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14 Unifying parameter learning and modelling complex
 15 systems with epistemic uncertainty using probability
 16 interval

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22 **Abstract**

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
 24 model, knowledge integration, uncertainty, modelling.

25 **1. Introduction**

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

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

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

- 45 • heterogeneous sources of knowledge (Web, data warehouse, experts,
 46 ...)
- 47 • mathematical formalisms used by different disciplines (differential equa-
 48 tions, graphs, cognitive maps, ...)
- 49 • various manipulated scales (molecular, cellular, population, ...)
- 50 • different forms of uncertainty [32, 36, 40] (natural randomness, impre-
 51 cision in expert opinions, data scarcity, vagueness, ...)

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

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

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

87 2. Imprecise probabilities and Dirichlet model

88 Let X be a variable¹ taking its values on the finite set $\mathcal{X} = \{x_1, \dots, x_n\}$,
 89 and $p : \mathcal{X} \mapsto [0, 1]$, $\sum_{x \in \mathcal{X}} p(x) = 1$ be a probability mass function over \mathcal{X} .
 90 $p(X)$ will denote the vector mass function, while $p(x)$ will denote the value
 91 taken by p for $X = x$. Such a mass function defines a measure $P_X(A) =$
 92 $\sum_{x \in A} p(x)$ for all $A \subseteq \mathcal{X}$.

93 2.1. Imprecise probability and credal sets

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

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

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

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

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

104 In a subjectivist tradition, the lower probability $\underline{P}_X(A)$ can be interpreted
 105 as the maximal price one would be willing to pay for the gamble which pays
 106 1 unit if event A occurs (and nothing otherwise) [61]. $\underline{P}_X(A)$ is therefore a
 107 measure of evidence in favour of event A , or in other words how much $K(X)$
 108 supports event A , while $\overline{P}_X(A)$ measures the lack of evidence against A .
 109 $K(X)$ can also be given a robust interpretation, in which it models imperfect

¹We adopt notations similar to those of [2, Ch.9] and [24].

110 knowledge of a precise, possibly frequentist, probability p . A credal set
 111 $K(X)$ contains a set $\mathcal{Ext}(K(X))$ of extreme probability masses, always finite
 112 in this paper, corresponding to the vertices of $K(X)$. Geometrically, $K(X)$
 113 may be equivalently specified by the convex hull (denoted CH) of the set
 114 $\mathcal{Ext}(K(X))$, i.e.

$$K(X) = CH\{\mathcal{Ext}(K(X))\}. \quad (4)$$

115 The *vacuous* credal set

$$K_v(X) = \{p(X) : p(x) \geq 0, \forall x \in \mathcal{X}, \sum_{x \in \mathcal{X}} p(x) = 1\} \quad (5)$$

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

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

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

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,
 124 while remaining expressive enough (they include both the vacuous and the
 125 precise models). We refer to De Campos *et al.* [11] for a detailed exposition,
 126 and will only limit 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 function-
 ing", "fully functioning"), and assume that previous experiments result in
 the following intervals

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

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:

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

127 Finding these vertices can be done by using classical tools of convex ge-
 128 ometry [39], or by using algorithms proper to a given representation (an
 129 Algorithm is provided by De Campos *et al.* [11]). The set $K(X)$ is repre-
 130 sented in Figure 1 in barycentric coordinates.

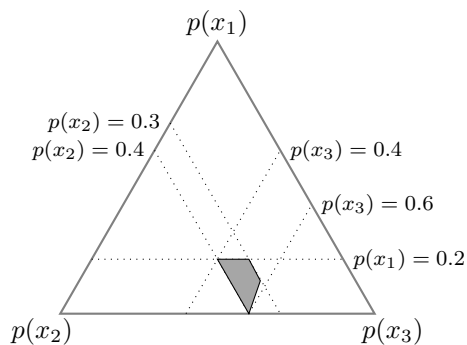


Figure 1: Example 1 credal set in Barycentric coordinates.

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

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

141 Let $\theta = (\theta_1, \dots, \theta_n)$ be a vector of chances such that θ_i corresponds to
 142 the chance that $X = x_i$. The prior distribution of vectors θ given by a
 143 Dirichlet model is then

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

144 where Γ is the gamma function. A very easy way to make this model imprecise
 145 is to let the vector ϵ_0 become imprecise, and more precisely to consider
 146 the set of Dirichlet models

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

147 with

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

148 the open $(n - 1)$ -dimensional unit simplex. When ξ_0 is precise, the first
 149 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
 150 used as estimates of $p(x_i)$, *i.e.*

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

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

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

153 and

$$\bar{E}(\theta_i | (s_0; \xi_0)) = \max_{\xi_0 \in \mathcal{T}} \xi_0(x_i) = 1. \quad (12)$$

154 The credal set corresponding to these bounds is then the vacuous one (5).

155 We may then receive additional information from various m sources. A
156 convenient way to encode this information is as a couple $s_k, \mathcal{P}_k, k = 1, \dots, m$,
157 with $\mathcal{P}_k \subseteq \mathcal{T}$ a convex polytope providing information about the possible
158 chances θ_i , and $s_k \in \mathbb{R}^+$ modelling the strength of the information. We can
159 then update the Dirichlet modelling our uncertainty about $\theta | (s_k; \xi_k)_{k=0}^m$ into

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

160 We can then use the posterior first moments to make inferences on chances
161 θ_i

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

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

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

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

163 where

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

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

164 These bounds then induce an updated credal set

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

165 that we can use as new knowledge. In practice, s_0 can be interpreted as
166 the number of "unseen" data, and $s_k = s_0$ means that the k th information
167 source has as much importance as our initial uncertainty.

168 *Remark 1.* The exact updated credal set

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

169 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
 170 (19) is thus an outer-approximation. Yet, the main advantages of using
 171 probability bounds as a basic representation are that

- 172 • their number of extreme points is bounded and relatively low, even
 173 when combining them through a weighted average. This is in general
 174 not the case if we consider averaging of heterogeneous simple repre-
 175 sentations: if we denote $|\mathcal{Ext}(\mathcal{P}_k)|$ the number of extreme points of
 176 the k th item of information, then their (Minkowsky) sum $\sum_{k=0}^m s_k \mathcal{P}_k$
 177 may have as much as $\prod_{k=0}^m |\mathcal{Ext}(\mathcal{P}_k)|$ extreme points, an exponentially
 178 growing number;
- 179 • they are easy to explain and to represent graphically (e.g., as imprecise
 180 histograms), therefore offering a convenient way to communicate with
 181 domain experts or users not specialized in mathematics or computer
 182 science. This is not the case of more complex representations such as
 183 belief functions (Section 3.4);
- 184 • except for requiring a finite space, they do not require specific assump-
 185 tions, such as the existence of an ordering between elements;
- 186 • they are expressive enough so that they can go from a fully precise
 187 probability to the complete ignorance model.

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

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

197 *Example 2.* Let $\mathcal{X} = \{x_1, x_2, x_3\}$ and $\mathcal{P} = \{\xi : \xi(x_2) \geq \xi(x_1), 1/2 \geq$
 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 $\{(0, 1, 0), (0, 0.5, 0.5),$
 200 $(0.5, 0.5, 0), (0.25, 0.25, 0.5)\}$ that are also extreme points of $K_\xi(X) = \{p :$
 201 $p(x_i) \leq \max_{\epsilon \in \mathcal{P}} \epsilon(x_i)\}$. However, the probability $(0.5, 0.25, 0.25)$ is an ex-
 202 treme point of $K_\xi(X)$ but not of $\tilde{K}_\xi(X)$.

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

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

212 *3.1. Precise evaluations*

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

$$\bar{\xi}^i = \underline{\xi}^i = f_i \quad (21)$$

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

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

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

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

226 *3.2. Numerical possibility distributions and fuzzy subsets*

227 A possibility distribution π is simply a mapping from $\{\xi^1, \dots, \xi^n\}$ to
 228 $[0, 1]$, with at least one element ξ^i such that $\pi(\xi^i) = 1$ [33]. In practice,
 229 we can see distribution π as an ordering $1 = \pi(\xi^{(1)}) \geq \dots \geq \pi(\xi^{(n)})$ of the
 230 elements x_1, \dots, x_n , from the most plausible to the least plausible one.

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

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

233 with $\pi(\xi^{(n+1)}) = 0$. $N(A_{(i)})$ can be associated to a lower probability bound
 234 of event $A_{(i)}$. In particular, the sets $A_{(i)}$ can be interpreted as nested sets
 235 with an associated lower confidence, these nested sets being built by starting

236 from the most plausible element $\xi^{(1)}$ and incrementally including the less
 237 plausible ones. Note that we may have $\pi(\xi^{(i)}) = \pi(\xi^{(i+1)})$, in which case
 238 elements $x_{(i-1)}$ and $x_{(i)}$ would be in the same confidence set.

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

$$\pi(\xi^k) = \min_{i: \xi^k \in A_i} 1 - \alpha_{i-1} \quad (24)$$

244 with $\alpha_0 = 0$.

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

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

250

$$\bar{\xi}^i = \pi(\xi^i) \quad (26)$$

251 *Example 4.* Assume that an expert is interrogated about the temperature
 252 in a room that can be in three states x_1, x_2, x_3 . Expert judges that x_2 is
 253 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:

$$N(\{\xi^2\}) = 0.5$$

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

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

254 which means that the expert has a confidence 0.5 that x_2 will be the observed
 255 state, a confidence 0.8 that the observed state will be either x_2 or x_3 , and
 256 finally is certain that the only observable states are x_1, x_2, x_3 . From these
 257 values can be deduced the values of the corresponding possibility distribution
 258 $\pi(\xi^1) = 0.2, \pi(\xi^2) = 1, \pi(\xi^3) = 0.5$.

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

266 *3.3. Probability boxes and clouds*

267 A probability box [35] $\underline{F}, \overline{F}$ is an imprecise cumulative distribution. It
 268 can be modelled by two discrete non-decreasing functions \underline{F} and \overline{F} from
 269 (ξ^1, \dots, ξ^n) to $[0, 1]$ such that $\underline{F}(\xi^i) \leq \overline{F}(\xi^i)$ for all i in $\{1, \dots, n\}$ and
 270 $\underline{F}(\xi^n) = \overline{F}(\xi^n) = 1$. The values $\underline{F}(\xi^i), \overline{F}(\xi^i)$ are interpreted as the following
 271 bounds

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

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

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

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

278

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

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

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

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

285 From it we can deduce the bounds

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

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

296 Up to now, what is the maximal number of extreme points of a p-box
 297 structure and how to efficiently enumerate them remains an open prob-
 298 lem. However, as p-boxes are a special case of belief functions, one can

299 use (potentially sub-optimal) algorithms and methods applicable to belief
 300 functions [17]. It is also clear that the maximal number of such points is
 301 bounded above by the maximal number of extreme point of a belief func-
 302 tion ($n!$). Classical p-boxes suffer from the fact that a natural order must
 303 exist on \mathcal{X} , and when no such order exists, then the average of generalized
 304 p-boxes relying on different orders will not be a p-box.

305 3.4. Belief functions and random sets

306 Formally, a random set or belief function, initially introduced by Demp-
 307 ster [30] and Shafer [57], is defined as a positive mapping $\nu : 2^{\{\xi^1, \dots, \xi^n\}} \rightarrow$
 308 $[0, 1]$ from the power set of $\{\xi^1, \dots, \xi^n\}$ to the unit interval, such that
 309 $\nu(\emptyset) = 0$ and $\sum_E \nu(E) = 1$. From this mapping can then be defined proba-
 310 bility bounds $Bel(A), Pl(A)$ for any event that are equal to

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

311 that induce an information \mathcal{P}_ν such that

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

312 In particular, this means that given a function ν , the bounds over elementary
 313 events are given by

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

314

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

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

319 *Example 6.* Assume again that we can meet four different situations x_1, x_2, x_3
 320 $, x_4$. Out of 20 observations, x_1, x_2, x_3, x_4 were each perfectly observed re-
 321 spectively 3, 2, 5, 6 times, we observed 3 times the set $\{x_2, x_3, x_4\}$ (excluding
 322 x_1) and 2 times the set $\{x_1, x_2, x_3\}$. Such observations can be modelled on
 323 $\xi^1, \xi^2, \xi^3, \xi^4$ by the mass

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

324

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

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

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

332 3.5. Fuzzy random variables

333 Fuzzy random variables have been given different interpretations in the
 334 literature, depending on the nature of the fuzzy elements. For example, a
 335 fuzzy random variable can be seen as a random phenomenon with precise
 336 observations that are fuzzy in nature, or as a random phenomenon with
 337 imprecise observations. We refer to [19, 21, 22] for a detailed discussion. In
 338 this paper, Fuzzy random variables are interpreted as conditional possibility
 339 measures [4, 21], which consist in putting positive masses, not on subsets,
 340 but on possibility distributions. They can be modelled by a set π_1, \dots, π_k
 341 where each distribution receives probability mass $p(\pi_i)$. As each π_i can in
 342 turn be turned into a mass function ν_{π_i} defined this time over subsets, it
 343 is always possible to come back from a fuzzy random variable to a classical
 344 mass function, simply by computing for any subset E the value

$$\nu(E) = \sum_{i=1}^k p(\pi_i) \nu_{\pi_i}(E).$$

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

352 3.6. Summary of types of knowledge

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

357 There are multiple ways to derive such bounds: for instance by instan-
 358 tiating multinomial confidence intervals over observations, by requiring lin-
 359 guistic opinions of the type "probable", "very probable" from the experts
 360 and then translating them into numerical evaluations [54], by simply re-
 361 quiring numerical evaluations from the experts, when having imprecise his-
 362 tograms, ...

363 Table 1 summarises the most common type of practical information one
364 can meet, to what type of information they correspond and how can be
365 computed the lower/upper values $\underline{\xi}^i$ and $\bar{\xi}^i$. These are the values (used as
366 a common mathematical tool) that are then combined and integrated into
367 the learning process developed in Section 2.2.

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| Model | Usual type of information | $\underline{\xi}^i$ | $\bar{\xi}^i$ |
|-----------------------|---|--|---|
| Precise values | Sample/simulation | f_i | f_i |
| Possibility | Lower confidence on nested sets Linguistic assessments | $1 - \max_{\xi \neq \xi^i} \pi(\xi^i)$ | $\bar{\xi}^i = \pi(\xi^i)$ |
| P-boxes and clouds | Lower/upper confidence on nested sets | $\max(0, \underline{F}(\xi^{(i)}) - \bar{F}(\xi^{(i-1)}))$ | $\bar{F}(\xi^{(i)}) - \underline{F}(\xi^{(i-1)})$ |
| Belief functions | Imprecise sample | $\nu(\xi^i)$ | $\sum_{\xi^i \in E} \nu(E)$ |
| 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 | \bar{f}_i |

Table 1: Summary of the different types of collectible information

368 4. Robust dynamic probabilistic graphical models

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

374 In practice, we need tool to represent these interactions, and to sim-
 375 plify the daunting task of specifying a full joint model. Credal networks
 376 are graphical (directed) models that aims at encoding our knowledge about
 377 variable interactions and at splitting the full joint into multiple, simple con-
 378 ditional models. This section introduces them, as well as their dynamical
 379 extension.

380 4.1. Credal networks

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

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

$$394 \quad K(\mathbf{X}) = CH \left\{ p(\mathbf{X}) : p(\mathbf{X}) = \prod_{i=1}^n p_i, p_i \in K_i \right\} \quad (33)$$

395 where $p_i = p(X_i | \mathbf{U}_i)$, \mathbf{U}_i denotes the set of parent nodes of the node X_i and
 396 $K_i = K(X_i | \mathbf{U}_i)$ is the closed convex set of probability mass function for
 397 the random variable X_i given \mathbf{U}_i . As mentioned in Section 2, it is sufficient
 398 to focus on $\mathcal{E}xt(K(X_i | \mathbf{U}_i))$ in Eq. (33).

399 In this work, we focus on the notion of strong independence and its ex-
 400 tension to dynamical models, as this is the most widely used independence
 401 notion within graphical models and the one that fits the best with a robust
 402 interpretation of probability sets. Other independence notions that may
 403 even have asymmetrical versions such as epistemic irrelevance remain com-
 404 putationally 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*

406 Let $\mathbf{X}(\mathbf{t}) = (X_1(1), \dots, X_n(1), \dots, X_1(\tau), \dots, X_n(\tau))$ be a discrete ran-
 407 dom vector process associated with the joint probability function $p(\mathbf{X}(\mathbf{t}))$
 408 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 mul-
 409 tivariate probability mass functions for $\mathbf{X}(\mathbf{t})$.

410 A dynamic credal network (CDN) [41] is a dynamic Bayesian network
 411 (DBNs) [51] where conditional probabilities $p(X_i(t) | \mathbf{U}_i(t))$ (noted p_i^t) are
 412 replaced by credal sets $K(X_i(t) | \mathbf{U}_i(t))$ (noted K_i^t). It is therefore a time-
 413 sliced model that can be used to describe a dynamic process or system².

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

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

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

422 *4.2.1. Independence in DCN*

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

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

We call this extension the *dynamic strong extension* and it is worth notic-
 ing that we can have $p_i^t \neq p_i^{t'}$ for $t, t' \in \llbracket 2, \tau \rrbracket$. 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 *repeti-*
tive 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 pos-
 sible 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 :

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

²It should be noted that the network itself is static, but is used to represent a dynamic process.

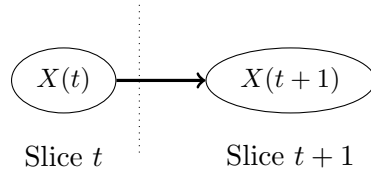


Figure 2: A simple dynamical graphical model

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

$$K(\mathbf{X}(\mathbf{t}))_{rp} = CH \left\{ \begin{array}{l} p(\mathbf{X}(\mathbf{t})) : p(\mathbf{X}(\mathbf{t})) = \prod_{i=1}^n \prod_{t=1}^{\tau} p_i^t, \\ p_i^2 \in K_i^2 \text{ and } p_i^t = p_i^2 \forall t \in \llbracket 2, \tau \rrbracket \end{array} \right\} \quad (37)$$

430 that we call the *dynamic repetitive extension*. We have $K(\mathbf{X}(\mathbf{t}))_{rp} \subseteq K(\mathbf{X}(\mathbf{t}))_{st}$,
 431 as $K(\mathbf{X}(\mathbf{t}))_{rp}$ is more constrained. In practice, the strong extension assumes
 432 that the dynamic network is ill-defined and that its behaviour can change
 433 between time slices, while the repetitive extension assumes that we seek a
 434 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 further-
 more that we have three time slices ($\tau = 3$), that $X(1) = 1$ is observed, and
 that

$$\begin{aligned} p(X(t) = 1 | X(t-1) = 0) &= 0.8, \\ p(X(t) = 1 | X(t-1) = 1) &\in [0.2, 0.5]. \end{aligned}$$

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

443 4.2.2. Inference algorithms in DCN

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

| Strong extension | | | | Repetitive extension | | | |
|------------------------|------|------|------|--|-----|-----|-----|
| 100 | 101 | 110 | 111 | 100 | 101 | 110 | 111 |
| $P(x(t) x(t-1)) = 0.5$ | | | | $P(x(2) x(1)) = 0.5, P(x(3) x(2)) = 0.2$ | | | |
| 0.1 | 0.4 | 0.25 | 0.25 | 0.1 | 0.4 | 0.4 | 0.1 |
| $P(x(t) x(t-1)) = 0.2$ | | | | $P(x(2) x(1)) = 0.2, P(x(3) x(2)) = 0.5$ | | | |
| 0.16 | 0.64 | 0.16 | 0.04 | 0.4 | 0.4 | 0.1 | 0.1 |

Table 2: Simple DCN extreme probabilities

$$p(\mathbf{X}_Q(t) | \mathbf{X}_E(t)) = \min_{p(\mathbf{X}(t)) \in K(\mathbf{X}(t))_\omega} \frac{\sum_{X_i(t) \in \mathbf{X}(t) \setminus \mathbf{X}_Q(t) \cup \mathbf{X}_E(t)} \prod_{i=1}^n \prod_{t=1}^{\tau} p_i^t}{\sum_{X_i(t) \in \mathbf{X}(t) \setminus \mathbf{X}_E(t)} \prod_{i=1}^n \prod_{t=1}^{\tau} p_i^t} \quad (38)$$

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

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

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

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

510 4.2.3. Robust parameter learning

511 Let p_{ijk}^t be the probability that $X_i(t) = x_k$, given that its parents have
 512 instantiation³ x_j (corresponding itself to a vector where j represents the

³Possible values of variables according to its discretization.

513 vector of parents of i), *i.e.*

$$p_{ijk}^t = p(X_i(t) = x_k | \mathbf{U}_i(t) = x_j) \quad \begin{array}{l} i = 1, \dots, n \\ j = 1, \dots, c_i \\ k = 1, \dots, r_i \end{array} \quad (39)$$

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

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

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

525 4.3. Practical robust parameter learning example

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

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

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

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

537 1. Precise measures are provided $\{(20, \text{Soft}), (20, \text{Hard}), (40, \text{Hard}), (60, \text{Soft})\}$
 538 leading to update by Eq. (19)

539 • $K_{(s_0, s_1)}(T|C = 20) = \{p_1 : \frac{1}{4} \leq p_{11} \leq \frac{3}{4}, p_{12} = 1 - p_{11}\},$

- 540 • $K_{(s_0, s_1)}(T|C = 40) = \{p_2. : 0 \leq p_{21} \leq \frac{1}{2}, p_{22} = 1 - p_{21}\},$
 541 • $K_{(s_0, s_1)}(T|C = 60) = \{p_3. : \frac{1}{2} \leq p_{31} \leq 1, p_{32} = 1 - p_{31}\}.$

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 • $\pi(T = \text{Hard}|C = 20) = 0.5, \quad \pi(T = \text{Soft}|C = 20) = 1$
 546 • $\pi(T = \text{Hard}|C = 40) = \pi(T = \text{Soft}|C = 40) = 1$
 547 • $\pi(T = \text{Hard}|C = 60) = 1, \quad \pi(T = \text{Soft}|C = 60) = 0.5$

548 meaning for instance that $P(T = \text{Hard}|C = 20) \leq 0.5$ leading to
 549 update

- 550 • $K_{(s_0, s_1, s_2)}(T|C = 20) = \{p_1. : \frac{1}{3} \leq p_{11} \leq \frac{5}{6}, p_{12} = 1 - p_{11}\},$
 551 • $K_{(s_0, s_1, s_2)}(T|C = 40) = \{p_2. : 0 \leq p_{21} \leq \frac{2}{3}, p_{22} = 1 - p_{21}\},$
 552 • $K_{(s_0, s_1, s_2)}(T|C = 60) = \{p_3. : \frac{1}{3} \leq p_{31} \leq \frac{5}{6}, p_{32} = 1 - p_{31}\}.$

553 3. A second expert provides more accurate estimation in terms of confi-
 554 dence

- 555 • $P(T = \text{Soft}|C = 20) \geq 95\%,$
 556 • $P(T = \text{Hard}|C = 40) \geq 60\%,$
 557 • $P(T = \text{Hard}|C = 60) \geq 95\%.$

558 which can be modeled again by a possibility distribution. This leads
 559 to update

- 560 • $K_{(s_0, \dots, s_3)}(T|C = 20) = \{p_1. : 0.49 \leq p_{11} \leq 0.875, p_{12} = 1 - p_{11}\},$
 561 • $K_{(s_0, \dots, s_3)}(T|C = 40) = \{p_2. : 0 \leq p_{21} \leq 0.6, p_{22} = 1 - p_{21}\},$
 562 • $K_{(s_0, \dots, s_3)}(T|C = 60) = \{p_3. : 0.25 \leq p_{31} \leq 0.64, p_{32} = 1 - p_{31}\}.$

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).

From this information lower and upper probability bounds over pa-
 rameters are given by

$$Bel(T = t|C = c) = \frac{Bel(T = t, C = c)}{Bel(T = t, C = c) + \sum_{t' \neq t} Pl(T = t', C = c)}$$

$$Pl(T = t|C = c) = \frac{Pl(T = t, C = c)}{Pl(T = t, C = c) + \sum_{t' \neq t} Bel(T = t', C = c)}$$

| | Focal sets | Type | | |
|-----------|--------------|------|------|-------------|
| | | Soft | Hard | {Soft,Hard} |
| Cellulose | 20 | 1 | 2 | 0 |
| | 40 | 4 | 6 | 1 |
| | 60 | 0 | 10 | 1 |
| | {20, 40} | 10 | 5 | 1 |
| | {20, 60} | 0 | 0 | 5 |
| | {40, 60} | 1 | 3 | 10 |
| | {20, 40, 60} | 0 | 0 | 8 |

Table 3: Focal sets occurrences

For example

$$Bel(T = \text{Soft}|C = 20) = \frac{1/68}{1/68 + 21/68} = 0.045$$

$$Pl(T = \text{Soft}|C = 20) = \frac{24/48}{24/48 + 2/48} = 0.926$$

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

- 567 • $K_{(s_0, \dots, s_4)}(T|C = 20) = \{p_1 : 0.4 \leq p_{11} \leq 0.89, p_{12} = 1 - p_{11}\},$
- 568 • $K_{(s_0, \dots, s_4)}(T|C = 40) = \{p_2 : 0.021 \leq p_{21} \leq 0.65, p_{22} = 1 - p_{21}\},$
- 569 • $K_{(s_0, \dots, s_4)}(T|C = 60) = \{p_3 : 0.2 \leq p_{31} \leq 0.67, p_{32} = 1 - p_{31}\}.$

570 5. Real-life case study

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

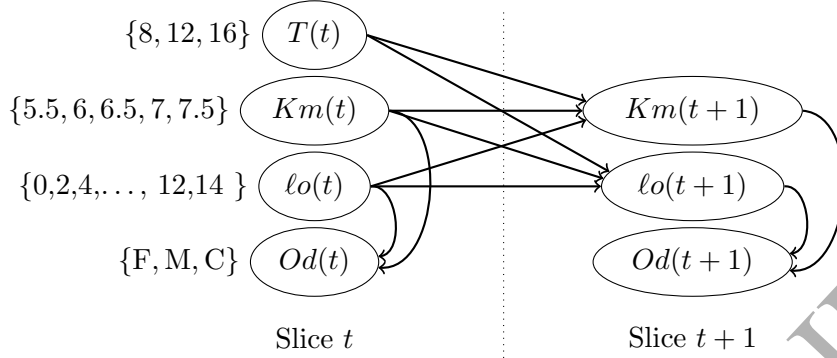


Figure 3: Structure of the dynamic credal network and the values of each variables representing the coupled dynamics Km growth versus lo consumptions influenced by temperature involving odour changes during the cheese ripening process (F=Fresh,M=Mushroom,C=Camembert).

582 5.1. Parameter learning

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

$$\begin{aligned}
 \mathbf{p}_1 &= p(Km(1)), \\
 \mathbf{p}_2 &= p(lo(1)), \\
 \mathbf{p}_3 &= p(T(1)), \\
 \mathbf{p}_4 &= p(Km(2)|(Km(1), lo(1), T(1))), \\
 \mathbf{p}_5 &= p(lo(2)|(Km(1), lo(1), T(1))), \\
 \mathbf{p}_6 &= p(Od(1)|(Km(1), lo(1)))
 \end{aligned}$$

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

586 1. Initialization (S_1).

587 All DCN parameters are initialized by:

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

593 With s_1 corresponding to the confidence level about experimental trials
 594 $S_{experiments}$, according to (19) we have:

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

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

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

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

604 where μ (the maximum specific growth rate of Km), $K_{lo}(T)$ (the
605 half saturation constant for growth), b (the decay coefficient) and
606 β (the yield coefficient for Km on lactose), depending on tempera-
607 ture, are tainted with stochastic and epistemic uncertainties, due to
608 the natural variability of yeast population and the imperfection of
609 the model. The background knowledge about parameters \mathbf{p}_1 , \mathbf{p}_2 , \mathbf{p}_4
610 and \mathbf{p}_5 are then updated regardless of the rest of network by using
611 a simulated database $S_{simulated}$ resulting from Monte Carlo simula-
612 tion coupled to interval analysis [4] leading to manage a joint ran-
613 dom set $([Km(t), \overline{Km}(t)], [lo(t), \overline{lo}(t)], T(t))_l$ associated with mass $\nu_l =$
614 $1/\#S_{simulated}$ such that for instance

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

615 where

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

616 and

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

617

and

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

618

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

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3. Integration of expert knowledge, (S_3).

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In cheese ripening, as in every complex food process, most of the control measures are performed on the basis of the expert's sensory perceptions. Indeed, experts have in mind the ripening process that they oversee and they are able to explain part of the complex reactions through their perception of quality changes [16]. Expert elicitation [48] informs us that during the exponential growing of the yeast Km , a characteristic fresh or lactic odour is released. Mushroom odour appears when the concentration of the yeast Km begins to stabilize and typical Camembert odour appears when the population of Km begins to decay. From this qualitative information, general rules may be deduced such as "it is impossible to have a Camembert odour with a weak (*resp.* high) concentrations of Km (*resp.* lo)". That means for several combinations of Km and lo concentrations, likely values about variable $Odour$ may be formalized by means of possibility distributions $\pi_{Odour}(\cdot|Km, lo)$. That is:

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- 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:

$$\pi_{Odour}(\text{Fresh}|j) = 1$$

$$\pi_{Odour}(\text{Mushroom}|j) = 0.8$$

$$\pi_{Odour}(\text{Camembert}|j) = 0.2$$

637

where $j = (Km \leq 6.5, lo \geq 8)$.

- 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:

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

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

640 Parameter \mathbf{p}_6 is then updated by using

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

641 where

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

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

644 5.2. Inference results and discussion

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

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

648 for the lower bounds where X may be Km , lo , $Odour$; $\mathbf{U}(t) = (lo(0), Km(0)$
649 $, T(0), \dots, T(t))$ and

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

650 by assuming $s_0 = s_1 = s_2 = s_3 = 1$ and the *repetitive independence*, since
651 we assume that transition probabilities remain the same along the process
652 (there is no reason to assume a change in the bacteria population behaviour),
653 but are ill-known due to insufficient experiments and information. Figure
654 4 displays the lower and upper simulated mean evolution of Km , lo , $Odour$
655 versus experimental data over the cheese ripening carried out at 12°C each
656 time a source of information is added. Supported by Table 4, we may observe
657 that the imprecision of simulated results well decreases (characterized by the
658 surface in gray).

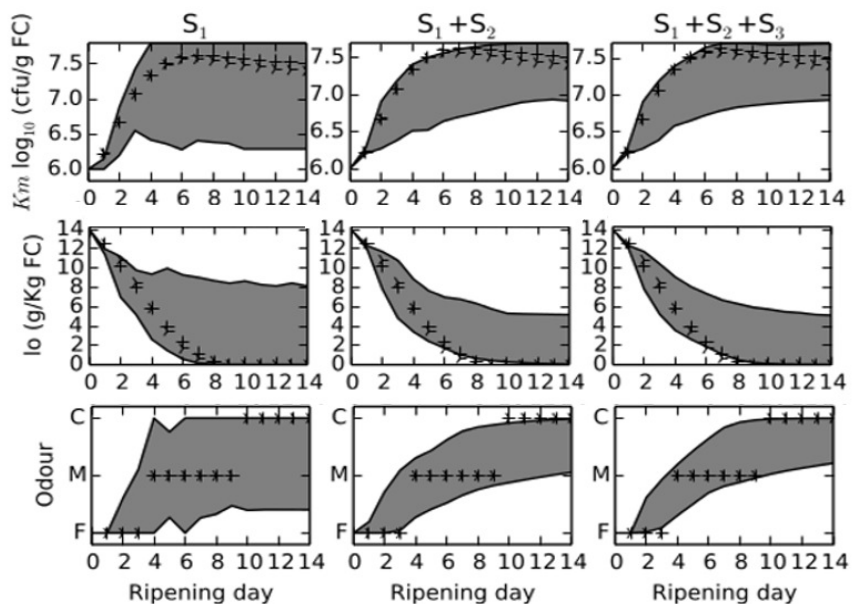


Figure 4: Incremental DCN average simulation versus raw data (dotted) of Km , lactose (lo) and Odour for a ripening carried out at and $T=12^{\circ}$ C each time a new source of information is integrated.

| | 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

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

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879 Vitae



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