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R. Susi  
H. Navarro  
P. Main  
M.A. Gómez-Villegas

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Av. Puerta de Hierro, S/N  
28040 Madrid  
Tlf. 913944035  
[buc\\_est@buc.ucm.es](mailto:buc_est@buc.ucm.es)

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# Perturbing the structure in Gaussian Bayesian networks

R. Susi<sup>a</sup>, H. Navarro<sup>b</sup>, P. Main<sup>c</sup> and M.A. Gómez-Villegas<sup>c</sup>

<sup>a</sup> *Departamento de Estadística e Investigación Operativa III,  
Universidad Complutense de Madrid, 28040 Madrid, Spain*

<sup>b</sup> *Departamento de Estadística, Investigación Operativa y Cálculo numérico  
UNED, 28040 Madrid, Spain*

<sup>c</sup> *Departamento de Estadística e Investigación Operativa,  
Universidad Complutense de Madrid, 28040 Madrid, Spain*

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## Abstract

In this paper we introduce a n-way sensitivity analysis for Gaussian Bayesian networks where we study the joint effect of variations in a set of similar parameters. Our aim is to determine the sensitivity of the model when the parameters that describe the quantitative part are given by the structure of the graph. Therefore, with this analysis we study the effect of uncertainty about the regression coefficients and the conditional variances of variables with their parents given in the graph.

If a regression coefficient between two variables,  $X_i$  and its parent  $X_j$ , is different from zero, there exists an arc connecting  $X_j$  with  $X_i$ . So, the study of variations in these parameters leads us to compare different dependence structures of the network, adding or removing arcs. This can be useful to determine the sensitivity of the network to variations in the qualitative part of the model, given by the graph.

The methodology proposed is implemented with an example.

*Key words:* Gaussian Bayesian networks, Sensitivity analysis, Kullback-Leibler divergence

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## Introduction

Probabilistic networks are graphical models of interactions between a set of variables where the joint probability distribution can be described in graphical terms.

This model consists of two parts: the qualitative and the quantitative part. The qualitative part is given by a graph useful to define dependences and independencies among variables. The graph shows us the set of variables of the model at nodes, and the presence/absence of edges represents dependence/independence between variables. The qualitative part of the model is related with the quantitative part. In the quantitative part, it is necessary to determine the set of parameters that describes the probability distribution of each variable, given its parents, to compute the joint probability distribution of the model.

Probabilistic networks have become an increasingly popular paradigm for reasoning under uncertainty situations, addressing such tasks as diagnosis, prediction, decision making, classification and data mining [1].

Bayesian networks (BNs) are an important subclass of probabilistic networks. In this subclass, the qualitative part is given by a directed acyclic graph (DAG), where the dependence structure is represented with arcs. Then, a BN is a probabilistic graphical model of causal interactions (although this restriction is not strictly necessary to have arcs at the graph). Moreover, in BNs the joint probability distribution can be factorized as the product of a set of conditional probability distributions, as can be seen in Section 1.

Building a BN is a difficult task, because it requires to determine the quantitative and the qualitative part of the network. Experts knowledge is important to fix the dependence structure between the variables of the network and to specify a large set of parameters. In this process, it is possible to work with a database of cases, nevertheless the experience and knowledge of experts is also necessary. As a consequence of the incompleteness of data and partial knowledge of the domain, the assessments obtained are inevitably inaccurate [2].

In this work, we focus on a subclass of Bayesian networks known as Gaussian Bayesian networks (GBNs). The quantitative part of a GBN is given by a set of univariate normal distributions for the conditional probability distribution of each variable given its parent in the DAG. Also, the joint probability distribution of the model is a multivariate normal distribution.

The quantitative part of a GBN, can be built with two kind of parameters: the means as marginal parameters and the corresponding conditional parameters.

Then, for each variable  $X_i$ , the experts have to give the mean of  $X_i$ , the regression coefficient between  $X_i$  and each parent  $X_j$ ,  $X_j \in Pa(X_i)$ , and the conditional variances of  $X_i$  given its parents in the DAG. This specification is easier for experts rather than others. Moreover, it is interesting because when the regression coefficient between two variables is different from zero, there is an arc between those variables in the DAG. Obviously, when a regression coefficient is zero there is no arc to join both variables and they are not parent and child.

Our interest is focused on studying the sensitivity of a GBN defined by the parameters introduced above. This subject has not been frequently treated in literature and also, the sensitivity analysis of the model to variations in these parameters permits the study of variations in the structure of the DAG. Actually, we can find different dependence structures with absence or presence of arcs, changing the zeros of the regression coefficients. Moreover, this analysis can be useful to work with a more simple structure of the network. In Section 3 we apply and discuss this technique.

The sensitivity analysis proposed in this work is a n-way sensitivity analysis. Then, we can study the joint effect of the variation of a set of similar parameters over the network's output.

The paper is organized as follows. In Section 1 we present some general concepts and introduce our running example. Section 2 describes the methodology used to study the sensitivity of the Gaussian model and the obtained results; this section discusses differences with other analyses developed to study the sensitivity in probabilistic networks. The second contribution of this paper is presented in Section 3, with the study of variations in the structure of the network, as a particular case of the analysis; these variations or changes are a direct result of disturbing the dependence structure of the model shown in the DAG. To check the analysis proposed and changes in the network dependence structure, we introduce an example. The paper ends with some conclusions and a brief discussion with some directions for further research.

## 1 General concepts

Throughout this paper, random variables will be denoted by capital letters. In the multidimensional case, boldface characters will be used.

The definition of a Bayesian network (BN) is given by a pair  $(\mathcal{G}, \mathcal{P})$ , where  $\mathcal{G}$  is the DAG with variables at nodes and dependence structure shown by the presence or absence of arcs between variables. And  $\mathcal{P}$  a set of conditional probability distributions having for each random variable the distribution of

$X_i$  given its parents in the DAG, i.e. ,  $P(X_i | pa(X_i)) \forall X_i$ .

The joint probability distribution of a BN can be defined in terms of the elements of  $\mathcal{P}$  as the product of the conditional probability distributions  $P(X_i | pa(X_i)) \forall X_i$ . That is,

$$P(\mathbf{X}) = \prod_{i=1}^n P(X_i | pa(X_i)). \quad (1)$$

Among others, Bayesian networks have been studied by authors like Pearl [3], Lauritzen [4] or Jensen and Nielsen [5].

It is common to consider BNs of discrete variables. Nevertheless, it is possible to work with some continuous distributions. For example, it is possible to describe a GBN as a BN where the variables of the model are Gaussian variables. Next, we introduce its formal definition.

**Definition 1 (Gaussian Bayesian network (GBN))** *A GBN is a BN where the joint probability density associated with the variables  $\mathbf{X} = \{X_1, \dots, X_n\}$  is a multivariate normal distribution  $N(\boldsymbol{\mu}, \Sigma)$ , given by*

$$f(\mathbf{x}) = (2\pi)^{-n/2} |\Sigma|^{-1/2} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})' \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\} . \quad (2)$$

$\boldsymbol{\mu}$  is the  $n$ -dimensional mean vector and  $\Sigma$  is the  $n \times n$  positive definite covariance matrix.

The conditional probability density for  $X_i$  ( $i = 1, \dots, n$ ) that satisfies (1), is a univariate normal distribution given by

$$X_i | pa(X_i) \sim N \left( \mu_i + \sum_{j=1}^{i-1} \beta_{ji} (x_j - \mu_j), v_i \right) \quad (3)$$

where  $\mu_i$  is the mean of  $X_i$ ,  $\beta_{ji}$  is the regression coefficient when  $X_i$  is regressed on its parents  $X_j \in Pa(X_i)$ , and  $v_i$  is the conditional variance of  $X_i$  given its parents. It can be pointed out that  $\beta_{ji} = 0$  if and only if there is no link from  $X_j$  to  $X_i$ .

The means of variables,  $\mu_i$ , are the elements of the  $n$ -dimensional mean vector  $\boldsymbol{\mu}$ . To get the covariance matrix  $\Sigma$  with  $v_i$  and  $\beta_{ji}$  we can define  $\mathbf{D}$  and  $\mathbf{B}$  matrices. Let  $\mathbf{D}$  be a diagonal matrix with the conditional variances  $v_i$ ,  $\mathbf{D} = \text{diag}(v)$ . Let  $\mathbf{B}$  be a strictly upper triangular matrix with the regression coefficients  $\beta_{ji}$  where  $X_j$  is a parent of  $X_i$ , for the variables in  $\mathbf{X}$  with  $j < i$ . Then, the covariance matrix  $\Sigma$  can be computed as

$$\Sigma = [(\mathbf{I} - \mathbf{B})^{-1}]^T \mathbf{D} (\mathbf{I} - \mathbf{B})^{-1} \quad (4)$$

For details see [6].

It is better to define GBN with the conditional parameters,  $v_i$  and  $\beta_{ji}$  for all the variables in the model, rather than with the covariance matrix, as we remark in Section 2. Experts can determine with more accuracy a conditional parameter of a variable given its parents in the DAG, rather than introducing a joint parameters involving all the variables of the model.

As the BN is defined, the model can be used to make inferences. This process, based on the Bayes theorem, is known as *probabilistic propagation*. And the first step is to compute an *initial network's output* given by the marginal distribution of any variable of the model running the dependence structure. Some times, there is a set of variables of the model whose states are known, that is, a set of observable variables with evidence. We can propagate the evidence over the network obtaining the *posterior network's output*. Variables with evidence are thus evidential variables,  $\mathbf{E}$ .

The evidence propagation consists in updating the probability distribution of a BN given the evidential variables. Then, we can compute the actual distribution of some nonobservable variables of interest as a posterior probability distribution given the evidence.

Several methods have been proposed in literature to propagate evidence in BNs (see [7] or [8]). For GBNs, some algorithms are based on methods performed for discrete BNs. However, most of the algorithms proposed to propagate the evidence in GBNs are based on computing the conditional probability distribution of a multivariate normal distribution, given a set of evidential variables.

After the evidence propagation, the posterior network's output is given by the conditional probability distribution of the variables of interest  $\mathbf{Y}$ , known the evidential variables  $\mathbf{E}$ . In GBNs the posterior network's output is a multivariate normal distribution given by  $\mathbf{Y}|\mathbf{E} = \mathbf{e} \sim N(\mu^{\mathbf{Y}|\mathbf{E}=\mathbf{e}}, \Sigma^{\mathbf{Y}|\mathbf{E}=\mathbf{e}})$ , with parameters

$$\mu^{\mathbf{Y}|\mathbf{E}=\mathbf{e}} = \mu_{\mathbf{Y}} + \Sigma_{\mathbf{Y}\mathbf{E}} \Sigma_{\mathbf{E}\mathbf{E}}^{-1} (\mathbf{e} - \mu_{\mathbf{E}}) \quad \text{and} \quad \Sigma^{\mathbf{Y}|\mathbf{E}=\mathbf{e}} = \Sigma_{\mathbf{Y}\mathbf{Y}} - \Sigma_{\mathbf{Y}\mathbf{E}} \Sigma_{\mathbf{E}\mathbf{E}}^{-1} \Sigma_{\mathbf{E}\mathbf{Y}} \quad (5)$$

Next, our working example of a GBN is introduced.

**Example 2** *The interest of the problem is about the duration of time that a machine works for. The machine is made up of 7 elements with random time*

to failure,  $X_i$  where  $i = 1, \dots, 7$ , are connected as shown in the DAG of Figure 1.

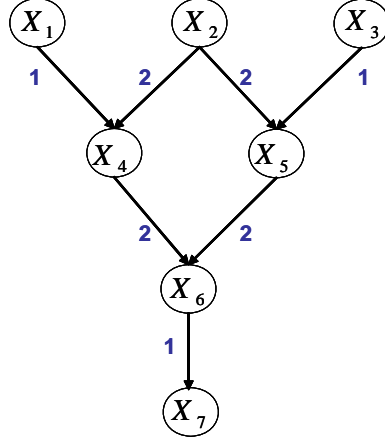


Figure 1: DAG of the GBN in Example 1

It is well-known that the time that each element is working is a normal distribution, being the joint probability distribution of  $\mathbf{X} = \{X_1, X_2, \dots, X_7\}$  a multivariate normal distribution.

Parameters given by experts are

$$\boldsymbol{\mu} = \begin{pmatrix} 1 \\ 3 \\ 2 \\ 1 \\ 4 \\ 5 \\ 8 \end{pmatrix} \quad \mathbf{B} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

Computing the prior network's output, we obtain that  $\mathbf{X} \sim N(\mathbf{x}|\boldsymbol{\mu},\Sigma)$  where

$$\boldsymbol{\mu} = \begin{pmatrix} 1 \\ 3 \\ 2 \\ 1 \\ 4 \\ 5 \\ 8 \end{pmatrix} \quad \Sigma = \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 2 & 2 \\ 0 & 1 & 0 & 2 & 2 & 8 & 8 \\ 0 & 0 & 2 & 0 & 2 & 4 & 4 \\ 1 & 2 & 0 & 6 & 4 & 20 & 20 \\ 0 & 2 & 2 & 4 & 10 & 28 & 28 \\ 2 & 8 & 4 & 20 & 28 & 97 & 97 \\ 2 & 8 & 4 & 20 & 28 & 97 & 99 \end{pmatrix}$$

For a specific case, evidence is given by  $\mathbf{E} = \{X_1 = 2, X_2 = 2, X_3 = 1\}$ . Then, after performing the evidence propagation, the posterior network's output given by the probability distribution of the rest of the variables is  $\mathbf{Y}|\mathbf{E} \sim N(\mathbf{y}|\boldsymbol{\mu}^{\mathbf{Y}|\mathbf{E}},\Sigma^{\mathbf{Y}|\mathbf{E}})$  with parameters

$$\boldsymbol{\mu}^{\mathbf{Y}|\mathbf{E}} = \begin{pmatrix} 0 \\ 1 \\ -3 \\ 0 \end{pmatrix} \quad \Sigma^{\mathbf{Y}|\mathbf{E}} = \begin{pmatrix} 1 & 0 & 2 & 2 \\ 0 & 4 & 8 & 8 \\ 2 & 8 & 21 & 21 \\ 2 & 8 & 21 & 23 \end{pmatrix}$$

## 2 Sensitivity in GBN

To build a BN is a difficult task and experts knowledge is necessary to define the model. As we introduced before, the assessments obtained for the parameters are usually inaccurate.

Sensitivity analysis is a general technique to evaluate the effects of inaccuracies in the parameters of the model on the model's output.

In BNs, the network's output, given by the marginal distribution of interest variables is computed with the parameter that specifies the quantitative part of BN. Then, they could be sensitive to the inaccuracies. However, every parameter will not require the same level of accuracy to reach a good behavior of the network; some parameters will typically have more impact on the network's output than others [2].

Sensitivity analysis can be developed varying one parameter and keeping the rest of network's parameters fixed. This is known as *one-way sensitivity analysis*.

sis. With a view to determining the effect of changing a set of parameters simultaneously, it is possible to develop an *n-way sensitivity analysis*. In this case, the analysis shows the joint effect of the variation of a set of parameters on the network’s output.

In recent years, some sensitivity analysis have been proposed in literature. Authors such as Laskey [9], Coupé, van der Gaag and Habbema [10], Kjærulff and van der Gaag [11], Bednarsky, Cholewa and Frid [12] and Chan and Darwiche [13] have already done research in this line. All of these works have succeeded in developing some useful sensitivity analysis techniques, but all are applied to discrete Bayesian networks.

The sensitivity in GBN has been studied by Castillo & Kjaerulff [14] and by Gómez-Villegas, Main & Susi [15,16].

Castillo & Kjaerulff [14] propose a one-way sensitivity analysis, based on [9], which investigates the impact of small changes in the network parameters.

The present authors, in a previous work [15], introduced a one-way sensitivity analysis. We propose a methodology based on computing a divergence measure as authors like Chan & Darwiche [13] do; nevertheless, we work with a different divergence measure due to the variables considered. To evaluate variations in the GBN we can compare the network’s output of two different models. The original model given by initial parameters assigned to the model and a perturbed model obtained after changing one of the parameters of the model. In [16], we have developed an n-way sensitivity analysis to study the joint effect of a set of parameters on the network’s output with the same settings.

Our approach differs from that of Castillo and Kjærulff [14] in the fact that we consider a global sensitivity measure rather than the evaluation of local aspects of distributions such as location and dispersion.

In the present paper we develop an n-way sensitivity analysis in the line of [16], but using the conditional specification of the model. Until now, all the sensitivity analyses proposed for GBNs [14, 15, 16] have studied variations in parameters of  $\boldsymbol{\mu}$  and  $\Sigma$ . In this work, we want to study variations in a set of parameters of  $\boldsymbol{\mu}$ ,  $\mathbf{D}$  and  $\mathbf{B}$ , specifically in a set of parameters of  $\mathbf{D}$  and  $\mathbf{B}$ , because  $\boldsymbol{\mu}$  is the mean vector and it is the same in both cases.

Note that for the specification of a network experts prefer to determine the regression coefficients for each  $X_i$ ,  $\beta_{ji} \forall X_j \in Pa(X_i)$ , and the conditional variance,  $v_i$ , rather than variances and covariances to build  $\Sigma$ . This specification of the network is easier to experts because it is clear and completes the dependence structure of the DAG. For that reason, experts can determine more accurately  $\beta_{ji}$  and  $v_i$  for all the variables in the GBN.

To develop a n-way sensitivity analysis we have to study a set of variations over  $\mathbf{B}$  and  $\mathbf{D}$  matrices. Remember that  $\mathbf{B}$  and  $\mathbf{D}$  are built with all the regression coefficients and the conditional covariances.

Moreover, with this technique we can study variations of the structure of the DAG. That is, the zeros in the  $\mathbf{B}$  matrix reflect absence of arcs between variables. As we introduced in a previous section,  $\mathbf{B}$  matrix, is a strictly upper triangular matrix made up of the regression coefficients of  $X_i$  given its parents  $X_j \in Pa(X_i)$ . Then, it is possible to determine the sensitivity of a GBN to changes in the structure of the DAG adding or removing an arc of the DAG. This analysis is introduced in Section 3.

Therefore we deal first with the comparison of the global models previous to the probabilistic propagation. It will give information about the effect of the different kind of perturbations in parameters and variables following the possibility of including evidence further.

In the next subsections we present and justify the usage of Kullback-Leibler divergence for analysis development and we describe the methodology and the obtained results for the n-way sensitivity analysis.

### 2.1 The Kullback-Leibler divergence

The Kullback–Leibler divergence (KL) is a non-symmetric measure that provides global information of the difference between two probability distributions (see [17] for more details).

The KL divergence between two probability densities  $f(w)$  and  $f'(w)$ , defined over the same domain, is given by

$$KL(f'(w)|f(w)) = \int_{-\infty}^{\infty} f(w) \ln \frac{f(w)}{f'(w)} dw .$$

With this notation the non-symmetric KL divergence is used, because  $f$  can be considered as a reference density and  $f'$  as a perturbed one.

For two multivariate normal distributions, the KL divergence is evaluated as follows:

$$KL(f'|f) = \frac{1}{2} \left[ \ln \frac{|\Sigma'|}{|\Sigma|} + tr \left( \Sigma \Sigma'^{-1} \right) + (\boldsymbol{\mu}' - \boldsymbol{\mu})^T \Sigma'^{-1} (\boldsymbol{\mu}' - \boldsymbol{\mu}) - \dim(\mathbf{X}) \right] \quad (6)$$

where  $f$  is the joint probability density of  $\mathbf{X} \sim N(\boldsymbol{\mu}, \Sigma)$ , and  $f'$  is the joint probability density of  $\mathbf{X}' \sim N(\boldsymbol{\mu}', \Sigma')$ .

We work with the KL divergence because it lets us study differences between two probability distributions in a global way rather than comparing their local features as in other sensitivity analyses. Moreover, we consider a non-symmetric measure because we propose to compare the original model, as the reference probability distribution, with some models, obtained after perturbing a set of parameters that describes the network. The original model is given by the initial parameters assigned to the network and the initial structure of the DAG, thereby, it is appropriate to consider this model as a reference.

## 2.2 Methodology and results

As in some previous works cited, the method developed in this work consists in comparing the network’s outputs under two different models.

We are going to work with the initial network’s output given by the marginal distribution of any variable. In this paper, we want to determine the set of parameters that will require a high level of accuracy independently of the evidence, because the model can be used in different situations with different cases of evidence.

Two models to be compared are: the original model and the perturbed one.

The original model is given by initial parameters associated with the quantitative part of the GBN, i.e., the initial values assigned by experts to the mean vector  $\boldsymbol{\mu}$  and to  $\mathbf{B}$  and  $\mathbf{D}$  matrices.

The perturbed model quantifies uncertainty in the parameters by introducing an additive perturbation. For each perturbed model we consider only one perturbation. Perturbations are a  $\boldsymbol{\delta}$  vector for the mean  $\boldsymbol{\mu}$ , and  $\boldsymbol{\Delta}_{\mathbf{B}}$  and  $\boldsymbol{\Delta}_{\mathbf{D}}$  for  $\mathbf{B}$  and  $\mathbf{D}$  matrices, respectively.  $\boldsymbol{\Delta}_{\mathbf{B}}$  and  $\boldsymbol{\Delta}_{\mathbf{D}}$  matrices have a specific structure similar to  $\mathbf{B}$  and  $\mathbf{D}$  matrices, respectively. Then,  $\boldsymbol{\Delta}_{\mathbf{B}}$  is a strictly upper triangular matrix formed with perturbations associated with the regression coefficients  $\beta_{ji}$ . And the matrix  $\boldsymbol{\Delta}_{\mathbf{D}}$  is diagonal, as  $\mathbf{D}$ , and rejoins variations associated with the conditional variances  $v_i$ .

Therefore, for the sensitivity analysis we have three different perturbed models, each one obtained after adding only one of the perturbations introduced ( $\boldsymbol{\delta}$ ,  $\boldsymbol{\Delta}_{\mathbf{B}}$  or  $\boldsymbol{\Delta}_{\mathbf{D}}$ ).

Computing the initial network’s outputs in both models, the original and the perturbed model, the joint distributions of the network are obtained.

To compare the joint distribution of the original model with the joint distribution of the perturbed model, we apply the KL divergence. Working with

three perturbed models, one for each perturbation, we obtain three different divergences.

With this sensitivity analysis we can evaluate uncertainty about one parameter like the mean vector or the  $\mathbf{B}$  and  $\mathbf{D}$  matrices, necessary to build the covariance matrix of the model.

Our next proposition introduces the expressions obtained for the KL divergence with a view to comparing the original model with anyone of the three perturbed model.

**Proposition 3** *Let  $(\mathcal{G}, \mathcal{P})$  be a GBN with parameters  $\boldsymbol{\mu}$ ,  $\mathbf{B}$  and  $\mathbf{D}$ , where  $\boldsymbol{\mu}$  is the mean vector of variables of the model, and  $\mathbf{B}$  and  $\mathbf{D}$  are the matrices of the regression coefficients and of the conditional variances, respectively, of any variable given their parents in the DAG. After computing the initial network's output given by the joint distribution, the quantitative part of the GBN is  $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ .*

For any set of variations of the parameters  $\boldsymbol{\mu}$ ,  $\mathbf{B}$  and  $\mathbf{D}$ , is obtained:

- (1) *When the perturbation  $\boldsymbol{\delta}$  is added to the mean vector, we compare the original model  $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  with the perturbed model  $\mathbf{X} \sim N(\boldsymbol{\mu}^\delta, \boldsymbol{\Sigma})$ , being  $\boldsymbol{\mu}^\delta = \boldsymbol{\mu} + \boldsymbol{\delta}$ . The expression obtained for the KL divergence is given by*

$$KL^\mu(f^\mu|f) = \frac{1}{2} [\boldsymbol{\delta}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\delta}] \quad (7)$$

- (2) *When the perturbation  $\boldsymbol{\Delta}_\mathbf{B}$  is added to  $\mathbf{B}$ , we compare the original model  $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  with the perturbed model  $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma}^{\boldsymbol{\Delta}_\mathbf{B}})$ , being  $\boldsymbol{\Sigma}^{\boldsymbol{\Delta}_\mathbf{B}} = [(\mathbf{I} - \mathbf{B} - \boldsymbol{\Delta}_\mathbf{B})^{-1}]^T \mathbf{D}(\mathbf{I} - \mathbf{B} - \boldsymbol{\Delta}_\mathbf{B})^{-1}$ . The expression obtained for the KL divergence is given by*

$$KL^\mathbf{B}(f^\mathbf{B}|f) = \frac{1}{2} [\text{trace}(\boldsymbol{\Sigma}\mathbf{K})] \quad (8)$$

where  $\mathbf{K} = \boldsymbol{\Delta}_\mathbf{B} \mathbf{D}^{-1} \boldsymbol{\Delta}_\mathbf{B}^T$ .

- (3) *When the perturbation  $\boldsymbol{\Delta}_\mathbf{D}$  is added to  $\mathbf{D}$ , we compare the original model  $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  with the perturbed model  $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma}^{\boldsymbol{\Delta}_\mathbf{D}})$ , being  $\boldsymbol{\Sigma}^{\boldsymbol{\Delta}_\mathbf{D}} = [(\mathbf{I} - \mathbf{B})^{-1}]^T (\mathbf{D} + \boldsymbol{\Delta}_\mathbf{D}) (\mathbf{I} - \mathbf{B})^{-1}$ . The expression obtained for the KL divergence is given by*

$$KL^\mathbf{D}(f^\mathbf{D}|f) = \frac{1}{2} \left[ \ln \frac{|\mathbf{D} + \boldsymbol{\Delta}_\mathbf{D}|}{|\mathbf{D}|} + \text{trace}((\mathbf{D} + \boldsymbol{\Delta}_\mathbf{D})^{-1} \mathbf{D}) - n \right] \quad (9)$$

The expression (9) can be computed with the conditional variances  $v_i$ , as

$$KL^{\mathbf{D}}(f^{\mathbf{D}}|f) = -\frac{1}{2} \left[ \sum_{i=1}^n \left( \ln \left( 1 - \frac{\delta_i}{v_i + \delta_i} \right) + \frac{\delta_i}{v_i + \delta_i} \right) \right]$$

where  $\delta_i$  is the variation of the conditional variance,  $v_i$ , of  $X_i$  given its parents in the DAG.

If there exists some inaccuracy in the conditional parameters describing a GBN, it is possible to carry out the proposed sensitivity analysis using the expressions given in Proposition 3. The calculation of the KL divergence for each case, can lead to determine the parameters that must be reviewed to describe the network more accurately.

When the KL divergence is close to zero, it is possible to conclude that the network is not sensitive to the proposed variations.

Our methodology can evaluate the perturbation effect with the conditional representation of GBN. It also makes possible the development of new lines of research to discover the transmission mechanism of the perturbations over the variables.

The next examples are used to illustrate the procedure described before. We also introduce two examples with different assumptions about the parameter's uncertainty.

**Example 4** *Working with the GBN given in Example 2, experts disagree on the values of some parameters. For example, the mean of  $X_6$  could be either 4 or 5 and the mean of  $X_7$  could be either 7 or 8. They also offer different opinions about the regression coefficient between  $X_4$  and its parent  $X_2$ , and between  $X_5$  and its parent  $X_2$ . Moreover, the conditional variances of  $X_2$ ,  $X_4$  and  $X_5$  also change. These uncertainties in  $\delta$ ,  $\Delta_{\mathbf{D}}$  and  $\Delta_{\mathbf{B}}$  give*

$$\delta = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ -1 \end{pmatrix} \quad \Delta_{\mathbf{B}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \Delta_{\mathbf{D}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

*For the sensitivity analysis each perturbed model is obtained after adding a*

perturbation given by  $\delta$ ,  $\Delta_{\mathbf{B}}$  or  $\Delta_{\mathbf{D}}$  to  $\mu$ ,  $\mathbf{B}$  or  $\mathbf{D}$ , respectively.

Computing the KL divergence for each perturbed model, we have that

$$\begin{aligned} KL^{\mu}(f^{\mu}|f) &= 0.5 \\ KL^{\mathbf{B}}(f^{\mathbf{B}}|f) &= 0.625 \\ KL^{\mathbf{D}}(f^{\mathbf{D}}|f) &= 0.204 \end{aligned}$$

Values obtained from the analysis proposed are rather small. Then, we can conclude that the network is not sensitive to the proposed perturbations.

Now, we introduce an example where more inaccurate parameters are considered, and the GBN is shown to be sensitive.

**Example 5** For the GBN in Example 2, experts now disagree on the values of more parameters. The uncertainties in  $\delta$ ,  $\Delta_{\mathbf{D}}$  and  $\Delta_{\mathbf{B}}$  give

$$\delta = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ -1 \\ -1 \end{pmatrix} \quad \Delta_{\mathbf{B}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \Delta_{\mathbf{D}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix}$$

Considering each time a different perturbed model and computing the KL divergence to compare both networks we obtain that

$$\begin{aligned} KL^{\mu}(f^{\mu}|f) &= 4.375 \\ KL^{\mathbf{B}}(f^{\mathbf{B}}|f) &= 12.625 \\ KL^{\mathbf{D}}(f^{\mathbf{D}}|f) &= 0.579 \end{aligned}$$

The obtained divergences are larger than in Example 4. When uncertainty is about the mean vector and about  $\mathbf{B}$  matrix we can conclude that the network is sensitive to the proposed perturbations about  $\mu$  and  $\mathbf{B}$ . Nevertheless, for uncertainty about conditional variances in  $\mathbf{D}$  the KL divergence is not large. Then, the GBN is not sensitive to the proposed perturbations of  $\mathbf{D}$ . Nevertheless, increasing in one unit the perturbations proposed in  $\Delta_{\mathbf{D}}$  the  $KL^{\mathbf{D}}(f^{\mathbf{D}}|f) > 1$ .

As can be seen with the uncertainty introduced in this example, not every inaccurate parameter requires the same level of accuracy to have a satisfactory behavior of the model. Changes about  $\mathbf{D}$  have less impact on the prior network's output than about  $\mathbf{B}$  or  $\boldsymbol{\mu}$ .

### 3 Perturbing the structure of a GBN

As we have introduced before, the regression coefficient of  $X_i$  given its parents,  $\beta_{ji}$ , shows the degree of association between  $X_i$  and its parents. When  $\beta_{ji} = 0$ , there is no arc in the DAG from  $X_j$  to  $X_i$ . Therefore, it is possible to study variations of the structure of the qualitative part of GBN (i.e., the DAG) by only perturbing  $\mathbf{B}$  matrix.

If we change the value of any  $\beta_{ji}$  to zero, being in the original model different from zero, then we are removing the arc between variables  $X_j$  and  $X_i$ . Otherwise, we can introduce the presence of dependence between two variables  $X_j$  and  $X_i$  changing some  $\beta_{ji} = 0$  to  $\beta_{ji} > 0$ , then adding an arc in the DAG.

To compare the original model with other with/without some arcs, i.e., introducing new dependences/independencies, it is possible to consider the sensitivity analysis in Section 2 when the perturbed model is given by adding  $\Delta_{\mathbf{B}}$ . That is, the perturbed model when uncertainty is about  $\mathbf{B}$ . In this case, we propose the calculation of expression (8). With the obtained result we can determine when variations in the structure of the DAG perturb or not the original network's output.

Sometimes experts do not agree with the qualitative part of the model. Then, this analysis is necessary to study uncertainty as regards the dependence structure at the DAG. Moreover, it can be very useful to compare the structure with another one detecting more dependences between variables. In some cases, more dependences can form a cycle in the DAG obtaining a structure impossible to build a GBN. Furthermore, with this analysis we can take away some arcs to work with the simplest structure that gives us the same accuracy than the original model.

In the next example, we will be looking for the simplest structure of the GBN introduced in Section 1, with a connected graph.

**Example 6** *We want to reduce the dependence structure of the GBN introduced in Example 1, keeping the graph connected .*

We can consider 4 different situations, corresponding to (a), (b), (c) and (d) in Figure 2.

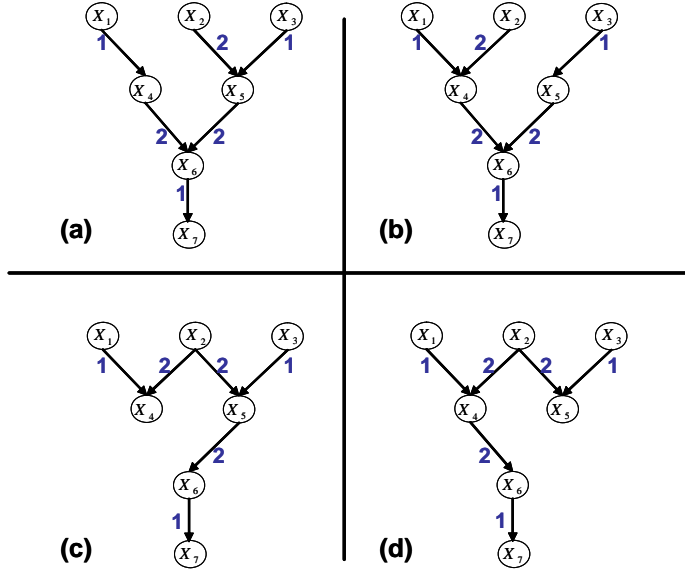


Figure 2: Four different situations removing arcs in the DAG, keeping all the variables connected

**Perturbed model (a)** The perturbed GBN in (a) shows variations at  $\mathbf{B}$ . The parameters that describe (a) are  $\boldsymbol{\mu}$ ,  $\mathbf{D}$  and  $\mathbf{B}^{\Delta_{\mathbf{B}}}$ , where  $\mathbf{B}^{\Delta_{\mathbf{B}}}$  is given by:

$$\mathbf{B}^{\Delta_{\mathbf{B}}} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

At  $\mathbf{B}^{\Delta_{\mathbf{B}}}$ , the arc between  $X_2$  and  $X_4$  has been removed, being at the perturbed model  $\beta_{24} = 0$ .

Computing the KL divergence, with expression (8), the obtained result is:

$$KL^{\mathbf{B}}(f^{\mathbf{B}}|f) = 2$$

**Perturbed model (b)** In the GBN shown at Figure 2 (b) the perturbed

model is obtained with  $\boldsymbol{\mu}$ ,  $\mathbf{D}$  and  $\mathbf{B}^{\Delta\mathbf{B}}$ , being  $\mathbf{B}^{\Delta\mathbf{B}}$

$$\mathbf{B}^{\Delta\mathbf{B}} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

In this perturbed model, the arc between  $X_2$  and  $X_5$  has been removed, changing to  $\beta_{25} = 0$ . Computing the expression (8) we obtain that:

$$KL^{\mathbf{B}}(f^{\mathbf{B}}|f) = 0.5$$

**Perturbed model (c)** The GBN in (c) is given by original parameters,  $\boldsymbol{\mu}$  and  $\mathbf{D}$ , and instead of  $\mathbf{B}$ , next  $\mathbf{B}^{\Delta\mathbf{B}}$  matrix:

$$\mathbf{B}^{\Delta\mathbf{B}} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Computing expression (8) we obtain that:

$$KL^{\mathbf{B}}(f^{\mathbf{B}}|f) = 12$$

**Perturbed model (d)** Finally, working the perturbed model (d) with  $\mathbf{B}^{\Delta\mathbf{B}}$

given by:

$$\mathbf{B}^{\Delta_{\mathbf{B}}} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The KL divergence is:

$$KL^{\mathbf{B}}(f^{\mathbf{B}}|f) = 20$$

With the obtained results, only the perturbed model (b) can replace the original model given in Example 2. Then, dependence between  $X_2$  and  $X_5$  can be removed.

As can be shown, it is not possible to remove the arcs between  $X_6$  and its parents,  $X_4$  and  $X_5$ , because perturbed models ((c) and (d)) are so much different from the original model. Finally, the arc between  $X_2$  and  $X_4$  could be removed but the KL divergence is larger than one, and it is better to consider this arc in the model.

## 4 Conclusion

This paper proposes a new contribution to the problem of sensitivity analysis in GBNs. Firstly, making possible the study of uncertainty in the conditional parameters given by experts. Then, it is possible to study variation of any mean, regression coefficient between a variable and its parents or conditional variance of variables in the model given its parents. And secondly, dealing with an n-way sensitivity analysis that gives a global vision of different kind of perturbations.

Also the sensitivity analysis of the model to variations of regression coefficients permits the study of changes of the qualitative part of the GBN, keeping the ancestral structure of DAG. In that way, we can change the dependence structure of the model adding or removing arcs between variables.

Finally we have evaluated and discussed the sensitivity analysis proposed with an example of a GBN.

Further research will focus on the application of the previous results to estab-

lish, more formally, the relative importance of arcs in a DAG to sensitivity. Also, the inclusion of evidence over some variables will be studied to evaluate the effect of conditional parameters perturbations on the network output.

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