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# Sensitivity analysis of Bayesian networks to parameters of the conditional probability model using a Beta regression approach

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## 12 Abstract

Ensuring the validity and credibility of Bayesian Belief Network (BBN) as a modelling tool for 13 14 expert systems requires appropriate methods for sensitivity analysis (SA), in order to test the 15 robustness of the BBN diagnostic and prognostic with respect to the parameterisation of the conditional probability model (CPM). Yet, the most widely used techniques (based on 16 17 sensitivity functions for discrete BBNs) only provide a local insight on the CPM influence, i.e. by varying only one CPM parameter at a time (or a few of them) while keeping the other ones 18 19 unchanged. To overcome this limitation, the present study proposes an approach for global SA 20 relying on Beta Regression using gradient boosting (potentially combined with stability selection analysis): it presents the benefit of keeping the presentation intuitive through a graph-21 22 based approach, while being applicable to a large number of CPM parameters. The 23 implementation of this approach is investigated for three cases, which cover a large spectrum of situations: (1) a small discrete BBN, used to capture medical knowledge, demonstrates the 24 25 proposed approach; (2) a linear Gaussian BBN, used to assess the damage of reinforced concrete structures, exemplifies a case where the number of parameters is too large to be easily 26 27 processed and interpreted (>40 parameters); (3) a discrete BBN, used for reliability analysis of 28 nuclear power plant, exemplifies a case where analytical solutions for sensitivity can hardly be derived. Finally, provided that the validity of the BBR model is carefully checked, we show that the proposed approach can provide richer information than traditional SA methods at different levels: (i) it selects the most influential parameters; (ii) it provides the functional relation between the CPM parameter and the result of the probabilistic query; and (iii) it identifies how the CPM parameters can lead to situations of high probability, while quantifying the confidence in the occurrence of these situations.

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Keywords: Bayesian Network; Sensitivity; Distributional Regression; Beta Distribution;
Gradient Boosting; Stability Selection.

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# 39 **1** Introduction

40 Bayesian Belief Network (BBN) is widely recognized as a valuable modelling tool for expert 41 systems (e.g. Russel et al., 2003). It has been applied in various complex domains, like 42 ecosystems (Milns et al., 2010), genetics and biology (Scutari et al., 2014), industry (Weber et al., 2012), finance forecasting (Malagrino et al., 2018), marine safety (Hänninen et al., 2014), 43 44 nuclear power plants (Kwag & Gupta 2017), coastal systems (Jäger et al., 2018), multi-hazard 45 risk assessments (Gehl and D'Ayala, 2016), etc. An expert system has the ability to represent 46 and reason on knowledge with the purpose of solving problems and giving advice (as defined 47 by Jackson, 1999), by relying on three components (i.e. knowledge base, observation base, 48 inference engine). Each of these components can benefit from the key features of BBN: (1) its 49 capability to represent expert knowledge and to combine and integrate expert knowledge with 50 information from any kind of sources, including experimental data, historical data, results from numerical simulations, etc.; (2) its high flexibility to model any causal relationships and to 51 52 explicitly display the relationship among variables using a network-based approach, which can 53 intuitively be understood by experts (Wiegerinck et al., 2010); and (3) its capability to answer 54 probabilistic queries about them and to find out updated knowledge of the state of a subset of 55 variables when other variables (the evidence variables) are observed. For instance, probabilistic 56 queries in reliability assessments may correspond to finding the probability values of some failure cause given the observed damage level of the considered system. See Appendix A for a 57 58 brief overview. The interested reader can also refer to Jensen (2001) for a complete introduction 59 to BBN.

Formally, BBN is based on the graphical representation of the probabilistic relations among 60 61 random variables by means of a directed acvelic graph composed of nodes (i.e. the states of the random variables) and arcs (i.e. dependency between nodes). See an example in Fig. 2A. The 62 nodes connected by an arc are called the parent and child nodes respectively. One child node 63 64 may have several parent nodes, meaning that this node is affected by several factors. Similarly, a parent node could have several child nodes, meaning that this factor may have influences on 65 66 several other factors. Conditional probabilities are the probabilities that reflect the degree of influence of the parent nodes on the child node. The probabilistic dependence (i.e. the relation 67 68 cause-effect) is represented via a table called a Conditional Probability Table (CPT) when the variables X (nodes) are discrete. In this case, the CPT entries correspond to the probability value 69  $P(X_i = k | Pa(X_i) = j)$  where k denotes the k<sup>th</sup> possible level (either a discrete value or a 70 category) that node  $X_i$  can take given that its parents  $Pa(X_i)$  takes the j<sup>th</sup> possible level. When 71 72 the variables are continuous, the conditional distribution given its parents can typically be represented by means of a continuous probability distribution. The most popular model is the 73 74 Gaussian distribution, as follows:

75

6 
$$P(X_i = y | Pa(X_i) = x) = G(y | m_0 + Zx, S)$$
 (Eq. 1)

77

where *G* is the Gaussian probability distribution whose mean is parameterized by a linear regression model with intercept  $m_0$  and regression coefficients *Z*, and *S* is the conditional variance.

81 When the nodes are both discrete and continuous, different hybrid techniques exist in the 82 literature (e.g., Murphy 1999; Shenoy, 2006; Beuzen et al., 2018).

Whatever the nature of the nodes, the pillar of any BBN-based results (either evidence 83 propagation or inference) is the specification of the parameters of the conditional probability 84 model (denoted CPM), i.e. the CPT entries or the regression coefficients of the linear Gaussian 85 regression model. This process is recognized in the literature as one of the most delicate part of 86 87 the BBN development (e.g., Chen & Pollino 2012; Druzdzel & van der Gaag 2000, etc.), which raises the question of confidence in the diagnosis or prognosis derived from the BBN-based 88 89 expert systems (see discussion by Pitchforth & Mengersen, 2013). In the validation framework of BBN, sensitivity analysis (SA) tools play a major role in order to study how the output of a 90

model varies with variation of the CPM parameters. Subsequently, the results from SA can be
used as a basis for parameter tuning, as well as for studying the robustness of the model output

93 to changes in the parameters (Coupé & van der Gaag 2002; Laskey et al. 1995).

94 For discrete BBNs, a widespread SA method relies on the use of sensitivity functions (Coupé 95 & van der Gaag 2002; Castillo et al., 1997), which describe how the considered output 96 probability varies as one CPT entry value is changed. Some recent extensions have been 97 proposed to conduct multi-way SA like the framework by Leonelli et al. (2017), i.e. SA when 98 several CPT entries are allowed to vary. Effects of parameter changes can be described by the 99 Chan-Darwiche (CD) distances (Chan-Darwiche 2002; 2005). The CD distance is used to 100 quantify global changes by measuring how the overall distribution behaves when one (or more) 101 parameter is varied. Likewise, SA approaches have been developed for continuous BBNs 102 (mostly based on linear Gaussian regression) either based on computing partial derivatives 103 (Castillo & Kjærulff 2003) or based on the use of divergence measures (Gómez-Villegas et al.,

104 2007), with generalisation to multi-way SA (Gómez-Villegas et al., 2013).

105 Yet, several limitations of the existing SA methods exist.

106 (1) The SA methods differ depending on the type of BBN (discrete, continuous, hybrid);

107 (2) Though simple and efficient to implement, the approach based on sensitivity functions
108 (combined with CD-distance analysis) remains local, because the values of only one parameter
109 of the CPM is varied, while the other ones are kept constant. Multi-way SA methods have been
110 proposed, but can rapidly become intractable. The SA procedure for Gaussian BBN presents
111 the same limitation as being based on partial derivatives;

(3) The SA is usually performed by focusing on one type of co-variation of the different
parameters (like proportional, uniform and order-preserving co-variation, see e.g., Renooij,
2014).

In the present study, we propose an alternative approach for SA, whose characteristics should complement the existing ones and overcome the afore-described limitations. The proposed approach should be:

Global: since the sensitivity of any BBN-based probability of interest is affected by
 multiple variations in the CPM parameters, the sensitivity is studied in a global manner
 and the different parameters are allowed to be varied all together;

- Generic: it should apply to any kind of BBN, i.e. discrete, Gaussian or hybrid, with
   limited restriction on the type of variations of the CPM parameters;
- Robust to the number of parameters: the number of parameters can rapidly increase (in
   relation with number of nodes), typically reaching several dozens even for a moderate
   number of BBN nodes, which can hamper the interpretation of any global SA;
- Concise: the presentation of the SA results should be as intuitive as the sensitivity
  function method by using a graph-based approach.

128 To do so, we address the problem of SA for BBN with the viewpoint of regression by 129 considering the BBN-based probabilistic queries *P* as the predictand and the CPM parameters 130 as the predictors (denoted C). In contrast to the classical regression model, which restricts the 131 analysis to the expected value of P as a function of C, we aim at estimating the full probabilistic variation of P by taking advantages of recent developments for distributional regression (e.g., 132 133 Koenker et al., 2013). In the subsequent sections, we first describe the principles of the proposed 134 method together with the implementation details (Sect. 2). In Sect. 3, we apply the approach to 135 a small discrete BBN (6 nodes) used to capture medical knowledge (adapted from Cooper 1984) 136 to exemplify the potentialities of the proposed approach. Then, in Sect. 4, two real cases are 137 used to investigate the applicability of the proposed approach. Finally, Sect. 5 discusses the 138 strengths and weaknesses of the proposed approach from the methodological and operational 139 viewpoints.

140

# 141 **2** Statistical methods

In this section, we first describe the principles underlying the development of the proposed approach (Sect. 2.1). We then provide the justifications for using Beta regression (Sect. 2.2) for sensitivity analysis of BBNs. Sect. 2.3 gives further technical details on the key ingredient of the procedure, namely the Boosted Beta Regression (BBR) technique. Finally, we describe how to check the adequacy of the BBR model to fit the data (Sect. 2.3).

147 **2.1 Overall procedure** 

148 The different steps of the procedure hold as follows:

Step1: generate perturbations of network's entry values *C* (i.e. the predictors) using, for
 instance, some random sampling techniques. For binary nodes, the CPT entries can be

- randomly perturbed using truncated Gaussian distributions (van der Gaag et al., 2013);
  for multi-level discrete nodes, it can be based on Dirichlet distributions (e.g., Young et al., 2009); for continuous Gaussian nodes, truncated Gaussian distributions can also be used if the purpose is to study the robustness to small-to-moderate variations; see also Gómez-Villegas et al. (2014) for alternative possible probability laws;
- Step 2: estimate the query probability of interest *P* derived from the inferences using
  the BBN. This probability value is the predictand;
- Step 3: establish the link between *C* and *P* using a regression model. We propose to rely
  on Beta regression models (see Sect. 2.1) using boosting-based fitting procedure (Sect.
  2.2) to deal with the potentially large number of predictors;
- Step 4: check the adequacy of the Beta model by checking that the residuals are well
  approximated by the standard normal distribution (see Sect. 2.4).

#### 163 **2.2** Use of Beta regression for BBN sensitivity analysis

We choose to rely on the Beta regression model (e.g., Ferrari and Cribari-Neto, 2004) due to different difficulties inherent to our case. The first difficulty is related to the nature of the predictand, which lies within the interval [0 ; 1]. This prevents from a direct application of ordinary least squares (linear) regression techniques, because bounded data (such as rates and proportions- or here probability values) are typically heteroskedastic (e.g., Cribari-Neto and Zeileis, 2010), which means that their variance depends on the predictors' values.

170 Second, the distributions of such data are typically asymmetric, and the normal assumption 171 underlying standard regression models might not be valid in our case. An alternative approach 172 is to use regression models that are based on a probability distribution suitable for handling 173 bounded data. A good candidate is the Beta law, whose density distribution d is defined as 174 follows:

175

176 
$$d(P, a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} P^{a-1} (1-P)^{b-1}$$
 (Eq. 2)

177

178 where  $\Gamma$  is the gamma function, (a,b) are the shape parameters. In the following, we preferably 179 use an alternative parametrisation  $(\mu,\sigma)$ , where  $\mu = \frac{a}{a+b}$  is the mean of *P* and  $\sigma = \frac{1}{(a+b+1)^{1/2}}$  is related to the variance of *P*, i.e.  $\mu(1 - \mu)\sigma^2$  (e.g., Schmid et al., 2013) The  $\sigma$ -parameter allows covering a large spectrum of density shapes as shown in Fig. 1 given different  $\mu$  and  $\sigma$  values. An additional difficulty is the inclusion of the boundary values at 0 and 1, because the density

*d* in Eq. 2 is not defined at these values. This can be overcome by means of a simple
transformation of *P* (Smithson and Verkuilen, 2006) as follows:

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186 
$$(P(n-1) + 0.5)/n$$
 (Eq. 3)

187 where *n* is the number of samples (i.e. the number perturbations performed to study the 188 sensitivity of *P*).

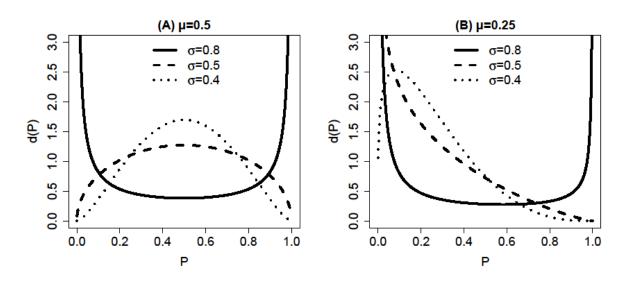
The joint analysis of both Beta parameters  $(\mu, \sigma)$  enables the BBN practitioners to investigate the sensitivity of the BBN with respect to two levels. The first level is related to the evolution of  $\mu$  as a function of the CPM parameters. These evolutions can be interpreted in a similar manner as the sensitivity functions used in the traditional SA for BBN, but it is worth noting that these functions are global; in the sense that they are constructed based on samples where all CPM parameters are allowed to vary all together.

195 In the present study, we propose to introduce a second level of analysis by allowing the Beta  $\sigma$ 196 parameter to vary as well. This is justified as follows:

- 197 when the Beta  $\sigma$  parameter is incorrectly taken to be constant, some efficiency loss in 198 the fitting process has been reported in the literature (e.g., Bayer and Cribari-Neto, 2017 199 and references therein);
- 200 a potentially large number of predictors have to be handled in the regression model and 201 we propose to select only one part of the CPM parameters that have influence on the 202 BBN probabilistic query *P* (see Sect. 2.3). This means that for fixed values of these 203 selected parameters, values of *P* can still vary due to perturbations of the CPM 204 parameters that were left out. The  $\sigma$  parameter is here used to describe this type of 205 variability;
- some algorithms for the estimation of BBN probabilistic queries are based on random
   sampling (like particle filter using logic sampling by Koller and Friedman (2009)),
   which may introduce some noise in the *P* estimates;

209 studying the evolution of  $\sigma$  enables the BBN practitioners to identify the sources of data 210 variability (e.g., Smyth and Verbyla, 1999) i.e. to study the influence on the uncertainty 211 of *P*. In this manner, the BBN practitioners can identify different probabilistic regimes; 212 e.g. situations where the probability of interest might switch from low to high values, 213 i.e. situations of low to high risk. Such situations can be highlighted by low and high 214 values of  $\mu$ . Values of  $\sigma$  are then useful to indicate the confidence in the occurrence of 215 such situations. For instance, high value of  $\mu$  (high average value of P) together with 216 low value of  $\sigma$  (low variance) provide strong evidence that changes in the considered 217 parameter(s) might surely lead to situations of high probability. High values for both Beta parameters show, however, that the situation of high probability might occur but 218 219 only with low confidence (i.e. high uncertainty).





221

*Figure 1. Probability density functions for the beta law. (A) mean*  $\mu$ =0.5; (*B*) *mean*  $\mu$ =0.25.

223

224 Given the transformation of P (Eq. 3), BBN sensitivity analysis can be performed using Beta 225 regression models (step 3 of the procedure) whose parameters are fitted using, for instance, 226 maximum likelihood techniques (Cribari-Neto and Zeileis 2010). Yet, the functional form of 227 the predictor-predictand relationship (e.g., quadratic or exponential) can hardly be specified in 228 advance in our case (except for specific cases, like binary discrete BBN) and the relationships 229 should preferably be learnt from the data. A possible option can rely on more advanced Beta 230 distribution regression techniques, for instance using generalized additive models for location, 231 scale and shape (GAMLSS, Rigby and Stasinopoulos, 2005), which allows deriving smooth

non-linear functional terms from the data, which correspond to the "partial effects" (more
formally introduced in Sect. 2.3). These terms are the key ingredients for sensitivity analysis,
because they hold the information of each parameter's individual effect on the considered Beta
parameter.

The difficulty in our case is, however, the possible large number of predictors, which can typically exceed several tens in real cases. This situation imposes the use of techniques for variable selection during the fitting process. A possible option is the combination of GAMLSS with boosting-based approach (Mayr et al., 2012), which is detailed in the next section.

#### 240 2.3 Boosted Beta Regression

In contrast to classical regression model, GAMLSS for Beta probability distribution aims at regressing the Beta parameters  $\theta = (\mu, \sigma)$  (or their transformation, e.g. via a log or a logit function) to the *p* predictor variables  $C = (c_1, c_2, ..., c_p)$ , e.g., the CPT entries for discrete BBN or the regression coefficients of a Gaussian BBN. In the following, we restrict the analysis to a semi-parametric additive formulation as follows:

246

247 
$$\theta = \eta_{\theta}(\boldsymbol{C}) = \beta_0 + \sum_{j=1}^J f_j(c_j | \beta_j)$$
(Eq. 4)

248

where  $\eta_{\theta}(.)$  is the link function that related the considered parameter  $\theta = (\mu, \sigma)$  with the predictor variables *C*;  $J \le p$ ,  $\beta_0$  is a constant and the functional term  $f_j(.)$  corresponds to a univariate smooth non-linear model like regression penalized regression P-spline models (Eilers and Marx 1996) with parameters  $\beta_j$ . These functional terms (termed as partial effect) hold the information of each parameter's individual effect on the considered Beta parameter.

The fitting is performed using the *gamboostLSS* algorithm of Mayr et al. (2012), which uses the Beta log-likelihood function (termed as risk) as an optimization criterion based on the component-wise gradient boosting technique (Bühlmann and Hothorn 2007, see further details in Appendix B). The approach is termed as BBR model (Boosted Beta Regression).

One advantage of using boosting techniques is to perform variable selection during the fitting process, which allows screening the parameters C which hold most information with respect to the conditional distribution of P. This is performed by assessing the individual fits of each 261 predictor variable, and by updating only the coefficient of the best-fitting predictor variable in 262 each iteration. Variable selection is carried out successively for the mean  $\mu$  and for the  $\sigma$ 263 parameter.

264 When the algorithm is stopped, the final model only contains the set of best-fitting predictors. 265 The number of boosting iterations controls the smoothness of the non-linear effects. Low values lead to sparse models with smooth functional terms, whereas large values lead to more complex 266 models with larger number of predictors and rougher functional terms. In practice, the selection 267 268 of the stopping parameter can be carried out using cross-validation procedures in order to 269 optimize the risk on observations left out (i.e. "out-of-bag") from the fitting process i.e. the out-270 of-bag risk, which corresponds here to the negative log-likelihood of the Beta distribution 271 calculated for the "out-of-bag" samples. To avoid optimizing two different stopping iterations, 272 i.e. one for each Beta parameter, the procedure can be enhanced using the noncyclic algorithm 273 of Thomas et al. (2018), which allows reducing the optimisation problem from a multi-274 dimensional to a one-dimensional problem.

In some situations, the resulting BBR model can still remain too rich to be easily interpretable by BBN practitioners. This procedure can be completed by the stability selection analysis (described in Appendix C), which allows screening the most influential variables in the BBR model.

In summary, the boosting-based approach allows to both select a limited number of influential predictors among all network's entry values *C*, and to derive the corresponding partial effects for each Beta parameter. Note that the identified predictors are not necessarily the same for  $\mu$ and for  $\sigma$ , and can be unique or multiple. The final results of the procedure are the partial effects (Eq. 4), which can directly be used to analyze the sensitivity of the considered Beta parameter to *C* as illustrated on the application cases (Sect. 3 and 4), by considering two levels of analysis (respectively related to the best estimate of *P* using  $\mu$ , and to the uncertainty of *P* using  $\sigma$ ).

#### 286 2.4 Model adequacy

Once the BBR model has been fitted, an important aspect is to check the model adequacy (step 4 of the procedure), i.e. how well the BBR model is appropriate to describe the randomly generated BBN-derived probabilities. This can be done by analysing the statistics of the residuals and checking whether their distribution is well approximated by the standard normal distribution (see e.g. Rigby and Stasinopoulos, 2005). Yet, contrary to ordinary least square regression, the raw response residuals  $r = P - \mu$  cannot be used, because they do not account for the heteroscedasticity of the model (i.e. the variance of *P* is a function of the Beta mean  $\mu$ , see Sect. 2.1).

In the following, we propose to keep the analysis of r in order to give information regarding the capability of the Beta mean to explain P. However, to properly validate the use of the Beta model, we rely on alternative residuals' formulations (see e.g., Pereira, 2019 and references therein). We focus here on three of the most widely-used ones described in Appendix D. The normality of these residuals is investigated by means of the normal Q-Q plot and by computing the coefficient of determination  $R^2$  as follows:

301

302 
$$R^2 = 1 - \frac{\sum_{i=1}^{i=N} (\hat{q}_i - q_i)^2}{\sum_{i=1}^{i=N} (q_i - \bar{q})^2}$$
 (Eq. 5)

303

where *N* is the number of quantile levels;  $q_i$  is the quantile of standard normal distribution at the i<sup>th</sup> level;  $\bar{q}$  is the mean of the quantile of standard normal distribution over the levels i=1...*N*;  $\hat{q}_i$  is the quantile of BBR residual at the i<sup>th</sup> level. The closer  $R^2$  to one, the better the agreement between the BBR residuals' quantiles and the ones of the standard normal distribution, hence the more satisfactory the adequacy of the BBR model. Furthermore, studying the evolution of *R*<sup>2</sup> as function of the number of random perturbations of *C* provides an option to estimate the minimum number of required permutations for the BBR model to be valid.

It should however be underlined that the residuals are analysed with the objective of checking that the Beta distribution is an appropriate model to explain the BBN-derived probabilities. Using them for another objective, for instance to compare different probability model families (e.g. Gamma, Gaussian) or to perform predictions, is made difficult by the use of boosting algorithms (see Hofner et al., 2016: Sect. 5.4). For these purposes, the use of the out-of-bag risk is recommended.

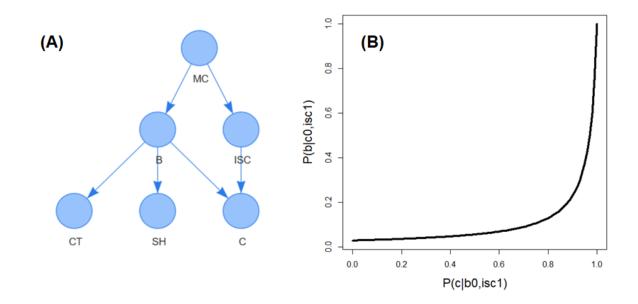
317

# 318 **3 Synthetic case study**

319 In this section, we consider a BBN of small number of nodes (described in Sect 3.1) to 320 exemplify the functionalities of the proposed approach (Sect. 3.2).

#### 321 3.1 Description

- We focus on the BBN adapted by van der Gaag et al. (2013) from Cooper (1984) in the field of
- 323 oncology. The network (as depicted in Fig. 2A) is composed of 6 nodes and 6 arcs.



324

Figure 2. A) Brain tumor structure network; B) Sensitivity function derived by van der Gaag et al. (2013)
showing the evolution of the probability of interest P(b/c0,isc1) as a function of the CPT entry
P(c/b0,isc1).

328

329 Node MC refers to metastatic cancer, which may potentially lead to the development of a brain 330 tumour (node B) and may give rise to an increased level of serum calcium (node ISC). The 331 presence of a brain tumour can be established from a CT scan (CT). Another indicator of the 332 presence of a brain tumour can be related to severe headaches (SH). A brain tumour or an 333 increased level of serum calcium are both likely to cause a patient to fall into a coma (C). The 334 conditional probabilistic relationships between the nodes (CPT entries) are provided in Table 335 1. We focus here on the probability P=P(b|c0,isc1), namely the probability to develop brain 336 tumor given the absence of coma and an increased level of serum calcium. The robustness of P 337 is studied with respect to the values of 13 CPT entries (Table 1).

338

339

[Table 1 about here]

#### 340 **3.2** Application

341 We now apply the proposed BBR approach. It starts with the random sampling of the 13 CPT 342 entry values using Gaussian distributions (with a standard deviation of 0.1 for all the 13 CPT 343 values) truncated at zero and one as proposed by van der Gaag et al. (2013). For each of the 344 randomly generated values of the CPT entries, the probability of interest P, i.e. P(b|c0,isc1), is 345 calculated through approximate Bayesian inference based on particle filter using logic sampling 346 (Koller and Friedman 2009). These values are then transformed using Eq. 3. 347 The minimum number of random perturbations of the BBN was chosen by studying the evolution of the  $R^2$  indicator values for the different residuals' formulations (see Sect. 2.3). Fig. 348

349 3A shows that the convergence can be considered reached for a minimum number of ten times

350 the number of CPT entries, i.e. 1,300 for which the  $R^2$  values all reach very satisfactory values

351 above 95%. The visual inspection of the normal Q-Q plots in Fig. 3B-D confirms the

satisfactory adequacy of the BBR model. We can however note some deviations for very lowquantile values but this is only indicated by one residuals' formulation (Fig. 3C). Besides,

taking into account the 95% confidence band (outlined by dashed lines in Fig. 3C), this

355 discrepancy can be considered low.

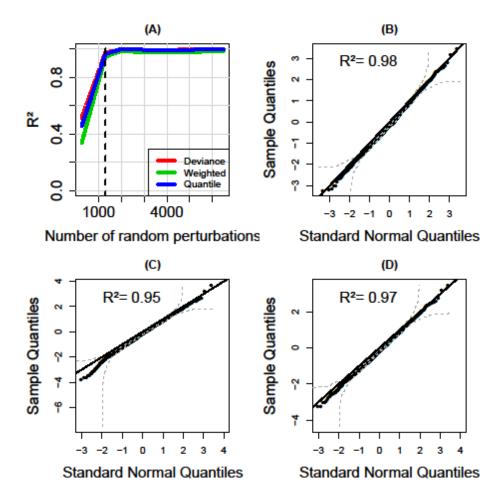


Figure 3. (A) Evolution of the R<sup>2</sup> indicator as a function of the number of random perturbations for the brain tumor BBN. Three residuals' formulations are considered (see Appendix D). The vertical dashed line indicates the selected number of random perturbations. For this number, normal Q-Q plots are provided considering different residuals: (B) deviance; (C) standardized weighted; (D) quantile. The dashed lines indicate the boundaries of the 95% confidence band based on the Kolmogorov-Smirnov statistic (Doksum and Sievers, 1976). The value of the R<sup>2</sup> indicator (Eq. 5) is also reported.

356

364 The histogram of the probability of interest P values is provided in Fig. 4A with mean and 365 standard deviation at respectively 0.18 and 0.14. Fig. 4B shows that the Beta mean is 366 informative regarding P and satisfactorily explains P, which is in agreement with the analysis 367 of the Q-Q plots (Fig. 3). Some deviations can however be noticed for very large values, but 368 may be related to the low number of data to perform the fitting (see the light colour in Fig. 4B 369 indicating a low density of dots). The optimal stopping iteration of BBR model is selected by a 370 5-fold cross validation procedure (combined with the noncyclic algorithm of Thomas et al., 371 2018) as illustrated in Fig. 4C.

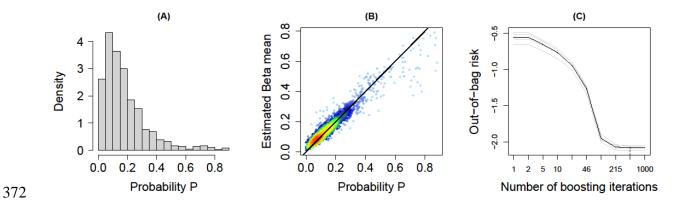
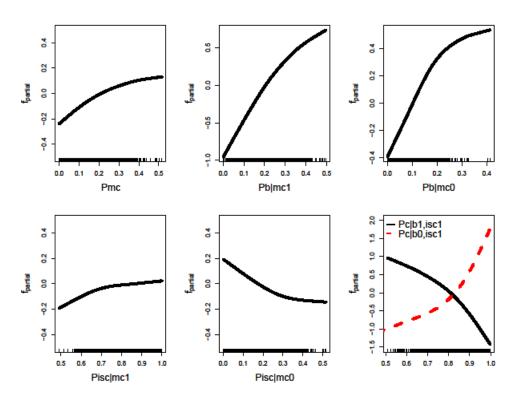


Figure 4. (A) Histogram of randomly generated P values for the brain tumor network; (B) Comparison
between the estimated Beta mean and P (the colours indicate the density of the dots); (C) Evolution of
the (out-of-bag) risk estimated using a 5-fold cross-validation procedure as a function of the number of
boosting iterations; the optimal stopping iteration is selected as the one minimizing the average risk
over all 5 cross-validation iterations (indicated by a vertical dashed line at 464).

Figure 5 and 6 respectively depicts the non-linear effects on  $\mu$  (logit-transformed) and  $\sigma$  (logittransformed) of the CPT entries selected by the boosting algorithm during the fitting of the BBR model. Different conclusions regarding the sensitivity of *P* to the CPT entries can be drawn:

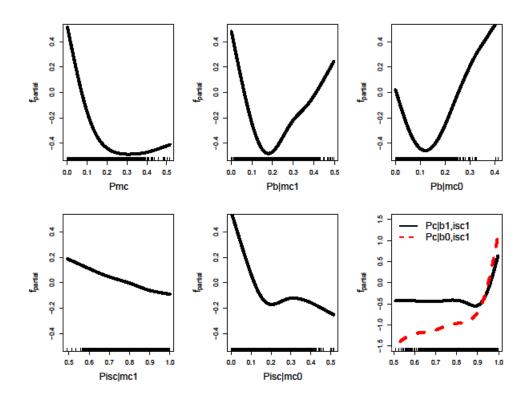
- Information on the importance ranking of the CPT entries can be derived. We show that
  only 7 out of the 13 CPT entries have been selected by the boosting algorithm, namely
  the CPT entries related to the nodes MC, ISC and C in direct relation with node B (see
  Fig. 2A);
- The individual contributions of the selected CPT entries in Figure 5 and 6 are global in
   the sense that they are constructed by accounting for the co-variations of all inputs
   (contrary to the traditional SA using sensitivity functions, which imposes the
   construction of the function by varying one input one at a time);
- 390-Information on the type of effect the CPT entries can be derived. We show that the CPT391entries' effect on the Beta mean  $\mu$  (logit-transformed) is monotonic but rarely linear. In392particular, the effect of P(c|b0,isc1) almost follows an exponential-like trend (outlined393by dashed red lines in Fig. 5, bottom right hard corner), which is in agreement with the394traditional SA of P (Fig. 2B) using a sensitivity function of polynomial form (as derived395by van der Gaag et al. 2013);

 $\begin{array}{rcl} 396 & - & \text{The effect on the Beta parameter } \sigma(\text{logit-transformed}) \text{ is also nonlinear with respect to} \\ 397 & & \text{the selected CPT entries, hence indicating that the CPT entries not only affect the best} \\ 398 & & \text{estimate of } P \text{ but also its precision, i.e. dispersion of the underlying Beta law.} \end{array}$ 



401 Figure 5. Partial effect of each CPT entry on  $\mu$  (logit-transformed) applied to the brain tumor network.

*Note the different scales of the x- and y-axis.* 



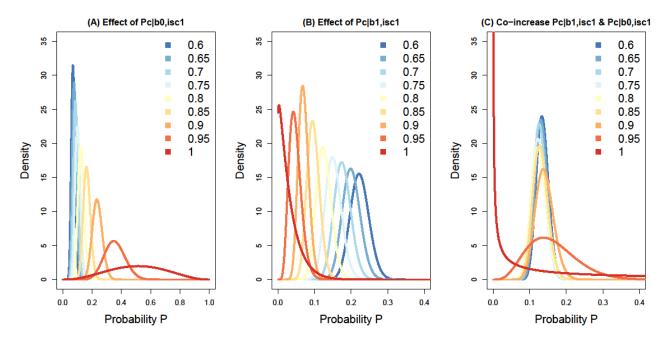
404 Figure 6. Partial effect of each CPT entry on σ(logit-transformed) applied to the brain tumor network.
405 Note the different scales of the x- and y-axis.

403

407 Since the partial effects in Fig. 5 and 6 are global, these can easily be used by varying each CPT 408 entries one-at-a-time or jointly. Figure 7(top) depicts the results of such analysis considering 409 the individual variation of P(c|b1,isc1) and of P(c|b0,isc1) on the Beta density function related 410 to *P* (while keeping the other CPT entry values at their original values as provided in Table 1). 411 When P(c|b0,isc1) is varied from low to high values (Fig. 7A), the corresponding Beta 412 density function is translated from low to high values, but with more and more 413 dispersion around the mode, which is more specifically amplified when P(c|b0,isc1) 414 exceeds value of  $\sim 0.9$ ;

When P(c|b1,isc1) is varied from low to high values (Fig. 7B), the effect on the Beta mode is opposite to the one due to the effect of P(c|b0,isc1). This exemplifies the decreasing trend outlined in Fig. 5 (bottom right hand corner): the mode is translated from high to low values with an effect on the dispersion less pronounced than for P(c|b0,isc1). This is in agreement with the lower partial effect outlined in Fig. 6(bottom right hand corner);

Finally, Figure 7C depicts the result of the analysis when both CPT entries are jointly
varied. This shows that the impact of both CPT entries is compensated when they are
jointly increased similarly: the Beta distributions remains "stuck" around 0.15 unless
both CPT entries reach very high values above 0.95.



425

Figure 7. (A) Evolution of the Beta law fitted to the P values given increasing values of P(c/b0,isc1)
from low (0.6) to high values (1.0); (B) Evolution of the Beta law fitted to the P values given increasing
values of P(c/b1,isc1) from low (0.6) to high values (1.0); (C) Evolution of the Beta law fitted to the P
values given increasing values (with same increment) of both P(c/b1,isc1) and P(c/b0,isc1).

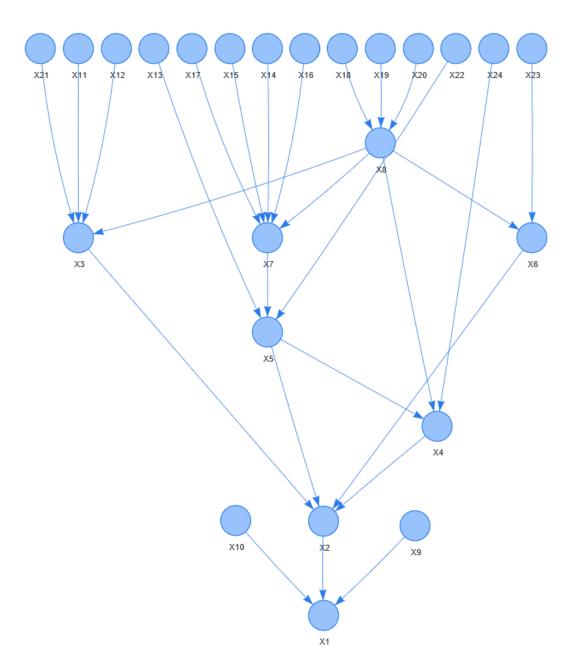
430

# 431 **4 Real-case applications**

In this section, we apply the BBR approach to real cases. First, a linear Gaussian BBN is considered for assessing the damage of reinforced concrete structures (Castillo and Kjærulff, 2003). This enables us to illustrate a situation where the number of parameters is large enough to hamper the interpretation, i.e. here more than 40 variables have to be processed (Sect. 4.1). Second, a discrete BBN is considered for reliability analysis. For this case, analytical sensitivity functions can hardly be derived since the interest is not the sensitivity to the values of the CPT entries directly, but the physical parameters, which determine them.

## 439 4.1 Reinforced-Concrete BBN

440 We investigate the robustness of the BBN presented in Castillo and Kjærulff (2003) for 441 assessing the damage of reinforced concrete structures (Fig. 8).



442

443 *Figure 8. Structure of the reinforced concrete network.* 

444

The BBN is composed of 24 continuous nodes, 27 arcs and more than 40 parameters. The random variables (see nodes' meaning in Table 2) are assumed to be normally distributed.

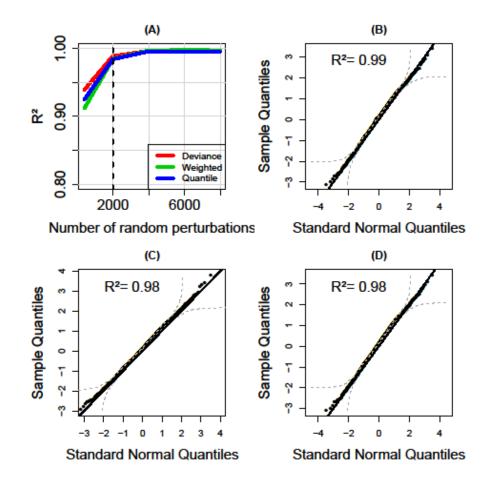
447

# [Table 2 about here]

449

450 The original parametrization of Castillo and Kjærulff (2003) follows the regression model in 451 Eq. 1 and assumes zero mean for all variables (i.e. nil intercept  $m_0$ ), and conditional standard 452 of 1.0 for observable nodes (i.e.  $X_9$ - $X_{24}$ ) and 1e<sup>-4</sup> otherwise (term denoted s<sub>0</sub> in Table 3). Values for the regression coefficients are provided in Table 3. In the following, we refer to these values 453 454 as the CPM best estimate for the BBN parametrization. 455 We investigate the robustness of the probability for the damage of the system  $X_1 \ge 1$  given the 456 evidence that the beam is weak  $X_{9} \ge 1$ , i.e.  $P = P(X_{1} \ge 1 | X_{9} \ge 1)$ . The CPM best estimates provided 457 in Table 3 are randomly perturbed using Gaussian laws truncated at zero (with mean correspond 458 to the values given in Table 3, standard deviation of 0.2 for the regression coefficients and of 459 0.5 for the intercept terms). In total 43 variables are considered. 460 461 [*Table 3 about here*] 462 463 Fig. 9A depicts the evolution of the  $R^2$  indicators considering the different residuals' formulations. This shows that a minimum of 2,000 random perturbations is required to consider 464 the BBR model adequate with  $R^2$  values above 98%. This is also confirmed by the visual 465

466 inspection of the normal Q-Q plot in Fig. 9B-D.





468 Figure 9. (A) Evolution of the  $R^2$  indicator as a function of the number of random perturbations for the

469 reinforced-concrete BBN. Three residuals' formulations are considered (see Appendix D). The vertical

470 dashed line indicates the selected number of random perturbations. For this number, normal Q-Q plots

471 are provided considering different residuals: (B) deviance; (C) standardized weighted; (D) quantile.

472 The dashed lines indicate the boundaries of the 95% confidence band based on the Kolmogorov-Smirnov

473 statistic (Doksum and Sievers, 1976). The value of the R<sup>2</sup> indicator (Eq. 5) is also reported.

474

Fig. 10A depicts the corresponding histogram of the randomly generated *P* values (with mean of 0.8 and standard deviation of 0.08). Fig. 10B shows that the Beta mean is very informative with a good agreement with *P*. The optimal stopping iteration of the regression model is selected based on a 5-fold cross validation procedure combined with the noncyclic algorithm as illustrated in Fig. 10C.

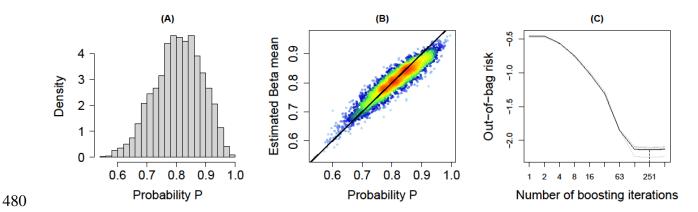
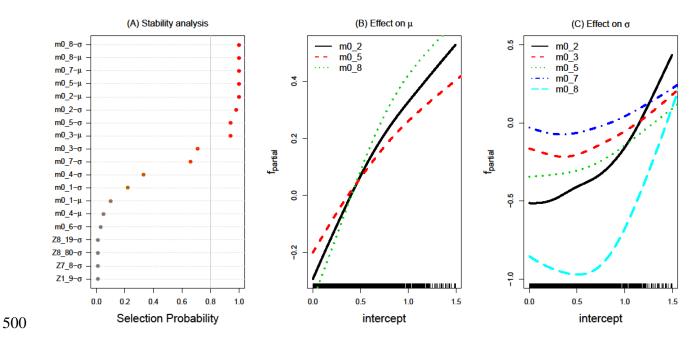


Figure 10. (A) Histogram of randomly generated P values for the concrete network; (B) Comparison between the estimated Beta mean and P (the colours indicate the density of the dots); (C) Evolution of the (out-of-bag) risk estimated using a 5-fold cross-validation procedure as a function of the number of boosting iterations; the optimal stopping iteration is selected as the one minimizing the average risk over all 5 cross-validation iterations (indicated by a vertical dashed line at 251).

487 The number of parameters of the conditional probability model is larger (almost four times) 488 than the case described in Sect. 3. In this case, despite the regularisation associated to the 489 boosting algorithm, the resulting BBR model can still remain too rich to be easily interpretable 490 by BBN practitioners. The direct application of the boosting algorithm ends up here with more 491 than 30 variables, i.e. analysing each of the partial effect may here not be practical. Therefore, 492 the analysis is completed by the stability selection analysis (described in Appendix C) to further 493 screen the most influential variables in the BBR model. Fig. 11A depicts the selection 494 probabilities for each CPM parameter with a threshold at 0.8 (see parametrisation in Appendix 495 C). This shows that only the intercept terms for node X<sub>2</sub>, X<sub>5</sub> and X<sub>8</sub> appear to be influential with 496 respect to the Beta mean  $\mu$  (logit-transformed), whereas only the intercept terms for node X<sub>2</sub>, 497 X<sub>3</sub>, X<sub>5</sub>, X<sub>7</sub> and X<sub>8</sub> appear to be influential with respect to the Beta parameter  $\sigma$  (logit-498 transformed). Interestingly, the nodes which affect the probability of interest are not necessarily 499 the ones in direct connections with  $X_1$  (see Fig. 8).



501 Figure 11. (A) Selection probability for each CPM parameter of the concrete network derived from the 502 stability selection analysis (Appendix C). (B) Partial effect of the intercept  $m_0$  of nodes  $X_2$ ,  $X_5$  and  $X_8$  on 503  $\mu$  (logit-transformed). (C) Partial effect of the intercept  $m_0$  of nodes  $X_2$ ,  $X_3$ ,  $X_5$ ,  $X_7$  and  $X_8$  on the  $\sigma$ 504 parameter (logit-transformed).

506 The non-linear effects for each selected CPM parameters are depicted in Fig. 11B,C. This shows 507 that the individual effect mainly corresponds to an increasing monotonic functions considering 508 both parameters of the Beta distribution; with a higher nonlinear effect of  $m_0$  of node X<sub>8</sub>. This 509 is confirmed by the Beta distribution's evolution with respect to the intercept parameter of node 510 X<sub>2</sub> and X<sub>8</sub> (Fig. 12A, B).

- 511 Fig. 12A shows that the increase of  $m_{0_2}$  mainly affects the increase of the best estimate 512 of *P* (with only slight effect on the dispersion), whereas Fig. 12B both affects the best 513 estimate and the dispersion, i.e. the larger  $m_{0_8}$ , the larger the mean value of *P* (i.e. the 514 riskier the situation), but also the larger the uncertainty on *P* (i.e. the occurrence of the 515 risky situation remains uncertain);
- 516 Fig. 12C shows the evolution of the Beta's distribution when both parameters are 517 increased similarly: we see that the combined increase amplifies the translation of the 518 Beta's distribution to very high values, i.e. risky situations (driven by both increasing 519 effects as shown in Fig. 12B). Despite the increase in  $\sigma$  during this process, the 520 occurrence of this risky situations remains of moderate-to-high confidence, which

521 suggests that changes in  $m_{0.8}$  and  $m_{0.2}$  might ultimately lead to the failure of the concrete 522 system.

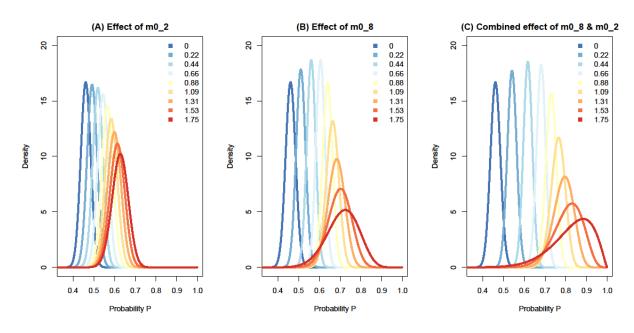


Figure 12. (A) Evolution of the Beta law fitted to the P values given increasing values of the intercept m<sub>0</sub> of node  $X_2$  from low (0.) to high values (1.75); (B) Evolution of the Beta law fitted to the P values given increasing values of the intercept m<sub>0</sub> of node  $X_8$  from low (0.) to high values (1.75); (C) Evolution

527 of the Beta law fitted to the P values given increasing values (with same increment) of both intercepts.

528

523

## 529 4.2 BBN-based reliability assessment

530 Figure 13 depicts the BBN constructed by Gehl and Rohmer (2018) for studying the problem 531 of station blackout (node SYS) following an earthquake at a given nuclear power plant (NPP) sub-system. The earthquake event is characterised by two intensity measures (nodes IM1 and 532 533 IM2 respectively corresponding to the peak ground acceleration and the spectral acceleration 534 at the first vibration period of the structure). The NPP sub-system is composed of a 5-story 535 reinforced-concrete structure hosting two emergency diesel generators (EDGs). Three damage 536 events (STR for structural damage and EDG for failure of the anchorage of the generators) are 537 considered.

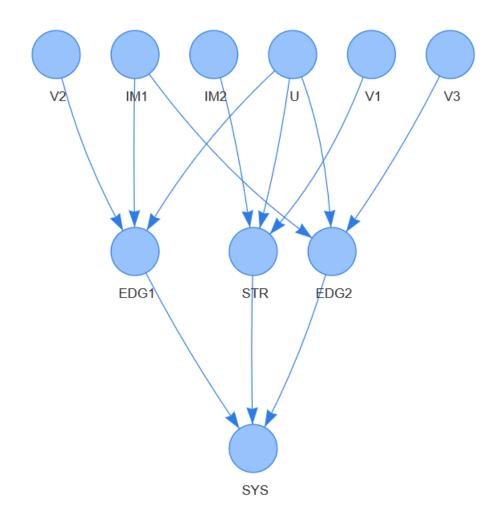


Figure 13. Structure of the network for studying the NPP subsystem reliability; IM1 and IM2 are
deterministic nodes representing intensity measure characterizing the earthquake event; Nodes U, V1,
V2 and V3 are zero-centered Gaussian random variables used to incorporate correlation. Only the
sensitivity to the parameters for the blue nodes is investigated.

543

544 The conditional probabilities of the failure states of STR, EDG1 and EDG2 are estimated 545 through fragility functions (i.e. probabilistic model that relates the failure probability to the 546 intensity measure IM), which are derived from non-linear seismic time histories applied to the 547 structure. Due to the observed statistical dependence between the failure events (i.e., due to the 548 common seismic loading applied to the three components), auxiliary variables U, V1, V2 and 549 V3 (described by a standard normal distribution) are added to the BBN following the approach 550 by Gehl and D'Ayala (2016). These variables result from the Dunnett-Sobel decomposition of 551 the correlation coefficients between the safety factors of the components as follows:

552 
$$Z_i = t_i \cdot U + \sqrt{1 - t_i^2} \cdot V_i$$
 (Eq. 6)

where  $Z_i$  is the standard score of the safety factor of component *i* ( $Z_1$  corresponds to STR,  $Z_2$  to EDG1, and  $Z_3$  to EDG2) and  $t_i$  is the Dunnett-Sobel coefficient that approximates the correlation between the failure events.

556 By definition, the failure of component *i* occurs if  $Z_i \leq -\beta_c$ , where  $\beta_c$  is the reliability index 557 expressed as follows:

558

559 
$$\beta_c = \frac{\alpha_i - \ln im}{\beta_i}$$
 (Eq. 7)

560

where  $\alpha_i$  and  $\beta_i$  are the fragility parameters (median and standard dispersion) of component *i*, under the common assumption of a cumulative lognormal distribution for the fragility function; *im* is the value of the intensity measure of interest (IM1 for EDG1 and EDG2, IM2 for STR, see Fig. 13).

Based on this framework, the CPT of the failure event of a component *i* is built by considering all combinations of discretized values {*im*; *u*; *v<sub>i</sub>*}, and by checking the following condition (Gehl and D'Ayala, 2016):

568

569 
$$\left(z_i = t_i \cdot u + \sqrt{1 - t_i^2} \cdot v_i\right) \le -\frac{\alpha_i - \ln im}{\beta_i}$$
 (Eq. 8)

570

571 For the sensitivity analysis, we do not consider the value of the CPT entries directly but the 572 physical parameters, which determine them, namely the parameters of the fragility curves, 573 (mean  $\alpha$  and standard deviation  $\beta$ ). The numerical values of the physical parameters considered 574 in this application are detailed in Table 4. The fragility curves' parameters were randomly 575 perturbed via a zero-centered Gaussian noise with standard deviation that is 10% of the original 576 values (termed as CPM best estimates in the following). For the parameters of Dunnett-Sobel 577 decomposition, the Gaussian noise is truncated at one. The probability of interest is here the 578 probability of the sub-system failure, i.e. P=P(SYS=1) given an earthquake event characterised

579	by intensity measures IM1 and IM2 of respectively 10 and 12.5 m <sup>2</sup> /s. In total, 9 parameters are
580	considered.
581	
582	[Table 4 about here]
583	
584	The selection of the minimum number of random perturbations is more difficult than for the
585	brain tumour or for the reinforced concrete case. Fig. 14A shows that at least 1,000 random
586	perturbations are necessary to reach $R^2$ values above 95%, but due to oscillations in the
587	evolution of the $R^2$ values, we preferably choose the largest number, i.e. >4,000. The visual
588	inspection of the normal Q-Q plots (Fig. 14C-D) also reveals some deviations for very high and
589	low quantiles (outside the range [-2 - 2]) though it should be noted that they remain within the
590	95% confidence band and with low-to-moderate magnitude. Contrary to the brain tumour case,
591	the three residuals' formulations all agree on the identification of the problem. A deeper
592	analysis show that these deviations correspond here to Beta distributions with very high mean
593	and very low variance values: the sensitivity should be analysed with care for these cases.

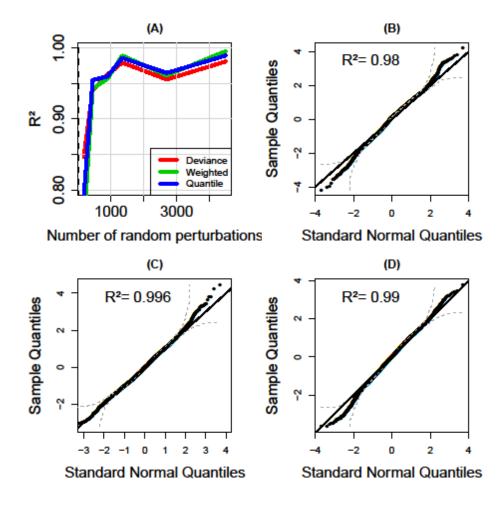


Figure 14. (A) Evolution of the R<sup>2</sup> indicator as a function of the number of random perturbations for the BBN-based reliability assessment. Three residuals' formulations are considered (see Appendix D). The vertical dashed line indicates the selected number of random perturbations. For this number, normal Q-Q plots are provided considering different residuals: (B) deviance; (C) standardized weighted; (D) quantile. The dashed lines indicate the boundaries of the 95% confidence band based on the Kolmogorov-Smirnov statistic (Doksum and Sievers, 1976). The value of the R<sup>2</sup> indicator (Eq. 5) is also reported.

594

The histogram of *P* values is provided in Fig. 15A with mean and standard deviation at respectively 0.65 and 0.26. Contrary to the reinforced-concrete BBN, the agreement with *P* is less satisfactory (Fig. 15B). A major part of the *P* values (see the warm colour indicating the density of dots in fig. 15B) appear to be reproduced by the Beta mean, but the scatter plot remains disperse. This type of analysis can be considered a complement to the analysis of the Q-Q plots (Fig. 14) and supports a cautious attitude with respect to the conclusions drawn from the sensitivity analysis. The optimal stopping iteration of the regression model is selected based

on a 5-fold cross validation procedure combined with the noncyclic algorithm as illustrated in

611 Fig. 15C.

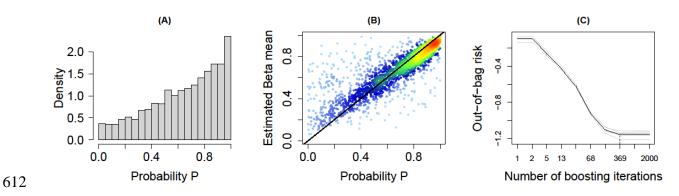


Figure 15. (A) Histogram of randomly generated P values for the NPP reliability network; (B)
Comparison between the P values and the estimated mean value provided by the Beta model; (C)
Evolution of the (out-of-bag) risk estimated using a 5-fold cross-validation procedure as a function of
the number of boosting iterations; the optimal stopping iteration is selected as the one minimizing the
average risk over all 5 cross-validation iterations (indicated by a vertical dashed line at 369).

618

The application of the boosting algorithm reveals that only the parameters of the fragility curves are selected. These are the only parameters identified as significant by the BBR approach, i.e. the correlation parameters  $t_{1-3}$  are discarded by the algorithm. Figure 16 provides the corresponding partial effects for both Beta law parameters.

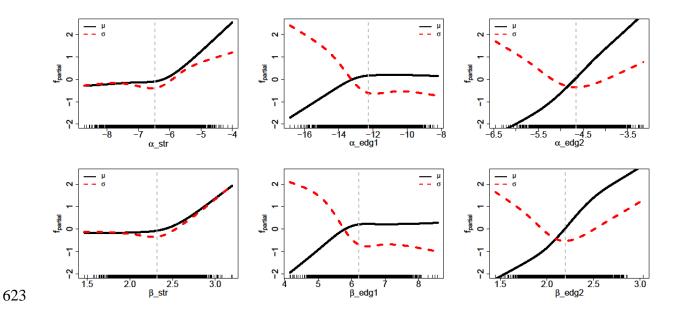


Figure 16. Partial effect of the fragility curve's parameters on  $\mu$  (logit-transformed) (black straight line) 625 and on  $\sigma$  (logit-transformed) (red dashed line). The vertical grey-coloured dashed line indicates the

627

626

628 Several observations can be made:

CPM best estimates of Table 4.

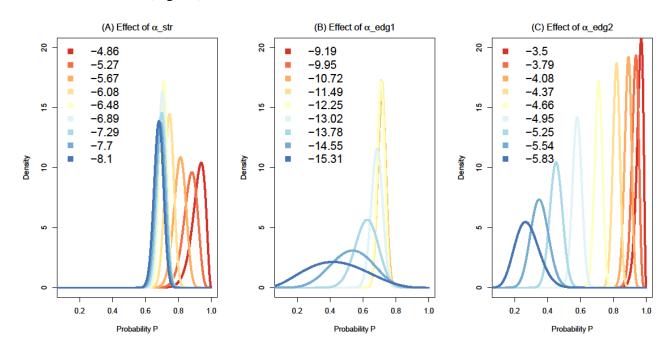
629 The parameters ( $\alpha$ \_str,  $\beta$ \_str) of the structural fragility curve (STR, Fig. 16, left) have 630 almost similar effect, whatever the Beta law parameter (logit-transformed); it 631 corresponds to a quasi- bilinear function, which remains quasi-constant below the CPM 632 best estimate then increases above it; from a risk viewpoint, this means that the damage 633 to the structure enhances the occurrence of risky situations, where the system failure's probability *P* might reach high values. Yet, the effect on  $\sigma$  parameter (logit-transformed) 634 also indicates that the confidence in the occurrence of this probabilistic regime is low; 635

The effects of the parameters ( $\alpha$  edg2,  $\beta$  edg2) of the second electrical generator's 636 637 fragility curve (EDG2, Fig. 16, right) are quasi-linear with respect to the Beta law mean 638  $\mu$ , but is non-monotonic with respect to the  $\sigma$  parameter (logit-transformed). This can 639 be schematically understood as a decrease of uncertainty on P (i.e. the Beta law 640 dispersion) when approaching the original value, then an increase above it;

641 The effect of the parameters ( $\alpha_{edg1}, \beta_{edg1}$ ) of the first electrical generator's fragility \_ curve (EDG1, Fig. 16, center) is more complex. The effect on the Beta mean  $\mu$  (logit-642 transformed) corresponds to a bilinear function, which increases at around the CPM best 643 644 estimate, then remains quasi-constant above it (i.e. to a lesser extent, it corresponds to 645 the opposite behaviour to the one for STR). The effect on the Beta parameter  $\sigma$ 646 corresponds to an inverted sigmoid, which reaches its lower horizontal plateau above 647 the CPM best estimate. This means that above their original values, parameters ( $\alpha_{edg1}$ ,  $\beta$  edg1) little affect the system failure's probability. 648

649 Fig. 17 illustrates how  $\alpha_{str}$ ,  $\alpha_{edg1}$  and  $\alpha_{edg2}$  act differently on the system failure. When 650 increasing  $\alpha$  str, the system failure starts increasing only for values well above the CPM best 651 estimates. This is shown by the Beta distributions, which remains "stuck" at moderate values 652 (around 0.6; see for cold colours in Fig. 17A). When increasing  $\alpha$  edg1, the resulting Beta distribution remains stuck at high value around 0.70-0.75 (note the evolution of the mode for 653 654 warm colours in Fig. 17B), hence leading to risky situations. The confidence in the occurrence

of such probabilistic regime is high as indicated by the low dispersion of the Beta distributions. When increasing  $\alpha_{edg2}$ , the Beta distribution continues to translate towards very high values above 0.90. Despite the very low dispersion of the Beta distribution, the confidence remains here moderate, because this situation corresponds to the one for which the normality of the residuals is not met (Fig. 14).



660

Figure 17. Evolution of the Beta distributions fitted to the P values given: (A) increasing values of the mean value of the fragility curve  $\alpha_{str}$ ; (B) increasing values of  $\alpha_{edg1}$ ; (C) increasing values of  $\alpha_{edg2}$ .

664

# 665 **5 Discussion**

Ensuring the validity and credibility of increasingly complex BBN-based expert systems 666 667 (Pitchforth & Mengersen, 2013; Kleemann et al., 2017; Marcot and Penman, 2019) requires a broad vision on the sensitivity to the CPM parameters. As outlined in the introduction, the most 668 669 widely used approach is based on sensitivity functions for discrete BBNs, and on partial 670 derivatives for continuous BBNs. Reasons are the intuitive interpretation of the results (thanks 671 to the graphical presentation) and the simplicity of the implementation. Yet, these approaches 672 only provide information on the local influence, in the sense that the parameters are varied "one-673 at-a-time". This means that it can only provide a restricted vision on sensitivity, because the 674 exploration of the sensitivity remains limited to a few CPM parameters, while the domain of 675 the other CPM parameters is left mostly unexplored (as thoroughly discussed by Saltelli et al.

(2019) with respect to sensitivity analysis practices). Multi-way SA methods have been
proposed (Leonelli et al., 2017; Gómez-Villegas et al., 2013), but they can rapidly become
intractable.

In this context, the proposed BBR approach can be considered more complete by providing global insight on the sensitivity by means of the partial effects (Fig. 4,10,13,14), which directly show the individual, possibly non-linear, effects of all CPM parameters. In Sect. 4, we have shown how the BBR approach can provide richer information than existing methods at multiple levels:

- Level (1): it selects the most influential parameters and it screens those that are of
   negligible influence (information that is generally unknown a priori);
- 686 Level (2): it provides the functional relation between the CPM parameters and the result
  687 of the probabilistic query. The proposed approach builds on a graphical presentation of
  688 the results, which eases the interpretation;
- Level (3): the practitioner can study how the combined effect of the CPM parameters
   can lead to different probabilistic regimes (e.g., situations of high probability values) by
   studying the evolution of the Beta mean. Furthermore, the practitioner can measure the
   confidence in the occurrence of the identified probabilistic regimes, by studying the
   effect on the Beta σ parameter.

Table 5 provides a summary of the strengths and weaknesses of the BBR approach with comparison to the approach based on sensitivity functions.

- 696
- 697

[Table 5 about here]

698

699 From an operational viewpoint, we tested the applicability of the BBR approach using different 700 application cases covering a large spectrum of situations, namely (1) a small discrete BBN, 701 used to capture medical knowledge, to exemplify the functionalities; (2) a linear Gaussian BBN, 702 used to assess the damage of reinforced concrete structures, exemplifies a case where the 703 number of parameters is too large to be easily processed and interpreted (>40 parameters); (3) 704 a discrete BBN, used for reliability analysis of nuclear power plant, exemplifies a case where 705 analytical solutions for sensitivity can hardly be derived. To ease the implementation, we 706 proposed a procedure based on random experiments, i.e. the BBN-based results are derived from randomly generated values of the CPM parameters. This procedure is generic, because it
can be applied to any CPM parameters whatever the type of the considered BBN: discrete (with
CPT entries), continuous (with regression coefficients), or hybrid.

However, it should be underlined that providing information on the global effect of the CPM parameters comes at the expense of a larger computational effort and complexity. The number of calls to the BBN inference engine is larger (typically >1,000) compared to the sensitivity functions, which may become problematic when the inference is difficult (hence time consuming) to perform.

715 The pillar of the BBR approach is the adequacy of the BBR model to explain the BBN-derived 716 probabilities. This adequacy should be carefully checked, and we propose here to investigate 717 the statistics of the residuals. In some situations, this might reveal situations where the 718 interpretation should be conducted with care as exemplified by the third application case. The 719 difficulties encountered for this case is also related to the characteristics of the sensitivity 720 analysis. Contrary to the brain tumour and to the reinforced concrete BBN, this case does not 721 consider the value of the CPM parameters directly, but the physical parameters that influence 722 them. This adds a level of complexity to the problem and make the BBR model more difficult 723 to fit.

Finally, it should be noted that the second application case shows that the BBR approach is robust even in the presence a large number of parameters (which can rapidly grow as a function of the number of BBN nodes). Yet, the applicability to complex cases with several hundreds of nodes (and thousands of parameters), like the pathfinder network (Heckerman et al., 1992), remains an open question especially regarding two aspects: (1) the capability of the combined "gradient boosting- stability selection analysis" to handle so many terms; (2) the complexity of the interpretation of the partial effects.

731

# 732 6 Summary and future research directions

The rapidly increasing advances of BBN for modelling of expert systems calls for the developments of robust methods for their validation and verification (e.g., Marcot and Penman, 2019). One major pillar to fulfil this purpose is sensitivity analysis. The proposed BBR approach broadens the scope of existing BBN sensitivity analysis methods by providing a larger vision (global) on the CPM influence. The approach has the advantage of being generic (it can be applied to any kind of BBN, i.e. discrete, Gaussian or hybrid), and robust to the number of
parameters (that can rapidly increase, typically reaching several dozens, even for moderate
number of BBN nodes).

741 Bringing the BBR approach to a fully operational state, raises different questions that should 742 be addressed in future work. The first line of future research should concentrate on the 743 intensification of the applicability tests using very large-scale BBNs. An important aspect to be 744 tested is the applicability to highly constraining situations where the number of variables largely 745 exceeds the size of the training database. In such cases, the performance of the stability selection 746 analysis should be more extensively investigated (see Meinshausen & Bühlmann, 2010; 747 Thomas et al., 2018). The second research direction should concentrate on improving the 748 interpretability of the results. The graphical representation of the partial effects is a strength of 749 the BBR approach but might lose its conciseness as the number of functional terms selected as 750 important largely increases (>100). We should take advantage of advances in distributional 751 regression methods that rely on trees like the one proposed by Grün et al. (2012) for Beta 752 regression. The presentation of the results using a network is expected to provide a more concise 753 and understandable presentation of the results. Finally, it should be underlined that the current 754 work has focused on only one part of the problem of uncertainties in BBNs. The CPM parameters constitute only one ingredient for BBN development; the second one being the DAG 755 756 specification, which has its own challenges as well, in particular when the learning is based on 757 data (see e.g., a comprehensive review by Heinze-Deml et al., 2018). To address the whole 758 spectrum of uncertainties in BBN building, sensitivity methods both covering DAG and CPM 759 learning would be beneficial. Again, a solution relying on trees is worth investigating, as 760 recently proposed to deal with psychometric networks (Jones et al., 2019).

761

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- the European Union's H2020-Euratom Programme under grant agreement N° 755439. The
- 765 analysis was performed using R packages bnlearn (available at: https://cran.r-
- 766 project.org/web/packages/bnlearn/index.html) for BBN building and queries, bnviewer
- 767 (<u>https://cran.r-project.org/web/packages/bnviewer/index.html</u>) for network visualisation, and
- 768 *gamboostLSS* (available at: <u>https://cran.r-project.org/web/packages/gamboostLSS/index.html</u>)
- for boosting of distributional regression model with BE() function of gamlss.dist package
- 770 (available at: <u>https://cran.r-project.org/web/packages/gamlss.dist/index.html</u>).

771

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- 906

## 907 Tables

908 Table 1. CPT entries for the brain tumor BBN. For instance P(c|b0,isc1) corresponds to the

909 probability of node C being in state 1 conditioned by the fact that node B is in state 0 and ISC

- 910 is in state 1. The meaning of the other probabilities should be understood following this
- 911 example.

NT 1		
Node	Conditional	
	probability	
MC	P(mc)=0.20	
В	P(b mc1)=0.20	
	P(b mc0)=0.05	
ISC	P(isc mc1)=0.80	
	P(isc mc0)=0.20	
С	P(c b1)=0.95;	
	P(c b1,isc1)=0.80	
	P(c b1,isc0)=0.80	
	P(c  b0,isc0)=0.05	
СТ	P(ct b1)=0.95	
	P(ct b0)=0.10	
SH	P(sh b1)=0.80	
	P(sh b0)=0.60	

912

913

Node	Description	
X1	Damage assessment	
X <sub>2</sub>	Cracking state	
X <sub>3</sub>	Cracking state in shear domain	
X4	Steel corrosion	
X5	Cracking state in flexure domain	
X <sub>6</sub>	Shrinkage cracking	
X <sub>7</sub>	Worst cracking in flexure domain	
X <sub>8</sub>	Corrosion state	
X9	Weakness of the beam	
X10	Deflection of the beam	
X <sub>11</sub>	Position of the worst shear crack	
X <sub>12</sub>	Breadth of the worst shear crack	
X <sub>13</sub>	Position of the worst flexure crack	
X14	Breadth of the worst flexure crack	
X15	Length of the worst flexure cracks	
X <sub>16</sub>	Cover	
X <sub>17</sub>	Structure age	
X <sub>18</sub>	Humidity	
X19	PH value in the air	
X <sub>20</sub>	Content of chlorine in the air	
X <sub>21</sub>	Number of shear cracks	
X <sub>22</sub>	Number of flexure cracks	
X <sub>23</sub>	Shrinkage	
X <sub>24</sub>	Corrosion	

- 916 Table 3. Definition of the CPM parameters of the concrete BBN; for instance  $m_{0_1}$ , is the
- 917 intercept of the regression model (Eq. 1) linking node  $X_1$  to its parents;  $Z_{1_2}$  is the regression
- 918 coefficient that models the relation between node  $X_1$  and  $X_9$ ;  $s_{0_1}$  is the corresponding standard
- 919 deviation.

Intercept	Regression	Standard
	coefficient	Deviation
<i>m</i> 0_1=0	Z1_9=0.3	<i>s</i> <sub>0_1</sub> =1e-4
	$Z_{1_2}=2$	
	$Z_{1_{10}}=0.$	
$m_{0_2}=0$	Z <sub>2_5</sub> =0.7	<i>s</i> <sub>0_2</sub> =1e-4
	Z <sub>2_4</sub> =0.5	
	Z <sub>2_6</sub> =0.3	
	Z <sub>2_3</sub> =0.7	
<i>m</i> <sub>0_3</sub> =0	Z <sub>3_8</sub> =0.3	<i>s</i> <sub>0_2</sub> =1e-4
	Z <sub>3_21</sub> =0.5	
	Z <sub>3_12</sub> =0.9	
	$Z_{3_{11}}=0.7$	
$m_{0_4}=0$	Z4_5=0.3	<i>s</i> <sub>0_4</sub> =1e-4
	$Z_{4_{24}}=0.7$	
	$Z_{4_8}=0.7$	
<i>m</i> 0_5=0	Z <sub>5_22</sub> =0.5	<i>s</i> <sub>0_5</sub> =1e-4
	$Z_{5_7}=0.9$	
	$Z_{5_{13}}=0.7$	
<i>m</i> <sub>0_6</sub> =0	Z6_23=0.3	<i>s</i> <sub>0_6</sub> =1e-4
	Z6_8=0.7	
<i>m</i> <sub>0_7</sub> =0	Z7_17=0.4	<i>s</i> <sub>0_7</sub> =1e-4
	Z7_16=0.4	
	Z <sub>7_15</sub> =0.6	
	Z <sub>7_14</sub> =0.6	
	Z7_8=0.6	
	$m_{0_{-1}}=0$ $m_{0_{-2}}=0$ $m_{0_{-3}}=0$ $m_{0_{-4}}=0$ $m_{0_{-5}}=0$ $m_{0_{-6}}=0$	$m_{0_1}=0$ $Z_{1_9}=0.3$ $Z_{1_2}=2$ $Z_{1_10}=0.$ $m_{0_2}=0$ $Z_{2_5}=0.7$ $Z_{2_4}=0.5$ $Z_{2_6}=0.3$ $Z_{2_3}=0.7$ $m_{0_3}=0$ $Z_{3_8}=0.3$ $Z_{3_11}=0.7$ $m_{0_4}=0$ $Z_{4_5}=0.3$ $Z_{4_8}=0.7$ $m_{0_5}=0$ $Z_{5_22}=0.5$ $Z_{5_7}=0.9$ $Z_{5_13}=0.7$ $m_{0_6}=0$ $Z_{6_8}=0.7$ $m_{0_7}=0$ $Z_{7_17}=0.4$ $Z_{7_15}=0.6$ $Z_{7_14}=0.6$

X8	$m_{0_{8}=0}$	$Z_{8_{20}}=0.8$	<i>s</i> <sub>0_8</sub> =1e-4
		$Z_{8_{19}}=0.9$	
		$Z_{8_{-}18}=0.5$	

# 922 Table 4. Parameters for constructing the CPT of the BBN-based reliability assessment

Parameter	Symbol	Original value
Mean and Standard deviation value of the log- normal fragility curve for STR	$\alpha_{\rm STR}, \beta_{\rm STR}$	-6.48, 2.32
Mean and Standard deviation of the log-normal fragility curve for EDG1	$\alpha_{\rm EDG1}, \beta_{\rm EDG1}$	-12.250, 6.22
Mean and Standard deviation of the log-normal fragility curve for EDG2	$\alpha_{\rm EDG2}, \beta_{\rm EDG2}$	-4.66, 2.20
Dunnett-Sobel decomposition's parameters	<i>t</i> <sub>1,2,3</sub>	0.914, 0.942, 0.999

Table 5. Summary of the strengths and weaknesses of the BBR method and of the approach

926 based on sensitivity functions.

Approach	Strengths	Weaknesses
Sensitivity function	It is simple to implement; It requires a low computational effort; The graphical representation is straightforward to interpret.	It is local: it focuses on the influence of one (or multiple) CPT parameters while the other ones are kept constant; It is restricted to the analysis of discrete BBNs; Multi-way SA can rapidly become intractable.
BBR	It provides insight in the global influence; It is simple to implement using random sampling, which is a generic procedure applicable to any types of BBNs; The results are intuitive to interpret based on a graphical presentation; It provides multilevel information on sensitivity; The combination of gradient boosting and stability selection increases the robustness to the number of parameters.	The number of calls to the BBN inference engine can be large (>1,000); The adequacy of the Beta model should be carefully checked; The demonstration of the applicability to very large-scale BBNs with hundreds of nodes and thousands of CPM parameters remains to be done.

#### Appendix A: Bayesian Belief Network Analysis 929

930 The analysis of Bayesian Belief Network relies on conditional probabilities. Consider X<sub>i=1,...,n</sub> 931 the *n* nodes of the BBN. The joint probability distribution can be expressed using conditional 932 probability as:

933

934 
$$P(X_1, X_2)$$

4 
$$P(X_1, X_2, ..., X_n) = \prod_{i=1}^n P(X_i | X_1, ..., X_{i-1})$$
 (Eq. A1)

935

936 This equation simplifies under the conditional independence assumption as:

937

938 
$$P(X_1, X_2, ..., X_n) = \prod_{i=1}^n P(X_i | Pa(X_i))$$
 (Eq. A2)

939 where  $Pa(X_i)$  corresponds to the parent nodes of  $X_i$ . For discrete nodes, the value of 940  $P(X_i | Pa(X_i))$  is the entry of the Conditional Probability Table. For continuous nodes,  $P(X_i | Pa(X_i))$  can be modelled by a continuous probability distribution whose parameters 941 942 depend on the values of the parent nodes.

943

944 Conditional queries aim at evaluating the conditional probability of some event, e.g. node  $X_i$ 945 takes up the value x when new information/observations become available, i.e. given new 946 "evidence" (denoted e), namely  $P(X_i = x | e)$ . This procedure, termed as query, relies on inference 947 techniques. Exact inference in a BBN is possible, but is generally not possible in large networks. 948 For networks, which contain a large number of nodes, arcs, or have nodes comprised of 949 variables with large numbers of levels, exact inference becomes too computationally intensive. 950 Among the possible approximate inference algorithms, the present study relies on the logic 951 sampling method (Koller and Friedman 2009), which works from the root nodes down to the 952 leaf nodes. First, a random draw from each of the leaf nodes is taken with probabilities equal to 953 the respective levels. The distributions for the next level of nodes can then be marginalized 954 based on the draws obtained from their parents. From these marginal distributions a random 955 draw is again taken respective of the categorical probabilities. This process is repeated until a 956 draw has been taken from every node in the network. This completed case represents a single 957 sample. After many samples have been taken, the samples are subsetted to the cases which 958 match the evidence of interest. Estimated probabilities can then be obtained for any node of 959 interest from this subset of the samples.

- 960
- 961

## 962 Appendix B: Gradient boosting within GAMLSS framework

We first describe the principles of model-based gradient boosting (Sect. B1), and describe howto apply it within the GAMLSS framework (Sect. B2).

#### 965 **B1 Gradient boosting**

This supervised learning technique (e.g., Bühlmann and Hothorn, 2007) combines an ensemble of simple regression models (termed as base-learners), such as linear regression models or regression splines of low degree of freedom, to estimate complex functional relationships. Consider the training dataset  $D = \{C^{(j)}, P^{(j)}\}_{j=1,...,n}$  where *C* is the vector of *p* predictor variables

970  $c_{i=1,...,p}$  and *P* is the variable of interest, whose expected value (possibly its transformed value) 971 is modelled by an additive model as follows:

972

973 
$$\eta(\mathbf{C}) = \beta_0 + \sum_{j=1}^J f_j(c_j | \beta_j)$$
 (Eq. B1)

974

975 where  $J \le p$ ,  $\beta_0$  is a constant intercept and the additive effects  $f_j(c_j | \beta_j)$  are pre-defined 976 univariate base-learners, which typically correspond to (semi-)parametric effects with 977 parameter vector  $\beta_j$ .

978 To estimate the parameters  $\beta_j$ , the boosting algorithm minimizes the empirical risk *R*, which 979 corresponds to the sum of loss function  $\rho$  over all training data:

980

981 
$$R = \sum_{j=1}^{n} \rho(P^{(j)}, \eta(\boldsymbol{C}^{(j)}))$$
 (Eq. B2)

982

where the loss function  $\rho$  can take different forms, such as the quadratic loss  $(P^{(j)} - \eta(\mathbf{C}^{(j)}))^2$ , which corresponds to the ordinary least square regression or more generally, it can correspond to the negative log-likelihood of the distribution of the variable of interest *P* (in the case considered here, this corresponds to the Beta distribution).

Among the different boosting algorithms, we focus on the component-wise gradient boosting approach of Bühlmann and Hothorn (2007). Instead of focusing on the true outcomes  $P = (P^{(1)}, P^{(2)}, ..., P^{(n)})$ , this procedure aims at fitting simple regression-type base learners h(.) one by one to the negative gradient vector of loss  $u = (u^{(1)}, u^{(2)}, ..., u^{(n)})$ . The objective is to approximate the j<sup>th</sup> effect  $f_j(c_j | \beta_j) = \sum_m h_j(.)$  at iteration *m* of the algorithm. Formally, *u* is evaluated 992 considering the current estimated (i.e. iteration *m*-1) additive predictor model  $\hat{\eta}^{[m-1]}(\boldsymbol{C}^{(j)})$  as 993 follows:

994

995 
$$\boldsymbol{u} = \left(-\frac{\partial}{\partial\eta}\rho(P,\eta)|_{\eta=\hat{\eta}^{[m-1]}(\boldsymbol{c}^{(j)}), P=P^{(j)}}\right)_{j=1,\dots,n}$$
(Eq. B3)

996

In every boosting iteration, each base-learner is fitted separately to the negative gradient vector.
The best-fitting base-leaner is then selected based on the residual sum of squares with respect
to *u* as follows:

1000

1001 
$$j^* = \underset{j \in 1, ..., J}{\operatorname{argmin}} \sum_{i=1}^n (u^{(i)} - h_j(\boldsymbol{C}^{(i)}))^2$$
 (Eq. B4)

1002

1003 The selected base-leaner is used to update the current predictor model as follows:

1004

1005 
$$\hat{\eta}^{[m]} = \hat{\eta}^{[m-1]} + s.h_{j*}(\mathcal{C})$$
 (Eq. B5)

1006 where s is a step length (with typical value of 0.1).

1007

The main tuning parameter is the number of iterations m, which directly determines the 1008 1009 prediction performance. If *m* is too large, rich models with large number of predictors and rough 1010 functional terms will be constructed (hence leading to overfitting), which might hamper the interpretability of the resulting model. If m is too low, sparse models with smooth functional 1011 1012 terms will be constructed but with the danger of missing some important predictor variables. In 1013 practice, the selection of m can be carried out using cross-validation procedures in order to 1014 optimize the predictive risk on observations left out from the fitting process i.e. the "out-of-1015 bag" risk which corresponds to the negative log-likelihood for the considered probabilistic 1016 distribution calculated for the "out-of-bag" samples.

1017

#### 1018 B2 Boosted GAMLSS

1019 The afore-described algorithm can be applied to the GAMLSS framework by cycling through 1020 the distribution parameters  $\theta$  in the fitting process (Thomas et al., 2018: Algorithm 1). In each 1021 iteration, the best fitting base-learner is evaluated for each distribution parameter, while the other ones remain fixed. For a probability distribution with two parameters (like the Beta
distribution), the update in the boosting algorithm at iteration *m* holds as follows:

1025 
$$\frac{\partial}{\partial \eta_{\theta_1}} \rho\left(P, \theta_1^{[m]}, \theta_2^{[m]}\right) \xrightarrow{\text{update}} \eta_{\theta_1}^{[m+1]}$$
 (Eq. B6)

1026 
$$\frac{\partial}{\partial \eta_{\theta_2}} \rho(P, \theta_1^{[m+1]}, \theta_2^{[m]}) \xrightarrow{\text{update}} \eta_{\theta_2}^{[m+1]}$$
 (Eq. B7)

1027

1028 In the original cyclic algorithm, (see algorithm 1 described by Thomas et al. (2018)), separate 1029 stopping values have to be specified for each parameter, which motivated the development of 1030 a noncyclic algorithm (algorithm 2 by Thomas et al. (2018)), which avoids optimizing two 1031 different stopping iterations and reducing the optimisation problem from a multi-dimensional 1032 to a one-dimensional problem.

1033

#### 1035 Appendix C: Stability Selection Analysis

1036 This appendix describes the procedure for stability selection (Meinhausen and Bühlmann, 1037 2010). Consider p predictor variables  $c_{j=1,...,p}$  and the predictand *P*. Based on n observations, the 1038 stability selection with boosting proceeds as follows:

- 1039 Step 1. Select a random subset of size [n/2] of the data (where [n/2] corresponds to the largest 1040 integer  $\leq n/2$ );
- 1041 Step 2. Fit a boosting model and continue to increase the number of boosting iteration until q
- 1042 base-learners are selected.  $\hat{S}_{[\frac{n}{2}]}$  corresponds to the set of selected variables;
- 1043 Step 3. Repeat steps 1 and 2 for  $b=1,\ldots,B$ ;
- 1044 Step 4. Compute the selection probabilities per base learner as follows:

1045 
$$P_{j} = \frac{1}{B} \sum_{b=1}^{B} \mathbf{I}_{\{j \in \hat{S}_{[\frac{n}{2}], b}\}}$$
(Eq. C1)

1046

1047 where **I**(A) is the indicator function, which reaches 1 if A is true, 0 otherwise.

1048 Step 5. Select all base-learners associated to a selection probability of at least *t*. The set of stable 1049 selected variables is thus  $\hat{S} = \{j: P_j \ge t\}$ .

Meinhausen and Bühlmann (2010) studied the error of selecting false positive variables (i.e.
noise variables) and showed that the selection procedure controls the per-family error rate
(*PFER*) and an upper bound is provided as follows:

1053

$$1054 \quad PFER \le \frac{q^2}{(2t-1)p} \tag{Eq. C2}$$

1055

where q is the number of selected variables per boosting iteration, p is the number of (possible) predictors and t is the selection threshold. In practice, at least two of these parameters have to be specified to run the procedure. In the application case of Sect. 4.1, we specified the upper bound of *PFER* (set up at 1) and q at 10. An extensive investigation of the applicability of this procedure for distributional regression within the boosted GAMLSS setting has been carried out by Thomas et al. (2018).

## 1062 Appendix D: Residuals for Beta regression

1063 The following appendix describes the main formulations of the residuals for Beta regression1064 based on Pereira (2019) and references therein.

- 1065 Let us consider the raw response residuals for the i<sup>th</sup> observation  $P_i$  defined as  $r_i = P_i \hat{P}_i$
- 1066 where  $\hat{P}$  is the mean  $\mu$  predicted by BBR model. For sake of presentation, let us consider the

1067 Beta parameter 
$$\varphi = \frac{1}{\sigma^2} - 1$$
 where  $\sigma$  is defined in Sect. 2.1

1068 The deviance residual is defined as:

1069 
$$r_i^{deviance} = r_i \cdot \sqrt{2|L(P,\varphi) - L(\mu,\varphi)|}$$
(Eq. D1)

1070 where the bivariate function L(.,.) holds as follows:

1071 
$$L(\mu, \varphi) = l\Gamma(\varphi) - l\Gamma(\varphi, \mu) - l\Gamma((1-\mu), \varphi) + (\mu, \varphi - 1) \cdot \log(P) + ((1-\mu), \varphi - 1) \cdot \log(1-P) (\text{Eq. D2})$$

- 1072 where  $l\Gamma(.)$  is natural logarithm of the absolute value of the gamma function.
- 1073
- 1074 The standardized weighted residual 1 originally introduced by Espinheira et al. (2008) is 1075 defined as follows:

1076 
$$r_i^{weighted} = \frac{P^* - \mu^*}{\sqrt{\nu}}$$
 (Eq. D3)

1077 where  $P^*$  is the quantile for the logistic distribution with location set up at zero and scale at one, 1078 and

1079 
$$\mu^* = \Gamma''(\mu, \varphi) - \Gamma''((1-\mu), \varphi)$$
 (Eq. D4)

1080 
$$v = \Gamma'''(\mu, \varphi) - \Gamma'''((1 - \mu), \varphi)$$
 (Eq. D5)

1081 where  $\Gamma''$  and  $\Gamma'''$  are respectively the second and third derivative of the  $\Gamma$  function.

1082

1083 The quantile residual is defined as:

1084 
$$r_i^{Quantile} = \Phi^{-1}(F(P, \mu, \varphi))$$
 (Eq. D6)

1085 where  $\Phi^{-1}$  is the inverse of the cumulative probability function of the standard normal 1086 distribution and F is the cumulative probability function of the Beta law.