Local Influence in Gaussian Bayesian networks

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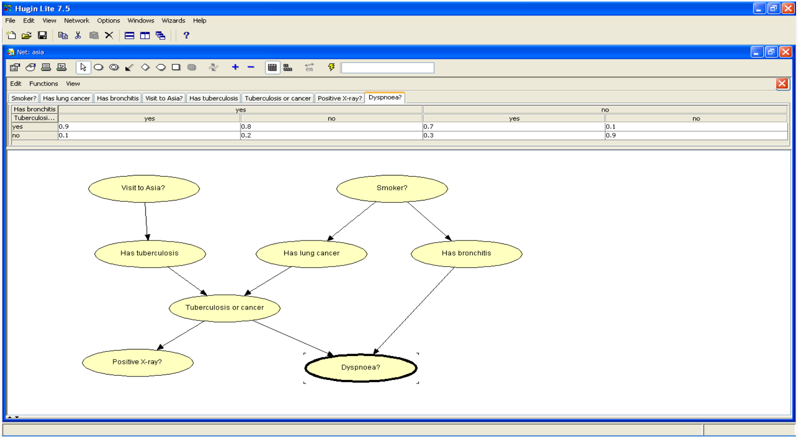
Bayesian networks

Definition

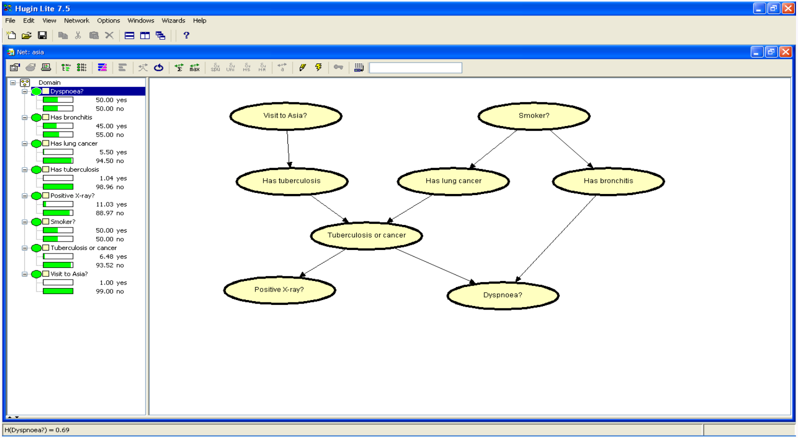
A Bayesian network is a couple $(\mathcal{G}, \mathcal{P})$*, where* $\mathcal{G}$ *is a DAG in which the nodes represent ordered random variables* $\mathbf{X} = \{X_1, \ldots, X_p\}$ *and the edges represent probabilistic dependencies.* $\mathcal{P} = \{P(X_1|pa(X_1)), \ldots, P(X_p|pa(X_p))\}$ *is a set of conditional probability distributions, where* $pa(X_i)$ *is the set of parents of node* X_i *in* $\mathcal{G}$*,* $pa(X_i) \subseteq \{X_1, ..., X_{i-1}\}$*.*
The set $\mathcal{P}$ *defines the associated joint probability distribution:*

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

Bayesian network: Asia



Evidence propagation: Asia



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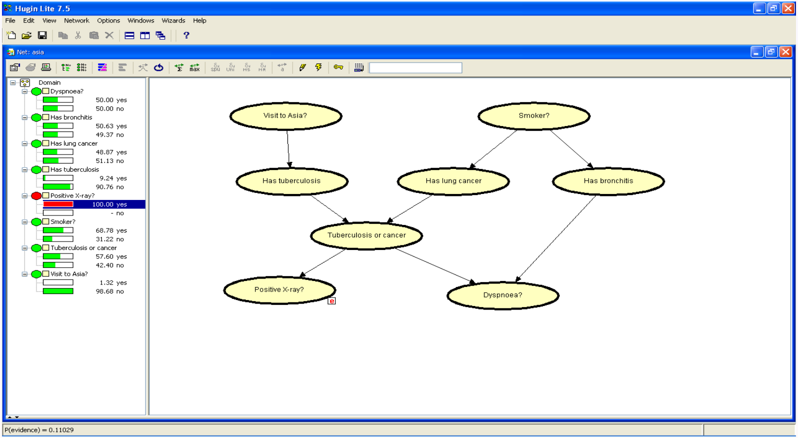


Gaussian Bayesian networks

Definition

A Gaussian Bayesian network (GBN) is a BN where the joint probability density of $\mathbf{X} = (X_1, ..., X_p)'$ *is a multivariate normal distribution* $N_p(\mu, \mathbf{\Sigma})$ *with* μ *the* $p-$*dimensional mean vector,* $\mathbf{\Sigma}$ *the* $p \times p$ *positive definite covariance matrix and the dependence structure is fixed in a DAG.*

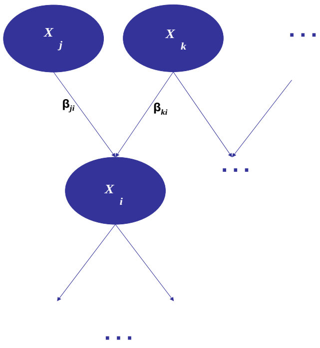
Gaussian Bayesian networks

Then, for every X_i $(i = 1, ..., p)$ given $pa(X_i) \subset \{X_1, ..., X_{i-1}\}$

$$f(x_i \mid pa(X_i)) \sim N_1(x_i \mid \mu_i + \sum_{j=1}^{i-1} \beta_{ji}(x_j - \mu_j), v_i)$$

with μ_i the X_i mean, β_{ji} the regression coefficients of X_i with respect to $X_j \in pa(X_i)$ and v_i the conditional variance of $X_i | pa(X_i)$

$\beta_{ji} = 0$ if X_j is not a parent of X_i



Conditional specification of the GBN

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- μ_i are the elements of the $p-$dimensional mean vector μ

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- v_i and β_{ji} are used to compute the covariance matrix $\boldsymbol{\Sigma}$

Conditional specification of the GBN

Let **D** be a diagonal matrix $\mathbf{D} = diag(\mathbf{v})$ with the conditional variances $\mathbf{v}' = (v_1, ..., v_p)$

$$\mathbf{D} = \begin{pmatrix} v_1 & & 0 \\ & \ddots & \\ 0 & & v_p \end{pmatrix}$$

Let **B** be a strictly upper triangular matrix with the regression coefficients β_{ji} where $j = 1, ..., i-1$.

$$\mathbf{B} = \begin{pmatrix} 0 & \beta_{12} & \dots & \beta_{1p} \\ & \ddots & & \\ & & \ddots & \beta_{p-1p} \\ 0 & & & 0 \end{pmatrix}$$

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Then,

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

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Study uncertainty about the parameters of the conditional specification of a GBN evaluating the effect of unknown prior hyperparameters.

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The Kullback–Leibler divergence is used to determine deviations of perturbed models from the original ones and to define a local sensitivity measure to compare prior and posterior deviations.

With the obtained results it is possible to decide the values to be chosen for the hyperparameters considered.

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The parameters to be considered now are

$$\{v_1, \beta_i, v_i\}_{i>1}$$

Next, we compute prior distributions, likelihood functions and posterior distributions for the parameters $\{v_1, \beta_i, v_i\}_{i>1}$.

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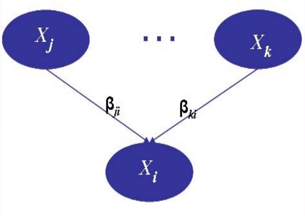
Orphan nodes (node/variable without parents in the DAG) are considered different from nodes with parents in the DAG.

Nodes with parents

Let be X_i a node with a nonempty set of parents $pa(X_i) \subset \{X_1, \dots, X_{i-1}\}$, that is, a node with parents in the DAG.



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$$\Rightarrow \pi(v_i) \propto \frac{\exp\left\{-\frac{\tau}{2v_i}\right\}}{v_i^{\left(\frac{\lambda+i-p}{2}+1\right)}}, v_i > 0$$

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- $\beta_i | v_i \sim N_{i-1}\left(0, \tau^{-1} v_i I_{i-1}\right)$ with the hyperparameter $\tau > 0$

  $\Rightarrow \underset{v_i>0}{\pi(\beta_i | v_i)} \propto \left(\frac{\tau}{v_i}\right)^{\frac{i-1}{2}} \exp\left\{-\frac{\tau}{2v_i}\beta_i^T \beta_i\right\}, \beta_i \in \mathbb{R}^{i-1}$

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- $\pi(\beta_i, v_i) = \pi(\beta_i | v_i)\pi(v_i)$, with $\beta_i \in \mathbb{R}^{i-1}$ and $v_i > 0$

Likelihood function

A random sample of size n is observed giving the next data matrix

For the variable X_i we consider the observations of its parents $pa(X_i)$

$$\left(\begin{array}{ccc|c|cc} x_{11} & x_{12} & \cdots & x_{1i} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2i} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{ni} & \cdots & x_{np} \end{array}\right) \qquad X_{pa_i} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1i-1} \\ x_{21} & x_{22} & \cdots & x_{2i-1} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{ni-1} \end{pmatrix}$$

$$x_i = (x_{1i}, x_{2i}, ..., x_{ni})^T \text{ observations of } X_i$$

Regression model:

$$x_i = X_{pa_i}\beta_i + \varepsilon_i \text{ for } i = 1, \ldots, p \text{ and } \varepsilon_i \sim N_n(0, v_i I_n)$$

Likelihood function

$$L(v_i, \beta_i; x_i, X_{pa_i}) \propto$$

$$\propto \frac{1}{(v_i)^{\frac{n}{2}}} \exp\left\{-\frac{1}{2v_i}\left[(n-(i-1))S_i^2 + (\beta_i - \hat{\beta}_i)^T X_{pa_i}^T X_{pa_i} (\beta_i - \hat{\beta}_i)\right]\right\}$$

for

$$\beta_i \in \mathbb{R}^{i-1}, v_i > 0$$

$$\hat{\beta}_i = \left(X_{pa_i}^T X_{pa_i}\right)^{-1} X_{pa_i}^T x_i$$

$$S_i^2 = \frac{x_i^T x_i - x_i^T X_{pa_i} \left(X_{pa_i}^T X_{pa_i}\right)^{-1} X_{pa_i}^T x_i}{n-(i-1)}$$

Posterior distribution

$$\pi(\beta_i, v_i | x_i X_{pa_i}) = \pi(\beta_i | v_i)\pi(v_i) L(v_i, \beta_i; x_i, X_{pa_i}) \propto \ldots$$

$$\propto \frac{\tau^{\frac{i-1}{2}}}{v_i^{\frac{\lambda+(i-p)+(i-1)+n}{2}+1}} \exp\left\{-\frac{1}{2v_i}\left[\tau + q_i + (\beta_i - \tilde{\beta}_i)^T M_i (\beta_i - \tilde{\beta}_i)\right]\right\}$$

with

$$\beta_i \in \mathbb{R}^{i-1}, v_i > 0$$

$$M_i = \tau I_{i-1} + X_{pa_i}^T X_{pa_i}$$

$$\tilde{\beta}_i = M_i^{-1} X_{pa_i}^T x_i$$

$$q_i = x_i^T x_i - x_i^T X_{pa_i} (M_i)^{-1} X_{pa_i}^T x_i$$

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- $\pi(v_i | x_i X_{pa_i}) \propto \frac{\tau^{\frac{i-1}{2}}}{v_i^{\frac{\lambda+(i-p)+n}{2}+1}} \exp\left\{-\frac{1}{2v_i}(\tau+q_i)\right\}, \; v_i > 0$

  $\Rrightarrow$ an Inverse-Gamma distribution $IG\left(\frac{\lambda+(i-p)+n}{2}, \frac{\tau+q_i}{2}\right)$

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  $\Rrightarrow$ an Inverse-Gamma distribution $IG\left(\frac{\lambda+(i-p)+n}{2}, \frac{\tau+q_i}{2}\right)$
- $\pi(\beta_i | v_i x_i X_{pa_i}) \propto \exp\left\{-\frac{1}{2v_i}\left[(\beta_i - \tilde{\beta}_i)^T M_i(\beta_i - \tilde{\beta}_i)\right]\right\}$,
  $\beta_i \in \mathbb{R}^{i-1}$
  $\Rrightarrow$ a normal distribution $N_{i-1}\left(\tilde{\beta}_i, v_i (M_i)^{-1}\right)$

Orphan nodes

X_i is an orphan node if X_i has no parents in the DAG, therefore there is no arc to X_i, then $\beta_{ji} = 0 \ \forall j < i$.

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The parameter to be studied is only v_i.

Prior distribution and likelihood function

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- Prior distribution:

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- Likelihood function:
  The data are the observations of X_i, $x_i = (x_{1i}, x_{2i}, ..., x_{ni})^T$, then

$$L(v_i; x_i) \propto \frac{1}{(v_i)^{\frac{n}{2}}} \exp\left\{-\frac{1}{2v_i}\left[x_i^T x_i\right]\right\}, v_i > 0$$

Posterior distribution

- Posterior distribution:

$$\pi(v_i|x_i) = \pi(v_i)L(v_i;x_i) \propto \frac{1}{v_i^{\frac{\lambda+(i-p)+n}{2}+1}} \exp\left\{-\frac{1}{2v_i}\left[\tau + x_i^T x_i\right]\right\}$$

$\Rightarrow$ an Inverse-Gamma distribution $IG\left(\frac{\lambda+(i-p)+n}{2}, \frac{\tau+x_i^T x_i}{2}\right)$

Divergence measure

We compute the Kullback-Leibler (KL) divergence to evaluate the effect of uncertainty in hyperparameters λ and τ, in terms of additive perturbations $\delta \in \mathbb{R}^+$.

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Then, we compute

$$\boxed{D_{KLprior} = D_{KL}(\pi^\delta(\beta_i, v_i) \mid \pi(\beta_i, v_i))}$$

and

$$\boxed{D_{KLposterior} = D_{KL}(\pi^\delta(\beta_i, v_i|x_i X_{pa_i}) \mid \pi(\beta_i, v_i|x_i X_{pa_i}))}$$

where $\pi^\delta(\cdot)$ is the perturbed model obtained by adding a $\delta \in \mathbb{R}^+$ perturbation to hyperparameters ($\lambda > p$, $\tau > 0$).

Sensitivity measure

To asses the sensitivity of the posterior to prior variations given by small perturbations in the hyperprior parameters, we introduce a local sensitivity measure given by

$$Sens_i = \lim_{\delta \to 0} \frac{D_{KLposterior}}{D_{KLprior}} = \lim_{\delta \to 0} \frac{D_{KL}(\pi^{\delta}(\beta_i, v_i | x_i X_{pa_i}) | \pi(\beta_i, v_i | x_i X_{pa_i}))}{D_{KL}(\pi^{\delta}(\beta_i, v_i) | \pi(\beta_i, v_i))}$$

Nodes with parents and orphan nodes

Nodes with parents

- $v_i \sim IG\left(\frac{\lambda+i-p}{2}, \frac{\tau}{2}\right)$ with $\lambda > p$ and $\tau > 0$
- $\beta_i | v_i \sim N_{i-1}\left(0, \tau^{-1} v_i I_{i-1}\right)$ with the hyperparameter $\tau > 0$

Orphan nodes

- $v_i \sim IG\left(\frac{\lambda+i-p}{2}, \frac{\tau}{2}\right)$ with $\lambda > p$ and $\tau > 0$

Hyperparameter perturbation $\lambda \Rightarrow \lambda + \delta$

KL divergence to compare prior distributions

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Original model $\pi(v_i) \sim IG\left(\frac{\lambda+(i-p)}{2}, \frac{\tau}{2}\right)$

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with $\Psi(x)$ the digamma function

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$$Sens_i(\lambda) = \frac{\Psi'\left(\frac{\lambda+(i-p)+n}{2}\right)}{\Psi'\left(\frac{\lambda+(i-p)}{2}\right)} < 1$$

with Ψ' the trigamma function

Hyperparameter perturbation $\tau \Rightarrow \tau + \delta$

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$$\text{Original model } \pi\left(\beta_i|v_i\right) \sim N_{i-1}\left(0, \tau^{-1} v_i I_{i-1}\right)$$

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$$D_{KLprior} = D_{KL}(\pi^{\delta}(\beta_i, v_i) \mid \pi(\beta_i, v_i)) =$$

$$\boxed{D_{KLprior} = \frac{\lambda+(i-p)+(i-1)}{2}\left[\left(\frac{\delta}{\tau}\right) - \ln\left(1+\frac{\delta}{\tau}\right)\right]}$$

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$$\text{Perturbed model } \pi^{\delta}(v_i|x_i X_{pa_i}) \sim IG\left(\frac{\lambda+(i-p)+n}{2}, \frac{\tau+\delta+q_i^{\delta}}{2}\right)$$

$$\text{with } q_i^{\delta} = x_i^T x_i - x_i^T X_{pa_i} \left(M_i^{\delta}\right)^{-1} X_{pa_i}^T x_i$$

and

$$\text{Original model } \pi(\beta_i|v_i x_i X_{pa_i}) \sim N_{i-1}\left(\tilde{\beta}_i, v_i \left(M_i\right)^{-1}\right)$$

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$$D_{KLposterior} = \frac{1}{2}\left[\ln \frac{|M_i|}{|M_i^{\delta}|} + \delta tr\left(M_i^{-1}\right) + \frac{\lambda+(i-p)+n}{\tau+q_i}\delta^2 \tilde{\beta}_i^T \left(M_i^{\delta}\right)^{-1} \tilde{\beta}_i\right] +$$
$$+\frac{\lambda+(i-p)+n}{2}\left[-\ln\left(1+\frac{\delta+\left(q_i^{\delta}-q_i\right)}{\tau+q_i}\right)+\frac{\delta+\left(q_i^{\delta}-q_i\right)}{\tau+q_i}\right]$$

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$$Sens_i\left(\tau\right) = \frac{\tau^2}{(\lambda+(i-p)+(i-1))}\left[\sum_{k=1}^{i-1}\frac{1}{(\lambda_k+\tau)^2}+\frac{\lambda+(i-p)+n}{\tau+q_i}2\tilde{\beta}_i^T M_i^{-1}\tilde{\beta}_i\right]+$$
$$+\frac{\lambda+(i-p)+n}{\lambda+(i-p)+(i-1)}\frac{\tau^2}{(\tau+q_i)^2}\left(1+\tilde{\beta}_i^T\tilde{\beta}_i\right)^2$$

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Same results than for nodes with parents

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KL divergence to compare prior distributions

$$D_{KLprior} = D_{KL}(\pi^{\delta}(v_i) \mid \pi(v_i)) =$$

$$\boxed{D_{KLprior} = \frac{\lambda + (i-p)}{2}\left[\left(\frac{\delta}{\tau}\right) - \ln\left(1 + \frac{\delta}{\tau}\right)\right]}$$

Hyperparameter perturbation $\tau \Rightarrow \tau + \delta$

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KL divergence to compare posterior distributions

$$D_{KLposterior} = D_{KL}(\pi^{\delta}(v_i|x_i) \mid \pi(v_i|x_i)) =$$

$$\boxed{D_{KLposterior} = \frac{\lambda+(i-p)+n}{2}\left[\frac{\delta}{\tau+x_i^T x_i} - \ln\left(1+\frac{\delta}{\tau+x_i^T x_i}\right)\right]}$$

Hyperparameter perturbation $\tau \Rightarrow \tau + \delta$

Sensitivity measure: $Sens_i(\tau)$

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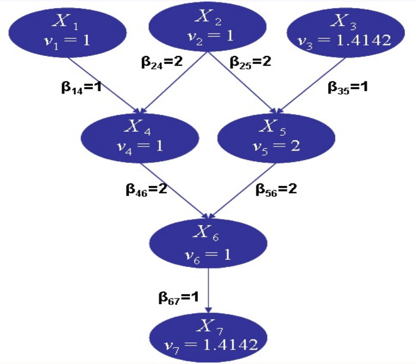
$$Sens_i(\tau) = \frac{\lambda+(i-p)+n}{\lambda+(i-p)} \frac{\tau^2}{\left(\tau+x_i^T x_i\right)^2}$$

GBN

Let us consider next GBN

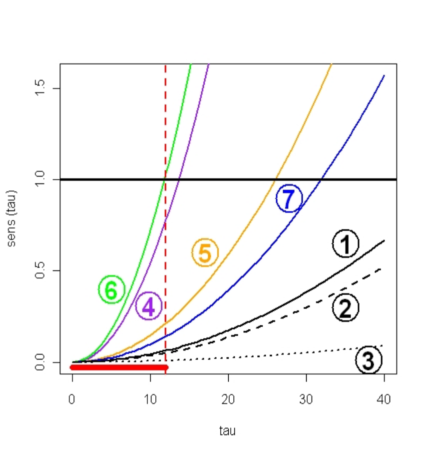


Hyperparameter perturbation $\lambda \rightarrow \lambda + \delta$

Sensitivity measures for different values of perturbed λ are computed, simulating an artificial sample of size $n = 1000$.

$\lambda \backslash X_i$	X_1	X_2	X_3	X_4	X_5	X_6	X_7
8	0.002	0.003	0.004	0.004	0.005	0.006	0.007
15	0.008	0.009	0.010	0.011	0.012	0.013	0.014
25	0.018	0.019	0.020	0.021	0.022	0.023	0.024
50	0.0428	0.043	0.044	0.044	0.045	0.046	0.047
150	0.125	0.126	0.127	0.128	0.128	0.129	0.129
500	0.330	0.331	0.331	0.332	0.332	0.333	0.333
1000	0.498	0.499	0.499	0.499	0.499	0.500	0.500
10000	0.909	0.909	0.909	0.909	0.909	0.909	0.909

Hyperparameter perturbation $\tau \longrightarrow \tau + \delta$



X_6 is the most sensitive node for all the values of τ, then if its sensitivity measure is restricted to be less than one, the rest of the nodes will be controlled. The red zone of recommended values corresponds to $\tau < 12{,}130363$.

Conclusions

In this work a sensitivity analysis to evaluate the effect of unknown prior hyperparameters in GBN is developed.

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This condition is always satisfied for the hyperparameter λ, whereas the hyperparameter τ needs a particular analysis for each network.

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Thank you!