $P_X(A) = \sum_{x \in A} p(x)$  for all  $A \subseteq \mathcal{X}$ .

# 93 2.1. Imprecise probability and credal sets

In general, identifying a single probability modelling our uncertainty 94 about some variable X requires a lot of data and/or knowledge. When such 95 knowledge is not available, a safer option is to model our uncertainty by 96 convex sets of probabilities, often called credal sets [47, 61, 2]. A credal 97 set associated with X, denoted K(X), is a convex set of probability masses 98 over  $\mathcal{X}$ . K(X) represents the uncertainty about the unknown value of the 99 variable X. From K(X) are defined upper and lower probability measures 100 of an event  $A \subseteq \mathcal{X}$  as 101

$$\overline{P_X}(A) = \sup_{p \in K(X)} \sum_{x \in A} p(x), \ \underline{P_X}(A) = \inf_{p \in K(X)} \sum_{x \in A} p(x).$$
(1)

and, in particular, for any element  $x \in \mathcal{X}$  we will have that the upper and lower probabilities are given by

$$\overline{p}(x) = \sup_{p \in K(X)} p(x), \tag{2}$$

$$\underline{p}(x) = \inf_{p \in K(X)} p(x) \tag{3}$$

In a subjectivist tradition, the lower probability  $\underline{P}_X(A)$  can be interpreted as the maximal price one would be willing to pay for the gamble which pays 1 unit if event A occurs (and nothing otherwise) [61].  $\underline{P}_X(A)$  is therefore a measure of evidence in favour of event A, or in other words how much K(X)supports event A, while  $\overline{P}_X(A)$  measures the lack of evidence against A. K(X) can also be given a robust interpretation, in which it models imperfect

<sup>&</sup>lt;sup>1</sup>We adopt notations similar to those of [2, Ch.9] and [24].

knowledge of a precise, possibly frequentist, probability p. A credal set K(X) contains a set  $\mathcal{E}xt(K(X))$  of extreme probability masses, always finite in this paper, corresponding to the vertices of K(X). Geometrically, K(X)may be equivalently specified by the convex hull (denoted CH) of the set  $\mathcal{E}xt(K(X))$ , i.e.

$$K(X) = CH\{\mathcal{E}xt(K(X))\}.$$

115 The *vacuous* credal set

$$K_v(X) = \{ p(X) : p(x) \ge 0, \ \forall x \in \mathcal{X}, \ \sum_{x \in \mathcal{X}} p(x) = 1 \}$$

that includes all probability masses over  $\mathcal{X}$  plays an important role, as it models total ignorance, and should be the starting point of any model. We refer to Walley [61, Sec. 5.5.] for a discussion about uniform probability distribution not being a good model of ignorance.

In this paper, we will also be especially interested in particular credal sets K(X) specified by means of *interval probability* 

$$K(X) = \{ p(X) : \ p(x) \in [l_x, u_x], \ 0 \le l_x \le u_x \le 1, \ \sum_{x \in \mathcal{X}} p(x) = 1 \}.$$
(6)

122 Indeed, such credal sets that focus over bounds of singletons have the advan-

123 tage to be easier to manipulate, simulate and represent than general ones,

<sup>124</sup> while remaining expressive enough (they include both the vacuous and the

precise models). We refer to De Campos *et al.* [11] for a detailed exposition,
and will only limits ourselves to necessary elements in this paper.

Example 1. Consider an example with three possibilities  $\mathcal{X} = \{x_1, x_2, x_3\}$  (e.g., the working states of a system such as "failing", "degraded functioning", "fully functioning"), and assume that previous experiments result in the following intervals

$$p(x_1) = [0; 0.2], \qquad p(x_2) = [0.3; 0.4], \qquad p(x_3) = [0.4; 0.6]$$

The credal set K(X) is the set of all precise probabilities  $P(X) = (p(x_1), p(x_2), (p(x_3)))$ within these interval bounds. Here K(X) is a polytope defined by the convex hull of its four vertices in a three dimensional space:

$$K(X) = CH\{(0, 0.4, 0.6); (0.2, 0.3, 0.5); (0.2, 0.4; 0.4); (0.1, 0.3, 0.6)\}$$

Finding these vertices can be done by using classical tools of convex geometry [39], or by using algorithms proper to a given representation (an Algorithm is provided by De Campos *et al.* [11]). The set K(X) is represented in Figure 1 in barycentric coordinates.



Figure 1: Example 1 credal set in Barycentric coordinates.

# 131 2.2. Robust Dirichlet model to learn K(X)

An important question is how the credal set K(X) can be instantiated 132 from actual evidence, or in other words how can we go from an initially 133 vacuous knowledge towards a more precise state of knowledge. An in-134 strumental tool to do that is to use a robustified version of the Dirichlet 135 model, also commonly referred to as the Imprecise Dirichlet Model (IDM) 136 [62, 7, 8, 60]. The basic model is based on two hyper-parameters: a positive 137 real value  $s_0$  associated to the strength of prior knowledge, and a vector 138  $\epsilon_0 = (\epsilon_0(x_1), \dots, \epsilon_0(x_n))$  associated to our initial beliefs about the probabil-139 ities of occurrence of elements  $x_i$ . 140

Let  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_n)$  be a vector of chances such that  $\theta_i$  corresponds to the chance that  $X = x_i$ . The prior distribution of vectors  $\boldsymbol{\theta}$  given by a Dirichlet model is then

$$\operatorname{Dir}(s_0;\xi_0)(\boldsymbol{\theta}) = \frac{\Gamma(s_0)}{\prod_{i=1}^n \Gamma(s_0\xi_0(x_i))} \prod_{i=1}^n \theta_i^{s_0\xi_0(x_i)-1}$$
(7)

where  $\Gamma$  is the gamma function. A very easy way to make this model imprecise is to let the vector  $\epsilon_0$  become imprecise, and more precisely to consider the set of Dirichlet models

$$\mathcal{M}_{(s_0;\xi_0)} = \{ \operatorname{Dir}(s_0;\xi_0)(\boldsymbol{\theta}) : \xi_0 \in \mathcal{T} \}$$
(8)

147 with

$$\mathcal{T} = \{\xi_0 : \ 0 < \xi_0(x_i) < 1 \ , \sum_{i=1}^n \xi_0(x_i) = 1\}$$
(9)

the open (n-1)-dimensional unit simplex. When  $\xi_0$  is precise, the first moments of  $\text{Dir}(s_0;\xi_0)$  are given by  $E(\theta_i|(s_0;\xi_0)) = \xi_0(x_i)$ , and they can be used as estimates of  $p(x_i)$ , *i.e.* 

$$E(\theta_i|(s_0;\xi_0)) = \xi_0(x_i) = p(x_i).$$
(10)

When starting from a vacuous prior knowledge  $\xi_0 \in \mathcal{T}$ , the bounds over the first moments become

$$\underline{E}(\theta_i|(s_0;\xi_0)) = \min_{\xi_0 \in \mathcal{T}} \xi_0(x_i) = 0 \tag{11}$$

153 and

$$\overline{E}(\theta_i|(s_0;\xi_0)) = \max_{\xi_0 \in \mathcal{T}} \xi_0(x_i) = 1.$$

The credal set corresponding to these bounds is then the vacuous one (5). We may then receive additional information from various m sources. A convenient way to encode this information is as a couple  $s_k, \mathcal{P}_k, k = 1, \ldots, m$ , with  $\mathcal{P}_k \subseteq \mathcal{T}$  a convex polytope providing information about the possible chances  $\theta_i$ , and  $s_k \in \mathbb{R}^+$  modelling the strength of the information. We can then update the Dirichlet modelling our uncertainty about  $\boldsymbol{\theta}|(s_k, \xi_k)_{k=0}^m$  into

$$\mathcal{M}_{(s_k;\xi_k)_{k=0}^m} = \left\{ \operatorname{Dir}\left( (s_k;\xi_k)_{k=0}^m \right) \left( \boldsymbol{\theta} \right) : \xi_k \in \mathcal{P}_k \; \forall k \right\}.$$
(13)

We can then use the posterior first moments to make inferences on chances  $\theta_i$ 

$$E(\theta_i|(s_k;\xi_k)_{k=0}^m) = p(x_i) = \frac{\sum_{k=0}^m s_k \xi_k(x_i)}{\sum_{k=0}^m s_k}$$
(14)

162 As information  $\mathcal{P}_k$  are imprecise, we again obtain bounds in the form

$$\underline{E}(\theta_i|(s_k;\xi_k)_{k=0}^m) = \underline{p}(x_i) = \frac{\sum_{k=0}^m s_k \underline{\xi}_k(x_i)}{\sum_{k=0}^m s_k},$$
(15)

$$\overline{E}(\theta_i|(s_k;\xi_k)_{k=0}^m) = \overline{p}(x_i) = \frac{\sum_{k=0}^m s_k \xi_k(x_i)}{\sum_{k=0}^m s_k}.$$
(16)

163 where

$$\underline{\xi}_k(x_i) = \inf_{\xi_k \in \mathcal{P}_k} \xi_k(x_i) \tag{17}$$

$$\overline{\xi}_k(x_i) = \sup_{\xi_k \in \mathcal{P}_k} \xi_k(x_i).$$
(18)

164 These bounds then induce an updated credal set

$$K_{(s_k;\xi_k)_{k=0}^m}(X) = \left\{ p : p(x_i) \in \left[ \frac{\sum_{k=0}^m s_k \xi_k(x_i)}{\sum_{k=0}^m s_k}, \frac{\sum_{k=0}^m s_k \overline{\xi}_k(x_i)}{\sum_{k=0}^m s_k} \right] \right\}$$
(19)

that we can use as new knowledge. In practice,  $s_0$  can be interpreted as the number of "unseen" data, and  $s_k = s_0$  means that the *k*th information source has as much importance as our initial uncertainty. 168 Remark 1. The exact updated credal set

$$\tilde{K}_{(s_k;\xi_k)_{k=0}^m}(X) = \left\{ \frac{\sum_{k=0}^m s_k \xi_k}{\sum_{k=0}^m s_k} : \ \xi_k \in \mathcal{P}_k, \ \forall k = 1, \dots, m \right\}$$
(20)

is a subset of  $K_{(s_k;\xi_k)_{k=0}^m}(X)$ , i.e.,  $\tilde{K}_{(s_k;\xi_k)_{k=0}^m}(X) \subseteq K_{(s_k;\xi_k)_{k=0}^m}(X)$ . The set (19) is thus an outer-approximation. Yet, the main advantages of using probability bounds as a basic representation are that

• their number of extreme points is bounded and relatively low, even when combining them through a weighted average. This is in general not the case if we consider averaging of heterogeneous simple representations: if we denote  $|\mathcal{E}xt(\mathcal{P}_k)|$  the number of extreme points of the kth item of information, then their (Minkowsky) sum  $\sum_{k=0}^{m} s_k \mathcal{P}_k$ may have as much as  $\prod_{k=0}^{m} |\mathcal{E}xt(\mathcal{P}_k)|$  extreme points, an exponentially growing number;

they are easy to explain and to represent graphically (e.g., as imprecise histograms), therefore offering a convenient way to communicate with domain experts or users not specialized in mathematics or computer science. This is not the case of more complex representations such as belief functions (Section 3.4);

except for requiring a finite space, they do not require specific assumptions, such as the existence of an ordering between elements;

they are expressive enough so that they can go from a fully precise
 probability to the complete ignorance model.

None of the other common practical models of information reviewed in Section 3 have all these advantages at once, making probability bounds a quite convenient model. Given this, using probability bounds seem a good general starting point in applications, not preventing one from investigating refined solutions if the results are unsatisfactory.

Of course, in some cases  $K_{(s_k;\xi_k)_{k=0}^m}(X)$  may be a poor outer-approximation, however we shall see in Section 5 that it does not necessarily lead to completely void conclusions. Previous studies [1] also suggest that this kind of approximation may be in average reasonable.

197 Example 2. Let  $\mathcal{X} = \{x_1, x_2, x_3\}$  and  $\mathcal{P} = \{\xi : \xi(x_2) \ge \xi(x_1), \frac{1}{2} \ge \xi(x_3), \sum_{i=1}^{3} \xi(x_i) = 1\}$  be an item of information. The credal set  $\tilde{K}_{\xi}(X)$ 198  $\xi(x_3), \sum_{i=1}^{3} \xi(x_i) = 1\}$  be an item of information. The credal set  $\tilde{K}_{\xi}(X)$ 199 over  $\{x_1, x_2, x_3\}$  obtained by (20) has four extreme points  $\{(0, 1, 0), (0, 0.5, 0.5), (0.5, 0.5, 0), (0.25, 0.25, 0.5)\}$  that are also extreme points of  $K_{\xi}(X) = \{p : p(x_i) \le \max_{\epsilon \in \mathcal{P}} \epsilon(x_i)\}$ . However, the probability (0.5, 0.25, 0.25, 0.25) is an ex-202 treme point of  $K_{\xi}(X)$  but not of  $\tilde{K}_{\xi}(X)$ .

### **3.** Review of practical sources of information

Building  $K_{(s_k;\xi_k)_{k=0}^m}(X)$  requires to obtain elements of information  $\mathcal{P}_k$ . 204 In this section, we review different practical models and the bounds they 205 induce over  $\xi_k(x_i)$ . We will also provide small examples illustrating what 206 kind of information they can model. For the sake of brevity, we will denote 207  $\xi(x_i)$  by  $\xi^i$  in this section. Note that our information is initially queried on 208 observed values  $x_i$ , to be then transferred as knowledge on the parameters  $\xi^i$ . 209 Hence we will consistently refer to knowledge about  $\xi^i$ , and to observation 210 or information about  $x_i$ . 211

212 3.1. Precise evaluations

The most simple models is when the knowledge  $\mathcal{P}$  is given by a precise vector, in which case  $\xi^i = f_i$  is a precise number, and we have

$$\overline{\xi}^i = \underline{\xi}^i = f_i \tag{21}$$

A classical way to obtain such precise evaluations is when observing  $m = (m_1, \ldots, m_n)$  experiments, where  $m_i$  is the number of times  $x_i$  was observed. In such a case, a classical choice is to take as strength  $s = m = \sum_{i=1}^{n} m_i$ and  $\mathcal{P}$  is the vector  $\mathbf{f} = (f_1, \ldots, f_n)$  where  $f_i = m_i/m$ .

*Example 3.* Assume we can observe three possibilities  $x_1, x_2, x_3$  (e.g., severity of a disease, importance of a bacterial population), and we observed 3 times  $x_1$ , 6 times  $x_2$  and one time  $x_3$ . We then have

$$f_1 = 0.3, f_2 = 0.6, f_3 = 0.1 \text{ and } s = m = 10$$
 (22)

Note that the more observations we accumulate, the stronger becomes this piece of knowledge. *s* can also be modulated to reflect the reliability of data. Note that this model is a degenerated case of probability intervals, and can therefore be exactly represented in our framework.

# 226 3.2. Numerical possibility distributions and fuzzy subsets

A possibility distribution  $\pi$  is simply a mapping from  $\{\xi^1, \ldots, \xi^n\}$  to [0,1], with at least one element  $\xi^i$  such that  $\pi(\xi^i) = 1$  [33]. In practice, we can see distribution  $\pi$  as an ordering  $1 = \pi(\xi^{(1)}) \ge \ldots \ge \pi(\xi^{(n)})$  of the elements  $x_1, \ldots, x_n$ , from the most plausible to the least plausible one.

Another instrumental way is to encode the possibility distribution through the necessity measure N. This necessity measure N is such that

$$N(A_{(i)} = \{\xi^{(1)}, \dots, \xi^{(i)}\}) = 1 - \pi(\xi^{(i+1)})$$
(23)

with  $\pi(\xi^{(n+1)}) = 0$ .  $N(A_{(i)})$  can be associated to a lower probability bound of event  $A_{(i)}$ . In particular, the sets  $A_{(i)}$  can be interpreted as nested sets with an associated lower confidence, these nested sets being built by starting from the most plausible element  $\xi^{(1)}$  and incrementally including the less plausible ones. Note that we may have  $\pi(\xi^{(i)}) = \pi(\xi^{(i+1)})$ , in which case elements  $x_{(i-1)}$  and  $x_{(i)}$  would be in the same confidence set.

In practice, an expert can provide a possibilistic information by giving confidence bounds over a collection of nested sets. Let  $A_1 \subseteq \ldots \subseteq A_m$  be such sets with associated confidence levels  $\alpha_1 \leq \ldots \leq \alpha_m$ , then it encodes the knowledge  $\mathcal{P}_{\pi} = \{\xi : \sum_{k=1}^{i} \xi^{(k)} \geq \alpha_i, \forall i\}$ . From the knowledge on sets  $A_1, \ldots, A_m$ , one can always come back to an associated distribution  $\pi$  using

$$\pi(\xi^k) = \min_{i:\xi^k \in A_i} 1 - \alpha_{i-1}$$

244 with  $\alpha_0 = 0$ .

Another possibility is to use the formal equivalence between a possibility distribution  $\pi$  and a fuzzy set having  $\pi$  for membership function. This means that an expert conveying information in the form of linguistic assessment [64] can also be modelled by possibility distributions. Deriving bounds on  $\xi^i$  from  $\mathcal{P}_{\pi}$  using the possibility distribution  $\pi$  is very easy, as

$$\underline{\xi}^{i} = 1 - \max_{\substack{\xi \neq \xi^{i}}} \pi(\xi) \tag{25}$$

250

$$\overline{\xi}^i = \pi(\xi^i) \tag{26}$$

(24)

*Example* 4. Assume that an expert is interrogated about the temperature in a room that can be in three states  $x_1, x_2, x_3$ . Expert judges that  $x_2$  is the most plausible state, then  $x_3$  and  $x_1$ , meaning that  $\xi^{(1)} = \xi^2, \xi^{(2)} = \xi^3, \xi^{(3)} = \xi^1$ . The expert provides the following confidence values:

$$N(\{\xi^2\}) = 0.5$$
$$N(\{\xi^2, \xi^3\}) = 0.8$$
$$N(\{\xi^2, \xi^3, \xi^1\}) = 1$$

which means that the expert has a confidence 0.5 that  $x_2$  will be the observed state, a confidence 0.8 that the observed state will be either  $x_2$  or  $x_3$ , and finally is certain that the only observable states are  $x_1, x_2, x_3$ . From these values can be deduced the values of the corresponding possibility distribution  $\pi(\xi^1) = 0.2, \ \pi(\xi^2) = 1, \ \pi(\xi^3) = 0.5.$ 

Alone, possibility distributions will often be simpler than probability intervals: they require less information (one value per element) and will have a maximal number of  $2^{|\mathcal{X}|-1}$  extreme points [56]. Yet the average of multiple sets  $\mathcal{P}_{\pi_1}, \ldots, \mathcal{P}_{\pi_m}$  would no longer be a possibility distribution, and the corresponding number of extreme points could explode. Also, possibility distributions cannot model precise probabilities, unless they are degenerate ones.

# 266 3.3. Probability boxes and clouds

A probability box [35]  $\underline{F}, \overline{F}$  is an imprecise cumulative distribution. It can be modelled by two discrete non-decreasing functions  $\underline{F}$  and  $\overline{F}$  from  $(\xi^1, \ldots, \xi^n)$  to [0,1] such that  $\underline{F}(\xi^i) \leq \overline{F}(\xi^i)$  for all i in  $\{1, \ldots, n\}$  and  $\underline{F}(\xi^n) = \overline{F}(\xi^n) = 1$ . The values  $\underline{F}(\xi^i), \overline{F}(\xi^i)$  are interpreted as the following bounds

$$\underline{F}(\xi^i) \le \sum_{i=1}^n \xi^i \le \overline{F}(\xi^i)$$

and we can denote by  $\mathcal{P}_{\underline{F} \leq \overline{F}}$  the knowledge modelled by a p-box. A p-box information provides us with estimates about the cumulated probabilities of events of the kind  $\{x_1, \ldots, x_i\}$ , hence assuming that the ordering induced by the indices do make sense.

In the case of p-boxes, the bounds over  $\xi^i$  are very easy to determine 277 [59], and are equal to

$$\underline{\xi}^{i} = \max(0, \underline{F}(\xi^{i}) - \overline{F}(\xi^{i-1}))$$
(27)

278

$$\overline{\xi}^{i} = \overline{F}(\xi^{i}) - \underline{F}(\xi^{i-1})$$
(28)

279 with the convention  $\underline{F}(\xi^0) = \overline{F}(\xi^0) = 0$ 

*Example* 5. Assume we have to assess the how likely it is that a bacterial population is below some threshold, or how likely it is that a component may function for a given period of time. The population sizes or time intervals may be discretized into  $x_1, x_2, x_3$ . Assume the following p-box has been given as information

$$\underline{F}(\xi^1) = 0.2, \underline{F}(\xi^2) = 0.7 \text{ and } \overline{F}(\xi^1) = 0.5, \overline{F}(\xi^2) = 0.9.$$

<sup>285</sup> From it we can deduce the bounds

$$\underline{\xi}^1 = 0.2, \underline{\xi}^2 = 0.2, \underline{\xi}^3 = 0.1 \text{ and } \overline{\xi}^1 = 0.5, \overline{\xi}^2 = 0.7, \overline{\xi}^3 = 0.3.$$

P-boxes usually rely on the fact that the set  $(\xi^1, \ldots, \xi^n)$  is naturally 286 ordered, and provide confidence bounds over sets of the kind  $\{\xi^1, \ldots, \xi^i\}$ . 287 However, one possibility is to extend this notion by considering that values 288  $\xi^i$  follows an arbitrary ordering  $\xi^{(1)} \leq \ldots \leq \xi^{(n)}$  (for example, from the least 289 to the most plausible element) and to ask to the expert to provide upper and 290 lower confidence bounds about the fact that the truth lies in  $\{x_{(1)}, \ldots, x_{(i)}\}$ , 291 thus obtaining  $F(\xi^{(i)})$  and  $\overline{F}(\xi^{(i)})$ . As in principle any ordering can be used, 292 this is indeed a generalization of p-boxes, known as comonotonic clouds [31]. 293 In particular, in the case where  $F(\xi^{(i)}) = 0$  for any *i*, we retrieve the notion 294 of possibility distribution as a special case. 295

<sup>296</sup> Up to now, what is the maximal number of extreme points of a p-box <sup>297</sup> structure and how to efficiently enumerate them remains an open prob-<sup>298</sup> lem. However, as p-boxes are a special case of belief functions, one can use (potentially sub-optimal) algorithms and methods applicable to belief functions [17]. It is also clear that the maximal number of such points is bounded above by the maximal number of extreme point of a belief function (n!). Classical p-boxes suffer from the fact that a natural order must exist on  $\mathcal{X}$ , and when no such order exists, then the average of generalized p-boxes relying on different orders will not be a p-box.

### 305 3.4. Belief functions and random sets

Formally, a random set or belief function, initially introduced by Dempster [30] and Shafer [57], is defined as a positive mapping  $\nu : 2^{\{\xi^1, \dots, \xi^n\}} \rightarrow [0, 1]$  from the power set of  $\{\xi^1, \dots, \xi^n\}$  to the unit interval, such that  $\nu(\emptyset) = 0$  and  $\sum_E \nu(E) = 1$ . From this mapping can then be defined probability bounds Bel(A), Pl(A) for any event that are equal to

$$Bel(A) = \sum_{E,E\subseteq A} \nu(E) \text{ and } Pl(A) = \sum_{E,E\cap A\neq\emptyset} \nu(E) = 1 - Bel(A^c)$$
(29)

311 that induce an information  $\mathcal{P}_{\nu}$  such that

$$\mathcal{P}_{\nu} = \left\{ \xi : \sum_{E \subseteq A} \nu(E) \le \sum_{\xi^i \in A} \xi^i \le \sum_{E \cap A \neq \emptyset} \nu(E), \ \forall A \right\}$$
(30)

In particular, this means that given a function  $\nu$ , the bounds over elementary events are given by

$$\underline{\xi^{i}} = Bel(\{\xi^{i}\}) = \nu(\{\xi^{i}\})$$
(31)

314

324

$$\overline{\xi}^{i} = Pl(\{\xi^{i}\}) = \sum_{\xi^{i} \in E} \nu(E)$$
(32)

Belief functions are instrumental to model frequencies of imprecise observations, for example when multiple exclusive options can be chosen in surveys, or when some sensors sometimes send back imprecise observations. They also include p-boxes, comonotonic clouds and possibilities as special cases.

Example 6. Assume again that we can meet four different situations  $x_1, x_2, x_3$ ,  $x_4$ . Out of 20 observations,  $x_1, x_2, x_3, x_4$  were each perfectly observed respectively 3, 2, 5, 6 times, we observed 3 times the set  $\{x_2, x_3, x_4\}$  (excluding  $x_1$ ) and 2 times the set  $\{x_1, x_2, x_3\}$ . Such observations can be modelled on  $\xi^1, \xi^2, \xi^3, \xi^4$  by the mass

$$\nu(\{\xi^1\}) = \frac{3}{20}, \nu(\{\xi^2\}) = \frac{2}{20}, \nu(\{\xi^3\}) = \frac{5}{20}, \nu(\{\xi^4\}) = \frac{6}{20},$$
$$\nu(\{\xi^1, \xi^2, \xi^3\}) = \frac{2}{20}, \nu(\{\xi^2, \xi^3, \xi^4\}) = \frac{3}{20}.$$

From this, we can for example deduce  $\underline{\xi}^3 = 0.25$  and  $\overline{\xi}^3 = 0.5$ .

Belief functions are general enough to deal with a lot of practical assessments, and share the properties of probability intervals that an average of belief functions is still a belief function. However, providing an intuitive graphical representation of a belief function is challenging, and their use may quickly lead to computational issues (e.g., their number of extreme points can be as high as  $\mathcal{X}$ ! [50])

### 332 3.5. Fuzzy random variables

Fuzzy random variables have been given different interpretations in the 333 literature, depending on the nature of the fuzzy elements. For example, a 334 fuzzy random variable can be seen as a random phenomenon with precise 335 observations that are fuzzy in nature, or as a random phenomenon with 336 imprecise observations. We refer to [19, 21, 22] for a detailed discussion. In 337 this paper, Fuzzy random variables are interpreted as conditional possibility 338 measures [4, 21], which consist in putting positive masses, not on subsets, 339 but on possibility distributions. They can be modelled by a set  $\pi_1, \ldots, \pi_k$ 340 where each distribution receives probability mass  $p(\pi_i)$ . As each  $\pi_i$  can in 341 turn be turned into a mass function  $\nu_{\pi_i}$  defined this time over subsets, it 342 is always possible to come back from a fuzzy random variable to a classical 343 mass function, simply by computing for any subset E the value 344



We obtain a weighted random sampling of subset E defining a belief function  $\nu$ . Fuzzy random variables in this context may be cast into the framework of belief functions leading to the same formal advantages and disadvantages of them (see Section 3.4). Fuzzy random variables can result, for instance, from Monte-Carlo simulations of physical models mixing possibilistic and probabilistic uncertainty [4], or from the random observation of fuzzy sets (modelling an ill-calibrated scale, for instance [18]).

# 352 3.6. Summary of types of knowledge

A final type of knowledge simply consists in directly providing bounds over the values of possible observations  $x_i$ . This means specifying, for each  $\xi^i$ , the bounds  $\underline{f}_i = \underline{\xi}^i$  and  $\overline{f}_i = \overline{\xi}^i$ . Such bounds are formally equivalent to probability intervals [11].

There are multiple ways to derive such bounds: for instance by instantiating multinomial confidence intervals over observations, by requiring linguistic opinions of the type "probable", "very probable" from the experts and then translating them into numerical evaluations [54], by simply requiring numerical evaluations from the experts, when having imprecise histograms, ... Table 1 summarises the most common type of practical information one can meet, to what type of information they correspond and how can be computed the lower/upper values  $\underline{\xi}^i$  and  $\overline{\xi}^i$ . These are the values (used as a common mathematical tool) that are then combined and integrated into the learning process developed in Section 2.2.

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			R
Model	Usual type of information		$\overline{\xi}^{i}$
Precise values	Sample/simulation	$f_i$	$f_i$
Possibility	Lower confidence on nested sets Linguistic assessments	$1 - \max_{\xi \neq \xi^i} \pi(\xi^i)$	$\overline{\xi}^i = \pi(\xi^i)$
P-boxes and clouds	Lower/upper confidence on nested sets	$\max(0, \underline{F}(\xi^{(i)}) - \overline{F}(\xi^{(i-1)}))$	$\overline{F}(\xi^{(i)}) - \underline{F}(\xi^{(i-1)})$
Belief functions	Imprecise sample	$ u(\xi^i)$	$\sum_{\xi^i \in E} \nu(E)$
Fuzzy random variable	Fuzzy sample	$\sum_{i=1}^k p(\pi_i) \nu_{\pi_i}(\xi^i)$	$\sum_{\xi^i \in E} \sum_{i=1}^k p(\pi_i) \nu_{\pi_i}(E)$
Probability bounds	Linguistic assessments Multinomial confidence regions	$\underline{f}_i$	$\overline{f}_i$
ACE	Table 1: Summary of the different types of collec	tible information	

# <sup>368</sup> 4. Robust dynamic probabilistic graphical models

When modeling complex systems, we are not interested in a single variable, but in multiple variables interacting with each others and evolving over time. In theory, our knowledge about these variables, their interaction and evolution can be represented by a credal set defined over the Cartesian product of the corresponding spaces.

In practice, we need tool to represent these interactions, and to simplify the daunting task of specifying a full joint model. Credal networks are graphical (directed) models that aims at encoding our knowledge about variable interactions and at splitting the full joint into multiple, simple conditional models. This section introduces them, as well as their dynamical extension.

# 380 4.1. Credal networks

Let  $\mathbf{X} = (X_1, \dots, X_n)$  be a discrete random vector associated with the joint probability mass function  $p(\mathbf{X})$  defined over  $\prod_{i=1}^{n} \mathcal{X}_i$ . Let  $K(\mathbf{X})$  be the closed convex set of multivariate probability mass functions describing our knowledge of  $\mathbf{X}$ .

A credal network (CN) [24, 23] is an extension of Bayesian networks 385 (BNs) where imprecision is introduced in probabilities by means of credal 386 sets [47]. When working with probability sets rather than precise proba-387 bilities, the notion of stochastic independence can be extended in several 388 ways [20]. Within graphical models, the most commonly used extension is 389 strong independence (also called a type 1 product of the marginals in [61]), 390 that induces the strong extension. It can be interpreted as a robust model 391 of a precise yet ill-known BN. Under the strong extension [23] hypothesis, 392 the joint credal set  $K(\mathbf{X})$  over  $\Omega_{\mathbf{X}}$  may be formulated as: 393

$$K(\mathbf{X}) = CH\left\{p(\mathbf{X}) : p(\mathbf{X}) = \prod_{i=1}^{n} p_i, p_i \in K_i\right\}$$
(33)

where  $p_i = p(X_i | \mathbf{U}_i)$ ,  $\mathbf{U}_i$  denotes the set of parent nodes of the node  $X_i$  and  $K_i = K(X_i | \mathbf{U}_i)$  is the closed convex set of probability mass function for the random variable  $X_i$  given  $\mathbf{U}_i$ . As mentioned in Section 2, it is sufficient to focus on  $\mathcal{E}xt(K(X_i | \mathbf{U}_i))$  in Eq. (33).

In this work, we focus on the notion of strong independence and its extension to dynamical models, as this is the most widely used independence notion within graphical models and the one that fits the best with a robust interpretation of probability sets. Other independence notions that may even have asymmetrical versions such as epistemic irrelevance remain computationally intractable [25, 49], except for specific network structures [9] that are usually less complex than the one generally considered here. 405 4.2. Dynamic credal networks

Let  $\mathbf{X}(\mathbf{t}) = (X_1(1), \dots, X_n(1), \dots, X_1(\tau), \dots, X_n(\tau))$  be a discrete random vector process associated with the joint probability function  $p(\mathbf{X}(\mathbf{t}))$ defined over  $\prod_{t=1}^{\tau} \prod_{i=1}^{n} \mathcal{X}_i(t)$ . Let  $K(\mathbf{X}(\mathbf{t}))$  be the closed convex set of multivariate probability mass functions for  $\mathbf{X}(\mathbf{t})$ .

A dynamic credal network (CDN) [41] is a dynamic Bayesian network (DBNs) [51] where conditional probabilities  $p(X_i(t) | \mathbf{U}_i(t))$  (noted  $p_i^t$ ) are replaced by credal sets  $K(X_i(t) | \mathbf{U}_i(t))$  (noted  $K_i^t$ ). It is therefore a timesliced model that can be used to describe a dynamic process or system<sup>2</sup>.

We assume the same *first-order Markov property* as for DBN, meaning that parents only originate from the same or previous time slice, and also that conditional models remain the same at each times slice, that is

$$K(X_i(t) \mid \mathbf{U}_i(t)) = K(X_i(2) \mid \mathbf{U}_i(2)), \ \forall t \in \llbracket 2, \tau \rrbracket.$$
(34)

Therefore, specifying the graphical structure of a DCN requires the same effort as the one of a DBN (that is, specifying only two consecutive time slices) but allows the user to provide conditional credal sets rather than probabilities if these latter cannot be reliably estimated (from data and/or experts).

## 422 4.2.1. Independence in DCN

Extending DBN to DCN requires to specify which kind of independence we consider within and also between each time-slice. We remind that we will only consider extensions relying on the strong independence (33). The most straightforward extension is to simply apply strong independence to the whole network, i.e.,

$$K(\mathbf{X}(\mathbf{t}))_{st} = CH\left\{p(\mathbf{X}(\mathbf{t})) : p(\mathbf{X}(\mathbf{t})) = \prod_{i=1}^{n} \prod_{t=1}^{\tau} p_i^t, p_i^t \in K_i^t\right\}$$
(35)

We call this extension the dynamic strong extension and it is worth noticing that we can have  $p_i^t \neq p_i^{t'}$  for  $t, t' \in [\![2, \tau]\!]$ . That is, we do not assume probabilities within each time-slice to be identical. However, when stepping to dynamic models, Condition (34) allows us to use the notion of *repetitive independence* (also called a *type 2 product* of the marginals in [61]). This condition states that if two variables X, Y have the same set of possible outcomes, that is  $\mathcal{X} = \mathcal{Y}$ , and can be assumed to be governed by the same probability distribution belonging to K(X), then the joint credal set K(X,Y) is :

$$K(X,Y) = CH\{p(X)p(X) : p(X) \in K(X)\}.$$
(36)

 $<sup>^2\</sup>mathrm{It}$  should be noted that the network itself is static, but is used to represent a dynamic process.



Figure 2: A simple dynamical graphical model

Adapting this notion of independence to DCN, so that probabilities of each time slice are assumed to be identical, leads to a second extension, i.e.,

$$K(\mathbf{X}(\mathbf{t}))_{rp} = CH \left\{ \begin{array}{l} p(\mathbf{X}(\mathbf{t})) : p(\mathbf{X}(\mathbf{t})) = \prod_{i=1}^{n} \prod_{t=1}^{\tau} p_{i}^{t}, \\ p_{i}^{2} \in K_{i}^{2} \text{ and } p_{i}^{t} = p_{i}^{2} \ \forall t \in [\![2,\tau]\!] \end{array} \right\}$$
(37)

that we call the dynamic repetitive extension. We have  $K(\mathbf{X}(\mathbf{t}))_{rp} \subseteq K(\mathbf{X}(\mathbf{t}))_{st}$ , as  $K(\mathbf{X}(\mathbf{t}))_{rp}$  is more constrained. In practice, the strong extension assumes that the dynamic network is ill-defined and that its behaviour can change between time slices, while the repetitive extension assumes that we seek a precise classical DBN who is partially known.

Example 7. Consider the very simple example where  $\mathcal{X} = \{0, 1\}$  and the 2-slice network given in Figure 2, which is nothing else than a two-state imprecise Markov chain, and an observed value X(1) = 1. Assume furthermore that we have three time slices ( $\tau = 3$ ), that X(1) = 1 is observed, and that

$$p(X(t) = 1 | X(t-1) = 0) = 0.8,$$
  
$$p(X(t) = 1 | X(t-1) = 1) \in [0.2, 0.5].$$

That is, the transition rates from state 0 are precisely known, but not the 435 one from state 1 (although staying in state 1 is clearly less likely). The 436 different extreme points over (X(1), X(2), X(3)) resulting from the strong 437 and repetitive extension are summarized in Table 2, in which we adopt the 438 notation x(t) for X(t) = 1 for simplification purposes. Each cell of the table 439 corresponds to a precise network obtained by a specific selection of extreme 440 points. The non-specified transition probabilities can be retrieved by the 441 formula p(X(t) = 1 | X(t-1) = 1) = 1 - p(X(t) = 0 | X(t-1) = 1).442

# 443 4.2.2. Inference algorithms in DCN

(D)CNs can be queried as in (D)BNs to get information about the state of a variable given evidence about other variables, with respect to the chosen network *extension*. However, the use of credal sets makes the updating problem much harder, as it becomes an optimization problem. As such, the computation of the lower bound on  $p(\mathbf{X}_Q | \mathbf{X}_E)$  requires to minimize a fraction containing polynomials :



$$\underline{p}(\mathbf{X}_{Q}(t) \mid \mathbf{X}_{E}(t)) = \min_{p(\mathbf{X}(t)) \in K(\mathbf{X}(t))_{\omega}} \frac{\sum_{X_{i}(t) \in \mathbf{X}(t) \setminus \mathbf{X}_{Q}(t) \cup \mathbf{X}_{E}(t)} \prod_{i=1}^{n} \prod_{t=1}^{n} p_{i}^{t}}{\sum_{X_{i}(t) \in \mathbf{X}(t) \setminus \mathbf{X}_{E}(t)} \prod_{i=1}^{n} \prod_{t=1}^{\tau} p_{i}^{t}}$$
(38)

with  $p(\mathbf{X}(\mathbf{t})) \in K(\mathbf{X})_{\omega}$  belonging to the dynamic strong extension ( $\omega = st$ ) 450 or dynamic repetitive extension ( $\omega = rp$ ) of the network. An upper bound can be obtained by maximizing (38). It is known that such a minimum (or 451 452 maximum) is obtained at a vertex of the dynamic strong/repetitive extension. 453 Depending on (1) the structure of network, (2) the number of modality 454 of variables and (3) the chosen extension (strong/repetitive), the updating 455 problem will be more or less complex to solve. Because inferences are already 456 hard in static credal networks, little work has been done on DCNs [41]. 457 By unrolling a two-time slice network over T time steps, the number of 458 possible vertex combinations goes from  $\prod_{i,t=0} # \mathcal{E}xt(K_i^t) \prod_{i,t=1} # \mathcal{E}xt(K_i^t)$  in 459 the case of repetitive independence, to  $\prod_{i,t=0} # \mathcal{E}xt(K_i^t) \prod_{i,t=1} # \mathcal{E}xt(K_i^t)^{\tau-1}$ 460 in the case of strong independence. Given the potential number of vertices, 461 approximate algorithms seem more appropriate regarding DCNs. 462

Many algorithms, exact and approximate, have been proposed to deal 463 with CN. Some are generalizations of well known (D)BNs algorithms. Among 464 the approximate algorithms, there are those that compute inner bounds, i.e. 465 bounds that are enclosed by the exact ones, outer bounds, which enclose 466 the exact ones, and those that perform randomly. The 2U algorithm [34] 467 performs an exact rapid inference in the case of binary tree-shaped (D)CNs 468 with the assumption of strong independence. The CCM transformation [15] 469 turns a (D)CN into a (D)BN by adding transparent nodes before performing 470 an Maximum A Posteriori (MAP) estimation over the latter to find the best 471 combination of vertices. It has the same complexity as credal network in-472

ference, that is  $NP^{PP}Complete$ , and performs poorly with separately spec-473 ified credal networks such as the one we used during our trials (because 474 of the sheer number of vertices). Optimization techniques such as branch 475 and bound over local vertices of credal sets [27, 13] are also well suited to 476 medium-sized networks and can be stopped at any time to give an approxi-477 mate answer. Other algorithms are based on a variable elimination scheme 478 from (D)BNs, such as Separable Variable Evaluation [26, 55] which keeps 479 the separately specified credal sets as separated as possible during propaga-480 tion, and can be mapped to an integer or a multi-linear program [29, 28]. 481 Regarding binary and DAG-shaped (DAG : Directed Acyclic Graph) credal 482 networks, algorithm L2U (Loopy 2U) [44] (similar to LBP (Loopy Belief 483 Propagation) [63]) produces either inner or outer approximations. Its effi-484 ciency is due both to the bounded cardinality of variables and to ignoring 485 loops. Another way to handle credal sets complexity is to represent them 486 by simpler means. Variational methods [43, 42] choose a family of functions 487 to approximate the exact combination of credal sets to decrease compu-488 tational costs. Those functions are optimized according to some criteria 489 until convergence and the inference is then realized in the network with the 490 original credal sets replaced by the new found functions. The  $A \setminus R(+)$  al-491 gorithm [27] uses interval probability arithmetic to approximate credal sets 492 in a propagation scheme in tree-shaped networks (with the use of some ad-493 ditional constraints limiting the information loss in its enhanced version). 494 The intervals produced are outer bounds of the real ones. Although those 495 algorithms are fast in medium-sized network, they either produce too many 496 approximations or are too complex to work with DCNs. Another popular 497 family of approximate algorithms producing inner bounds is based on Monte-498 Carlo sampling [38]. Several methods have been proposed to better guide 499 the search (simulated annealing [12], genetic algorithms [14]) among the ver-500 tices of the (conditional) local credal sets, but they require some tuning for 501 more accurate results, otherwise they can lead to poor approximations. 502

Although there exist several inference algorithms, none allows to do inference, in a realistic and practical way, on networks capable of representing global complex system of Life Sciences. In further inferences, we used a simple Monte-Carlo sampling algorithm [38] which has the advantage to be a good starting point, as it applies with the same easiness to *dynamic repetitive* and *strong extensions* (with a faster convergence for *dynamic repetitive extension*).

# 510 4.2.3. Robust parameter learning

Let  $p_{ijk}^t$  be the probability that  $X_i(t) = x_k$ , given that its parents have instantiation<sup>3</sup>  $x_j$  (corresponding itself to a vector where j represents the

<sup>&</sup>lt;sup>3</sup>Possible values of variables according to its discretization.

<sup>513</sup> vector of parents of i), *i.e.* 

$$p_{ijk}^{t} = p(X_{i}(t) = x_{k} | \mathbf{U}_{i}(t) = x_{j}) \qquad \begin{array}{l} i = 1, \dots, n \\ j = 1, \dots, c_{i} \\ k = 1, \dots, r_{i} \end{array}$$
(39)

where  $r_i$  is the number of values that node *i* can take and  $c_i$  is the number 514 of distinct configurations of  $\mathbf{U}_i(t)$ . Parameter learning consists in estimat-515 ing  $p_{ij}^t$  faced with available information [45, 10]. For the sake of clarity, 516 parameters  $p_{ij}^t$  will be denoted  $p_{ij}$  since parameters  $p_{ij}^t$  are time-invariant in 517 the case of repetitive extension assumption and it is sufficient to only con-518 sider information limited to each time slice in the case of strong extension 519 assumption. According to section 2.2, for all  $i \in \{1, \ldots, n\}$ ;  $j \in \{1, \ldots, c_i\}$ 520 the credal set  $\tilde{K}_{(s_l;\xi_l)_{l=0}^m}(X_i | \mathbf{U}_i = x_j)$  may be approximated by using the 521 outer credal set  $K_{(s_l;\xi_l)_{l=0}^m}(X_i | \mathbf{U}_i = x_j)$  defined by 522

$$K_{(s_l;\xi_l)_{l=0}^m}(X_i|\mathbf{U}_i = x_j) = \left\{ p_{ij}: \ p_{ijk} \in [\underline{p}_{ijk}, \overline{p}_{ijk}], \sum_k p_{ijk} = 1 \right\}$$
(40)

where  $[\underline{p}_{ijk}, \overline{p}_{ijk}]$  is estimated and updated from Eq. (19) according to the available sources of knowledge  $(S_0, \ldots, S_m)$ .

# 525 4.3. Practical robust parameter learning example

Wood is essentially composed of cellulose (denoted C) that is a polymer 526 whose quantity characterizes the nature of wood (denoted T) namely hard-527 wood or softwood. Imagine that we want to determine the kind of wood 528 according to its chemical composition tainted with uncertainties, that is we 529 are interested in P(T|C). For the sake of clarity, we choose  $C = \{x_1 =$ 530  $20\%, x_2 = 40\%, x_3 = 60\%$  meaning that there is 20%, 40% or 60% of cel-531 lulose inside wood,  $T = \{x_1 = \text{Soft}, x_2 = \text{Hard}\}$  and all sources  $s_i$  have the 532 same confidence level, *i.e.*  $s_i = 1$  for all *i*. We thus need to estimate the 533 following parameters: 534

$$p_{jk} = p(T = x_k | C = x_j) \tag{41}$$

according to the available knowledge described in the following. The credal sets  $K(T|C = x_j)$  are initialized by

$$K_{s_0}(T|C=x_j) = \{p_{j.} : p_{jk} \ge 0, \sum_k p_{jk} = 1\}, \ \forall j = 1, \dots, 3$$
(42)

Precise measures are provided {(20, Soft), (20, Hard), (40, Hard), (60, Soft)}
 leading to update by Eq. (19)

539

$$K_{(s_0,s_1)}(T|C=20) = \{p_{1.}: \frac{1}{4} \le p_{11} \le \frac{3}{4}, p_{12}=1-p_{11}\},\$$

540	• $K_{(s_0,s_1)}(T C=40) = \{p_{2.}: 0 \le p_{21} \le \frac{1}{2}, p_{22}=1-p_{21}\},\$
541	• $K_{(s_0,s_1)}(T C=60) = \{p_{3.}: \frac{1}{2} \le p_{31} \le 1, p_{32} = 1 - p_{31}\}.$
542	2. A first expert says that the more cellulose there is, the harder the
543	wood. This information may be formalized by means of the following
544	fuzzy numbers or possibility distribution (see Section 3.2):
545	• $\pi(T = \text{Hard} C = 20) = 0.5,  \pi(T = \text{Soft} C = 20) = 1$
546	• $\pi(T = \text{Hard} C = 40) = \pi(T = \text{Soft} C = 40) = 1$
547	• $\pi(T = \text{Hard} C = 20) = 1$ , $\pi(T = \text{Soft} C = 20) = 0.5$
548 549	meaning for instance that $P(T = \text{Hard} C = 20) \le 0.5$ leading to update
550	• $K_{(s_0,s_1,s_2)}(T C=20) = \{p_1: \frac{1}{3} \le p_{11} \le \frac{5}{6}, p_{12} = 1-p_{11}\},\$
551	• $K_{(s_0,s_1,s_2)}(T C=40) = \{p_{2.}: 0 \le p_{21} \le \frac{2}{3}, p_{22} = 1 - p_{21}\},\$
552	• $K_{(s_0,s_1,s_2)}(T C=60) = \{p_{3.}: \frac{1}{3} \le p_{31} \le \frac{5}{6}, p_{32} = 1-p_{31}\}.$
553	3. A second expert provides more accurate estimation in terms of confi-
554	dence
555	• $P(T = \text{Soft} C = 20) \ge 95\%$ ,
556	• $P(T = \text{Hard} C = 40) \ge 60\%$ ,
557	• $P(T = \text{Hard} C = 60) \ge 95\%.$
558	which can be modeled again by a possibility distribution. This leads
559	to update
560	• $K_{(s_0,\ldots,s_3)}(T C=20) = \{p_{1.}: 0.49 \le p_{11} \le 0.875, p_{12}=1-p_{11}\},\$
561	• $K_{(s_0,\ldots,s_3)}(T C=40) = \{p_{2.}: 0 \le p_{21} \le 0.6, p_{22}=1-p_{21}\},\$
562	• $K_{(s_0,\ldots,s_3)}(T C=60) = \{p_{3.}: 0.25 \le p_{31} \le 0.64, p_{32} = 1 - p_{31}\}.$
563	4. Defective sensors and measurements provide joint imprecise observa-
564	tions, summarized in Table 3 and producing a joint belief function
565	(Section $3.4$ ).
	$\checkmark$ From this information lower and upper probability bounds over pa-
	rameters are given by
X /	Bel(T = t, C = c)
<i>y</i>	$Bel(T = t   C = c) = \frac{Bel(T = t, C = c)}{Bel(T = t, C = c) + \sum_{t' \neq t} Pl(T = t', C = c)}$
	Pl(T = t, C = c)
	$Pl(T = t   C = c) = \frac{Pl(T = t, C = c)}{Pl(T = t, C = c) + \sum_{t' \neq t} Bel(T = t', C = c)}$
	22

		T	ype	
	Focal sets	Soft	Hard	${Soft, Hard}$
	20	1	2	0
س	40	4	6	1
lose	60	0	10	1
[llu]	$\{20, 40\}$	10	5	1
Ge	$\{20, 60\}$	0	0	5
	$\{40, 60\}$	1	3	10
	$\{20, 40, 60\}$	0	0	8

Table 3: Focal sets occurrences

¥,

For example

$$Bel(T = Soft|C = 20) = \frac{1/68}{1/68 + 21/68} = 0.045$$
$$Pl(T = Soft|C = 20) = \frac{24/48}{24/48 + 2/48} = 0.926$$

Credal set  $K_{(s_0,\ldots,s_4)}$  is then updated by 566

• 
$$K_{(s_0,\ldots,s_4)}(T|C=20) = \{p_1: 0.4 \le p_{11} \le 0.89, p_{12} = 1 - p_{11}\},\$$

• 
$$K_{(s_0,\dots,s_4)}(T|C=40) = \{p_2: 0.021 \le p_{21} \le 0.65, p_{22} = 1-p_{21}\}$$

• 
$$K_{(s_0,\ldots,s_4)}(T|C=60) = \{p_{3.}: 0.2 \le p_{31} \le 0.67, p_{32} = 1-p_{31}\}$$

### 5. Real-life case study 570

To illustrate the feasibility and practical use of our approach in a real 571 case, we have focused on the ripening process of the Camembert type soft 572 mould cheese that represents an ecosystem and a bioreactor difficult to ap-573 prehend from a global point of view [37, 52]. Based on recent works carried 574 out by Baudrit et al. [5]; Sicard et al. [48], a simplified sub-structure 575 of dynamic Bayesian networks has been extracted (see Figure 3) provid-576 ing a qualitative representation of the coupled dynamics of yeast behaviour 577 Kluyveromyces marxianus (Km, colony forming unit/g of Fresh Cheese in 578 decimal logarithmic scale) with its lactose substrate (lo, g/Kg of Fresh 579 Cheese) influenced by temperature  $(T, {}^{o}C)$  inside the ripening chamber and 580 involving odour changes  $(Od = \{Fresh, Mushroom, Camembert\}\}$ . 581



Figure 3: Structure of the dynamic credal network and the values of each variables representing the coupled dynamics Km growth versus lo consumptions influenced by temperature involving odour changes during the cheese ripening process (F=Fresh,M=Mushroom,C=Camembert).

# 582 5.1. Parameter learning

Assuming *repetitive extension* for computational reason mentioned in Section 4.2.2, we present, in the following, how parameters

$$\begin{aligned} p_1 &= p(Km(1)), \\ p_2 &= p(lo(1)), \\ p_3 &= p(T(1)), \\ p_4 &= p(Km(2)|(Km(1), lo(1), T(1))), \\ p_5 &= p(lo(2)|(Km(1), lo(1), T(1))), \\ p_6 &= p(Od(1)|(Km(1), lo(1))) \end{aligned}$$

may be estimated by using the robust hybrid parameter learning when we have several sources of knowledge (denoted  $S_i$ ) tainted with stochastic and epistemic uncertainty.

586 1. Initialization  $(S_1)$ .

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All DCN parameters are initialized by:

- An experimental database  $S_{experiments}$  of six cheese ripening trials carried out for temperatures varying from T = 8 to 16 °C is available.
- the vacuous credal sets leading to bracket parameters by [0,1] when no information is available.

With  $s_1$  corresponding to the confidence level about experimental trials  $S_{experiments}$ , according to (19) we have:

$$p_{ijk} \in \left[\frac{s_1 f_{ijk}}{s_0 + s_1}, \frac{s_0 + s_1 f_{ijk}}{s_0 + s_1}\right]$$
(43)

where  $f_{ijk}$  represents the observed frequency corresponding to sample information in Table 1 and linked to Section 3.1.

2. Integration of partial mechanistic model tainted with uncertainties  $(S_2)$ . The yeast Km is one of the dominant species in the yeast flora of Camembert cheeses and its principal activity is the consumption of lactose (lo) [46]. Models to determine the growth of microorganisms have been studied in the fermentation industry [58], and the description of the growth of Km is obtained by performing material balances on biomass Km and lactose lo [3]:

$$(S) \begin{cases} \frac{dKm}{dt} = \mu \frac{lo}{K_{lo} + lo} Km - b \cdot Km \\ \frac{dlo}{dt} = -\frac{\mu}{\beta} \frac{lo}{K_{lo} + lo} Km \end{cases}$$
(44)

where  $\mu$  (the maximum specific growth rate of Km),  $K_{lo}(T)$  (the 604 half saturation constant for growth), b (the decay coefficient) and 605  $\beta$  (the yield coefficient for Km on lactose), depending on tempera-606 ture, are tainted with stochastic and epistemic uncertainties, due to 607 the natural variability of yeast population and the imperfection of 608 the model. The background knowledge about parameters  $p_1$ ,  $p_2$ ,  $p_4$ 609 and  $p_5$  are then updated regardless of the rest of network by using 610 a simulated database  $S_{simulated}$  resulting from Monte Carlo simula-611 tion coupled to interval analysis [4] leading to manage a joint ran-612 dom set  $([\underline{Km}(t), \underline{Km}(t)], [\underline{lo}(t), lo(t)], T(t))_l$  associated with mass  $\nu_l =$ 613  $1/\#S_{simulated}$  such that for instance 614

$$a_{jk} \in \left[\frac{s_1 f_{4jk} + s_2 \xi_{4jk}}{s_0 + s_1 + s_2}, \frac{s_0 + s_1 f_{4jk} + s_2 \overline{\xi}_{4jk}}{s_0 + s_1 + s_2}\right]$$
(45)

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$$\underline{\xi}_{4jk} = \frac{bel(j,k)}{bel(j,k) + \sum_{l \neq k} pl(l,j)} \text{ and } \overline{\xi}_{4jk} = \frac{pl(j,k)}{pl(j,k) + \sum_{l \neq k} bel(l,j)}$$
(46) and

$$pl(j,k) = \sum_{\substack{l, [\underline{k}\underline{m}(t+1), \overline{k}\overline{m}(t+1)]_l \cap \{km_k\} \neq \emptyset \\ [\underline{k}\underline{m}(t), \overline{k}\overline{m}(t)]_l \cap \{km_j\} \neq \emptyset \\ [\underline{lo}(t), \overline{lo}(t)]_l \cap \{lo_j\} \neq \emptyset \\ T_l(t) = T_j}$$
(47)

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and

$$bel(j,k) = \sum_{\substack{l, \{km_k\} \subseteq [\underline{km}(t+1), \overline{km}(t+1)]_l \\ \{km_j\} \subseteq [\underline{km}(t), \overline{km}(t)]_l \\ \{lo_j\} \subseteq [\underline{lo}(t), \overline{lo}(t)]_l \\ T_l(t) = T_j}$$
(48)

This kind information is linked to Sections 3.4, 4.3 and corresponds to Belief functions in Table 1.

- 3. Integration of expert knowledge,  $(S_3)$ .
- In cheese ripening, as in every complex food process, most of the con-622 trol measures are performed on the basis of the expert's sensory per-623 ceptions. Indeed, experts have in mind the ripening process that they 624 oversee and they are able to explain part of the complex reactions 625 through their perception of quality changes [16]. Expert elicitation 626 [48] informs us that during the exponential growing of the yeast Km, 627 a characteristic fresh or lactic odour is released. Mushroom odour 628 appears when the concentration of the yeast Km begins to stabilize 629 and typical Camembert odour appears when the population of Km630 begins to decay. From this qualitative information, general rules may 631 be deduced such as "it is impossible to have a Camembert odour with 632 a weak (resp. high) concentrations of Km (resp. lo)". That means for 633 several combinations of Km and lo concentrations, likely values about 634 variable Odour may be formalized by means of possibility distributions 635  $\pi_{Odour}(.|Km, lo)$ . That is: 636
  - When there is a high (*resp.* weak) concentration of lactose (*resp.* the yeast Km), having a fresh odour is the most plausible state, followed by Mushroom and Camembert odours, which can be formalized as the following possibility distribution:

$$\pi_{Odour}(\text{Fresh}|j) = 1$$
  
$$\pi_{Odour}(\text{Mushroom}|j) = 0.8$$
  
$$\pi_{Odour}(\text{Camembert}|j) = 0.2$$

where  $j = (Km \le 6.5, lo \ge 8)$ .

• When there is a medium concentration of lactose and Km, the Mushroom odour is the most plausible state but we cannot exclude having Fresh or Camembert odours, formalized by:

 $\pi_{Odour}(\text{Fresh}|j) = 0.2$  $\pi_{Odour}(\text{Mushroom}|j) = 1$  $\pi_{Odour}(\text{Camembert}|j) = 0.2$  638

- where j = (Km = 7, 2 < lo < 8).
- When having very weak (*resp.* high) concentration of lactose (*resp.* the yeast Km), the Camembert odour is the most plausible state, followed by Mushroom and Fresh odours, formalized by:

$$\pi_{Odour}(\text{Fresh}|j) = 0.2$$
  
$$\pi_{Odour}(\text{Mushroom}|j) = 0.8$$
  
$$\pi_{Odour}(\text{Camembert}|j) = 1$$

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where j = (Km > 7, lo < 2).

Parameter  $p_6$  is then updated by using

$$p_{6jk} \in \left[\frac{s_1 f_{6jk} + s_3 \xi_{6jk}}{s_0 + s_1 + s_3}, \frac{s_0 + s_1 f_{6jk} + s_3 \overline{\xi}_{6jk}}{s_0 + s_1 + s_3}\right]$$
(49)

641 where

$$\overline{\xi}_{6jk} = \pi_{Odour}(k|j) \text{ and } \underline{\xi}_{6jk} = 1 - \max_{l \neq k} \pi_{Odour}(l|j)$$
 (50)

This kind of information is linked to the Section 3.2 and correspondsto possibilistic model in Table 1.

# 644 5.2. Inference results and discussion

<sup>645</sup> We attempt to estimate the lower and upper mean time evolution of Km, <sup>646</sup> *lo* and *Odour* for a temperature control according to the previous parameter <sup>647</sup> learning. That is

$$\underline{E}(X(t)|\mathbf{U}(t)) = \sum_{k} x_k \underline{p}(X(t) = x_k |\mathbf{U}(t))$$
(51)

for the lower bounds where X may be Km, lo, Odour;  $\mathbf{U}(t) = (lo(0), Km(0))$  $, T(0), \dots, T(t))$  and

$$\underline{p}(X(t) = x_k | \mathbf{U}(t)) = \inf_{p \in K(X(t) | \mathbf{U}(t))} p(X(t) = x_k | \mathbf{U}(t))$$
(52)

by assuming  $s_0 = s_1 = s_2 = s_3 = 1$  and the repetitive independence, since 650 we assume that transition probabilities remain the same along the process 651 (there is no reason to assume a change in the bacteria population behaviour), 652 but are ill-known due to insufficient experiments and information. Figure 653 4 displays the lower and upper simulated mean evolution of Km, lo, Odour654 versus experimental data over the cheese ripening carried out at  $12^{\circ}$ C each 655 time a source of information is added. Supported by Table 4, we may observe 656 that the imprecision of simulated results well decreases (characterized by the 657 surface in gray). 658



Figure 4: Incremental DCN average simulation versus raw data (dotted) of Km, lactose (lo) and Odour for a ripening carried out at and  $T=12^{\circ}$  C each time a new source of information is integrated.

	Km	lactose	Odour
Source 1	18.62	105.38	20.91
Source 1 & 2	11.37	71.06	13.77
Source 1& 2& 3	11.03	71.32	10.99

Table 4: Area between the lower and upper bounds of the simulated mean time evolution

# 659 6. Conclusion

There are complex dynamical processes for which no deterministic model 660 describing the complete process exists. In such cases, dynamic credal net-661 works are convenient models that allow to include expert knowledge, data 662 and variable interaction in a single framework. They allow a faithful repre-663 sentation of incomplete knowledge or scarce data, that are inherent to the 664 complexity of bio-physicochemical phenomena occurring in Life Sciences. In 665 this paper, we attempted to implement a practical methodology coupling 666 interval analysis and Dirichlet model in the framework of dynamical credal 667 networks for building mathematical model capable of representing complex 668 systems. Moreover, the concepts of dynamic repetitive and strong exten-669 sions have been proposed. While the latter can be seen as a straightforward 670 extension of classical credal networks, the former considers repetitive inde-671 pendence to allow the model to preserve a temporal regularity. Methodology 672 has been applied to a simplified real-case study concerning microbial popu-673 lation growth involving sensory evolution during cheese ripening. These ex-674 periments have shown that including information reduces imprecision about 675 result simulations. Next tools should consider to manipulate, to combine 676 convex sets in order to not lose information during incremental parameter 677 learning. In further works, DCNs should enable us to determine the contri-678 bution of imprecision and/or incompleteness on the outcomes of a model in 679 order to know if an ambiguous answer is due to a lack of information or due 680 to a random phenomenon. That is, we plan to develop refined sensitivity 681 analysis techniques based on their use. They should thus determine key 682 variables and/or key phenomena for which it will be necessary to acquire 683 more information. Finally, we also plan to investigate their usefulness in 684 determining optimal commands. 685

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879 Vitae



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