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SCREENING STRONG PAIRWISE RELATIONSHIPS FOR FAST BAYESIAN NETWORK STRUCTURE LEARNING

IFSS 2018

Thibaud Rahier, Sylvain Marié, Stéphane Girard, Florence Forbes

September 7, 2018

INRIA - Schneider Electric



I - Bayesian network structure learning

II - Determinism and Bayesian networks

III - Structure learning with (quasi-)determinism screening

IV - Experiments

V - Discussion

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Setting

- $\mathbf{X} = (X_1, \dots, X_n)$: tuple of categorical random variables
- $D = \{(x_1^{(m)}, \dots, x_n^{(m)})\}_{1 \leq m \leq M}$: dataset w/ M i.i.d observations of \mathbf{X}

I-1. BAYESIAN NETWORKS

Setting

- $\mathbf{X} = (X_1, \dots, X_n)$: tuple of categorical random variables
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Bayesian network: $\mathcal{B} = (\mathcal{G}, \Theta)$ where

- $\mathcal{G} = (\mathcal{V}, \mathcal{A})$: DAG structure with
 - $\mathcal{V} = \llbracket 1, n \rrbracket$ vertices associated to the n variables
 - $\mathcal{A} \subset \mathcal{V}^2$ set of arcs
 - $\pi(i)$ the set of parents of i in \mathcal{G}

Factorization of the joint distribution:

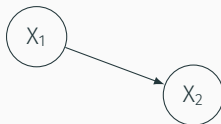
$$P(X_1, \dots, X_n) = \prod_{i=1}^n P(X_i | \mathbf{X}_{\pi(i)})$$

- Θ : parameters of the local $P(X_i | \mathbf{X}_{\pi(i)})$

I-2. BAYESIAN NETWORKS: EXAMPLE

$\mathcal{B} = (G, \Theta)$: two node Bayesian network

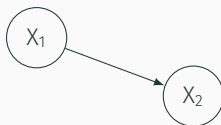
$G = (\{1, 2\}, \{(1, 2)\})$



I-2. BAYESIAN NETWORKS: EXAMPLE

$\mathcal{B} = (G, \Theta)$: two node Bayesian network

$$G = (\{1, 2\}, \{(1, 2)\})$$



$$\Theta = \{\Theta_1, \Theta_2\}$$

- $\Theta_1 = \{\theta_{x_1}\}_{x_1}$ parameters of distribution of X_1 , i.e.:

$$\forall x_1 \in \text{Val}(X_1), \theta_{x_1} = P(X_1 = x_1).$$

- $\Theta_2 = \{\theta_{x_2|x_1}\}_{x_1, x_2}$ parameters of conditional dist. $X_2|X_1$, i.e.:

$$\forall (x_1, x_2) \in \text{Val}(X_1) \times \text{Val}(X_2), \theta_{x_2|x_1} = P(X_2 = x_2 | X_1 = x_1).$$

I-3. BAYESIAN NETWORK STRUCTURE LEARNING

Score&search-based BN structure learning

For a scoring function $s : \text{DAG}_V \rightarrow \mathbb{R}$, BNSL_s comes down to:

$$\hat{G} \in \underset{G \in \text{DAG}_V}{\text{argmax}} s(G)$$

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Some scoring functions

Most scoring functions are based on the log-likelihood $l_D(\Theta)$:

$$l_D(\Theta) = \log(P_{\Theta}(D)) = \sum_{m=1}^M \sum_{i=1}^n \log \left(\theta_{x_i^{(m)} | x_{\pi(i)}^{(m)}} \right)$$

As the MaxLogLikelihood score (MLL), (leads to complete graphs):

$$s_D^{\text{MLL}}(G) = \max_{\Theta \in \Theta_G} l_D(\Theta).$$

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As the Bayesian information criterion score (BIC):

$$s_D^{\text{BIC}}(G) = \underbrace{\max_{\Theta \in \Theta_G} l_D(\Theta)}_{s_D^{\text{MLL}}(G)} - \frac{\log(M)}{2} d(G),$$

I-3. BAYESIAN NETWORK STRUCTURE LEARNING

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As the Bayesian Dirichlet equivalent score (BDe):

$$s_D^{\text{BDe}}(G) = \log \left(\underbrace{P(G)}_{\text{Structure prior}} \int_{\Theta \in \Theta_G} \underbrace{P(D|\Theta, G)}_{\text{Likelihood}} \underbrace{P(\Theta|G)}_{\text{Dirichlet prior}} d\Theta \right) \propto P(G|D)$$

I - Bayesian network structure learning

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Conditional Shannon entropy

The conditional Shannon entropy of X_i knowing X_j is defined as

$$H(X_i|X_j) = - \sum_{x_i, x_j} p(x_i, x_j) \log(p(x_i|x_j))$$

$H(X_i|X_j) = 0$ if and only if the value of X_i is entirely determined by the value of X_j

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$H(X_i|X_j) = 0$ if and only if the value of X_i is entirely determined by the value of X_j

Linking the entropy with MLL score

The MLL score can be rewritten as

$$s_D^{\text{MLL}}(G) = -M \sum_{i=1}^n H^D(X_i | \mathbf{X}_{\pi(i)})$$

Definitions: determinism and quasi-determinism

The relationship $X_i \rightarrow X_j$ is **deterministic** wrt D iff

$$H^D(X_i|X_j) = 0$$

The relationship $X_i \rightarrow X_j$ is **ϵ -quasi deterministic** wrt D iff

$$H^D(X_i|X_j) \leq \epsilon$$

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$$H^D(X_i|X_j) \leq \epsilon$$

Definition: deterministic DAGs

A DAG G is **deterministic wrt D** iff for every $i \in V$ st $\pi(i) \neq \emptyset$,

$$H^D(X_i|\mathbf{X}_{\pi(i)}) = 0$$

(analogous definition for quasi-deterministic DAGs)

II-3. OPTIMAL BN WITH THE MAXLIKELIHOOD SCORE (1/2)

Proposition 1: Deterministic trees and the MLL score

If $T \in \text{DAG}_V$ is a **deterministic tree** (single-parented DAG) wrt D then T is a solution of BNSL_{MLL} :

$$S_D^{\text{MLL}}(T) = \max_{G \in \text{DAG}_V} S_D^{\text{MLL}}(G)$$

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Proposition 2: Deterministic forests and the MLL score

Let $F \in \text{DAG}_V$ be a **deterministic forest**, and $R(F) \subset V$ its **roots**. If G_R is a solution of BNSL_{MLL} on $\{X_j, j \in R(F)\}$, then $F \cup G_R$ is a solution of BNSL_{MLL} on $\{X_1, \dots, X_n\}$:

$$s_D^{\text{MLL}}(F \cup G_R) = \max_{G \in \text{DAG}_V} s_D^{\text{MLL}}(G)$$

I - Bayesian network structure learning

II - Determinism and Bayesian networks

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IV - Experiments

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Summary of the theoretical results

- If we can relate all variables by a single deterministic tree, then this tree is a optimal solution to $BNSL_{MLL}$
 - If we can relate subsets of the variables by deterministic trees, solving $BNSL_{MLL}$ narrows down to the roots of the trees
- Let's search for deterministic subtrees before solving BNSL!

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→ Let's search for deterministic subtrees before solving BNSL!

What if the target BNSL score is not MLL score ?

Intuition: trees have very small complexity and are therefore also interesting wrt scores such as **BIC** or **BDe**.

III-1. (QUASI-)DETERMINISTIC SCREENING: IDEA

Summary of the theoretical results

- If we can relate all variables by a single deterministic tree, then this tree is a optimal solution to $BNSL_{MLL}$
- If we can relate subsets of the variables by deterministic trees, solving $BNSL_{MLL}$ narrows down to the roots of the trees

→ Let's search for deterministic subtrees before solving BNSL!

What if the target BNSL score is not MLL score ?

Intuition: trees have very small complexity and are therefore also interesting wrt scores such as **BIC** or **BDe**.

What about quasi-determinism ?

Empirical determinism is rare, however very strong relationships (i.e. very low conditional entropies) are common

→ Let's search for quasi-deterministic subtrees before solving BNSL!

Algorithm 1 Bayesian network structure learning with quasi deterministic screening (qds-BNSL)

Input: D, ϵ , sota-BNSL

- 1: Compute F_ϵ by running **qd-screening** with D and ϵ
- 2: Identify $R(F_\epsilon) = \{i \in \llbracket 1, n \rrbracket \mid \pi^{F_\epsilon}(i) = \emptyset\}$, the set of F_ϵ 's roots.
- 3: Compute $G_{R(F_\epsilon)}^*$ by running sota-BNSL on $\mathbf{X}_{R(F_\epsilon)}$
- 4: $G_\epsilon^* \leftarrow F_\epsilon \cup G_{R(F_\epsilon)}^*$

Output: G_ϵ^*

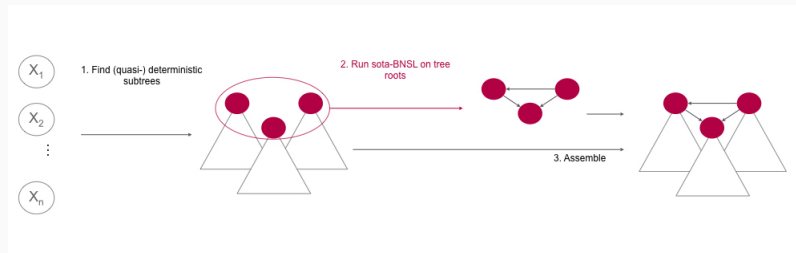
III-2. BNSL WITH QD-SCREENING: ALGORITHM

Algorithm 2 Bayesian network structure learning with quasi deterministic screening (qds-BNSL)

Input: D , ϵ , sota-BNSL

- 1: Compute F_ϵ by running **qd-screening** with D and ϵ
- 2: Identify $R(F_\epsilon) = \{i \in \llbracket 1, n \rrbracket \mid \pi^{F_\epsilon}(i) = \emptyset\}$, the set of F_ϵ 's roots.
- 3: Compute $G_{R(F_\epsilon)}^*$ by running sota-BNSL on $X_{R(F_\epsilon)}$
- 4: $G_\epsilon^* \leftarrow F_\epsilon \cup G_{R(F_\epsilon)}^*$

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Algorithm 3 Bayesian network structure learning with quasi deterministic screening (qds-BNSL)

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- 3: Compute $G_{R(F_\epsilon)}^*$ by running sota-BNSL on $X_{R(F_\epsilon)}$
- 4: $G_\epsilon^* \leftarrow F_\epsilon \cup G_{R(F_\epsilon)}^*$

Output: G_ϵ^*

Complexity

- **qd-screening:** $O(n^2)$
- **qds-BNSL:** calls **sota-BNSL** on $|R(F_\epsilon)| \leq n$ variables (exact BNSL: $O(2^p)$, heuristics are very time-intensive as well)

We expect qds-BNSL to be faster than sota-BNSL when $|R(F_\epsilon)| < n$ (Rahier et al., 2018)

I - Bayesian network structure learning

II - Determinism and Bayesian networks

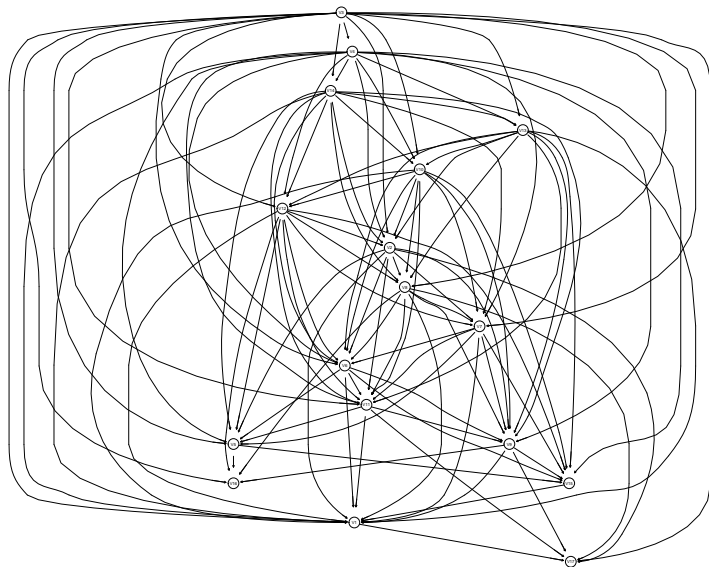
III - Structure learning with (quasi-)determinism screening

IV - Experiments

V - Discussion

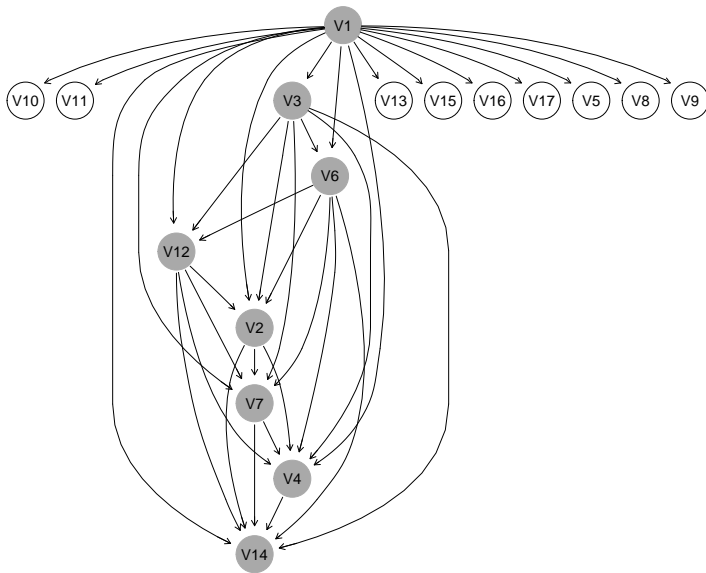
IV-1. BAYESIAN NETWORKS LEARNT ON THE MSNBC DATASET: BASELINE

BN learnt on dataset 'msnbc' with sota-BNSL

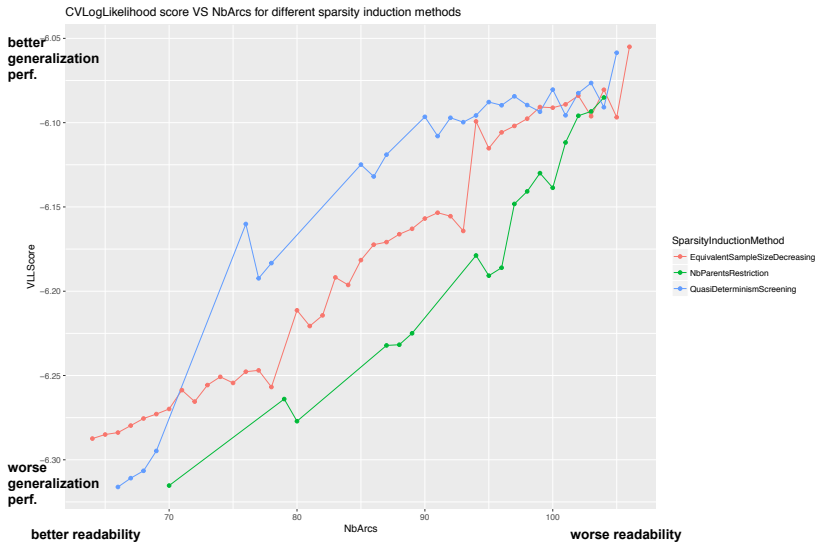


IV-1. BAYESIAN NETWORKS LEARNT ON THE MSNBC DATASET: QDS

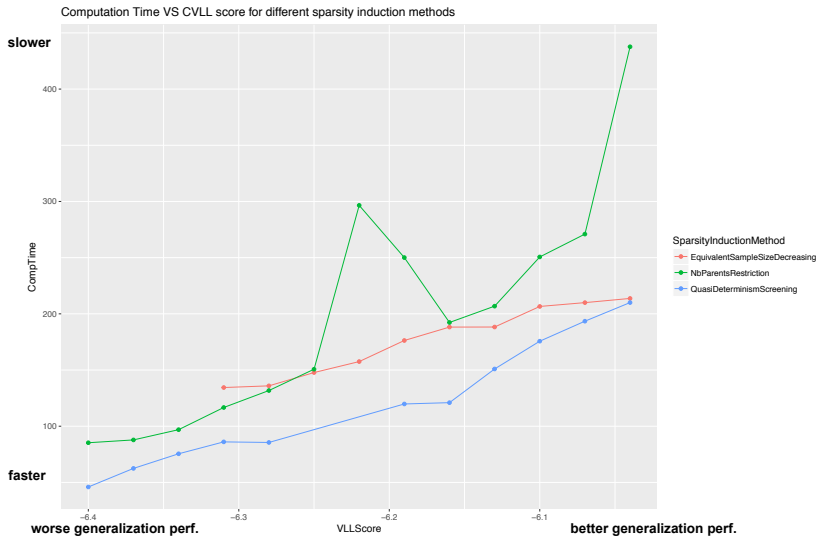
BN learnt on dataset 'msnbc' with qds-BNSL (eps_0.5)



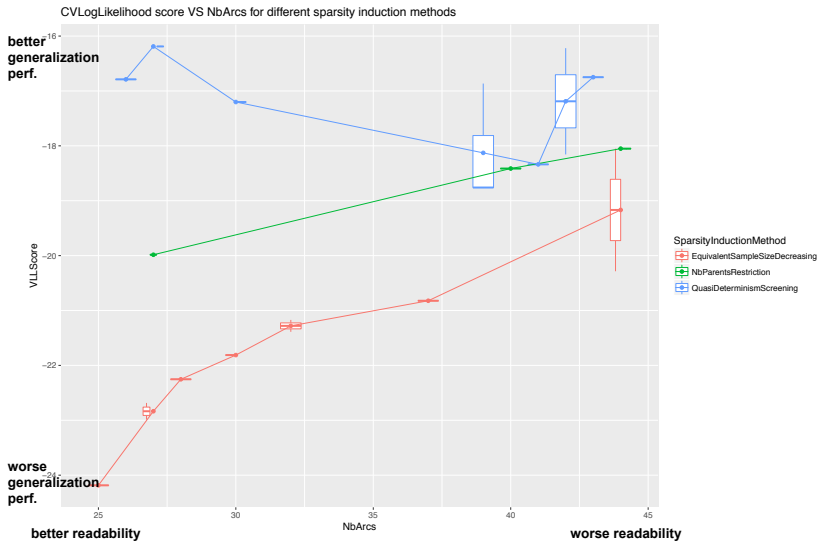
IV-2. PERFORMANCE/READABILITY TRADEOFF - MSNBC DATASET



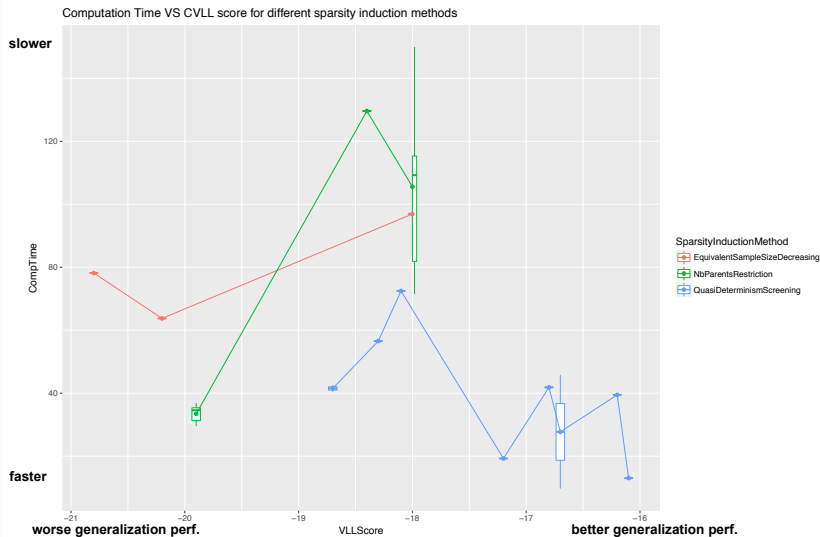
IV-3. PERFORMANCE/COMPUTATION TIME TRADEOFF - MSNBC DATASET



IV-4. PERFORMANCE / READABILITY TRADEOFF - PIU DATASET



IV-5. PERFORMANCE/COMPUTATION TIME TRADEOFF - PIU DATASET



I - Bayesian network structure learning

II - Determinism and Bayesian networks

III - Structure learning with (quasi-)determinism screening

IV - Experiments

V - Discussion

Summary

- Deterministic screening is **consistent wrt the MLL score**
- BN learnt via qds-BNSL have often have a very interesting **performance-vs-readability** tradeoff, and are consistently **faster** to compute for a given performance score than with usual methods

However these properties depend highly on the dataset

Summary

- Deterministic screening is **consistent wrt the MLL score**
- BN learnt via qds-BNSL have often have a very interesting **performance-vs-readability** tradeoff, and are consistently **faster** to compute for a given performance score than with usual methods

However these properties depend highly on the dataset

Perspectives

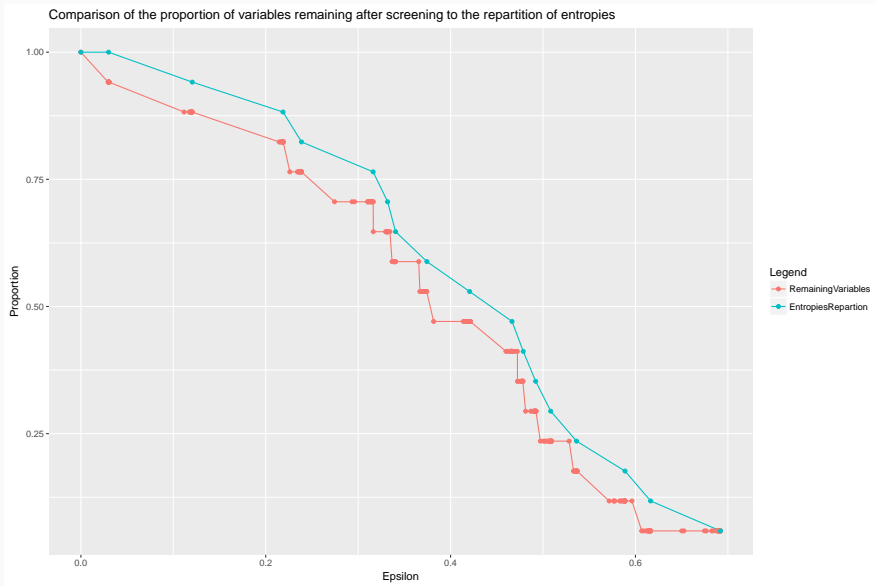
In the future we plan to

- Search for **guarantees** of qds-BNSL wrt scores as BIC, BDe or CVLL
- Look for a **criteria** that enables us to choose ϵ in a principled way

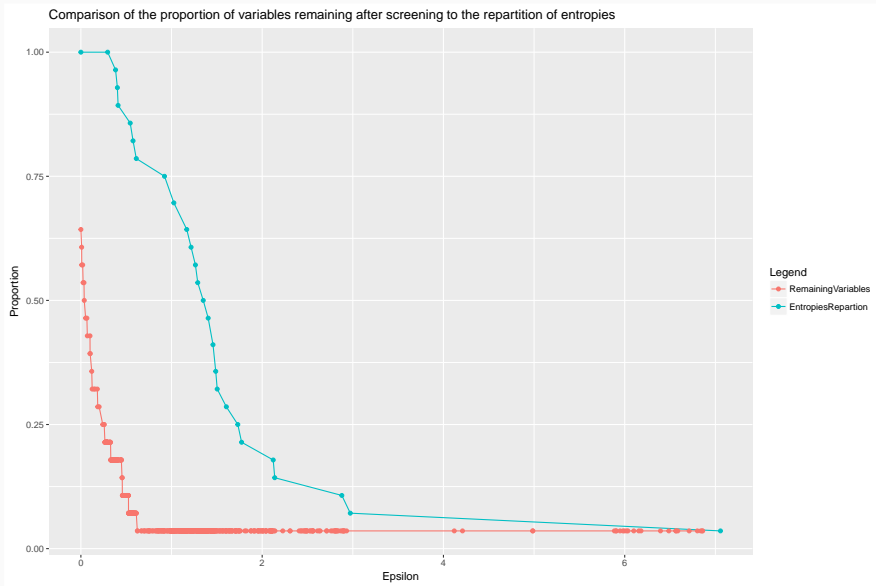
THANK YOU

MORE RESULTS

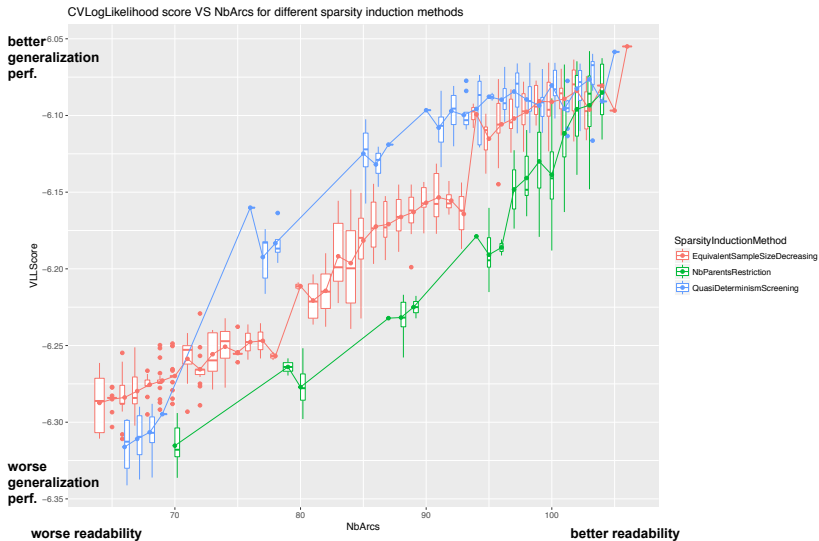
V-2. CANDIDATE CRITERION FOR CHOICE OF ϵ - MSNBC DATASET



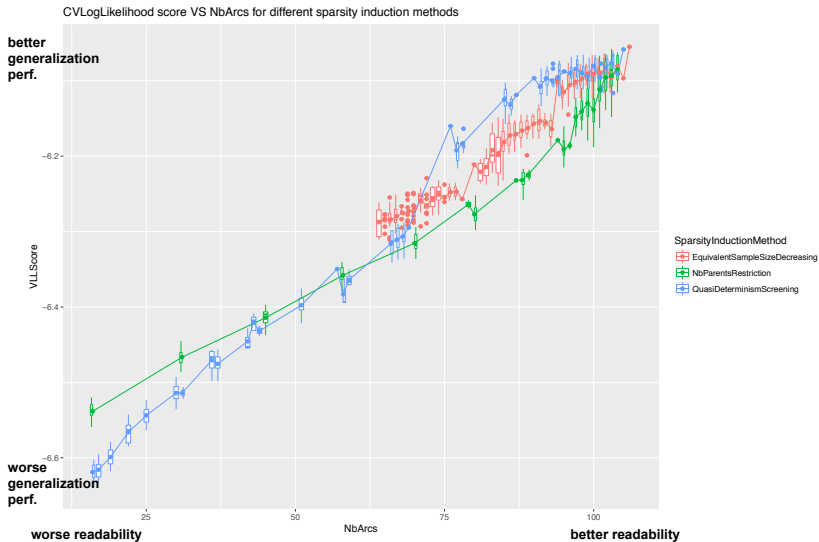
V-3. CANDIDATE CRITERION FOR CHOICE OF ϵ - PIU DATASET



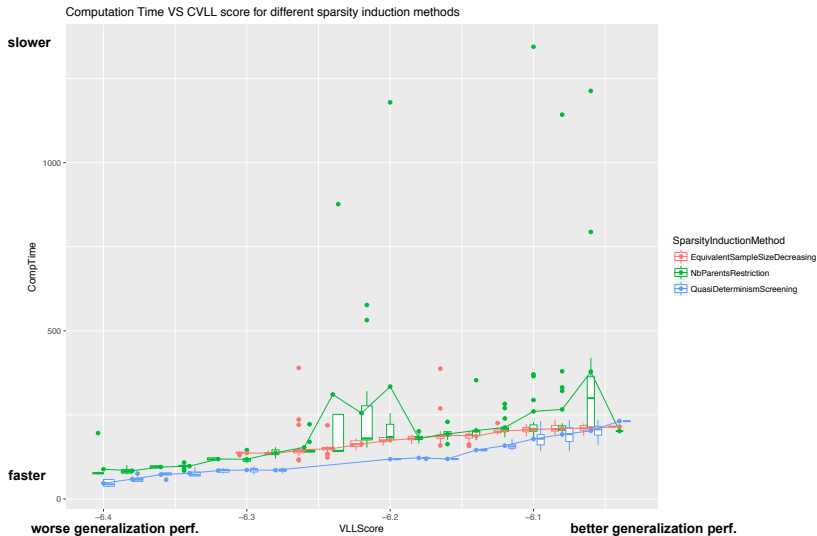
APP 1. PERFORMANCE/READABILITY TRADEOFF - MSNBC DATASET (1/2)



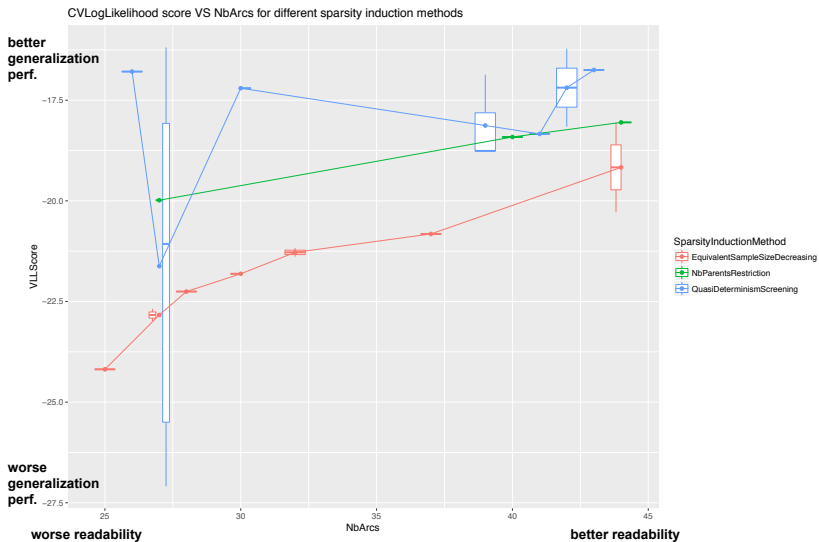
APP 1. PERFORMANCE/READABILITY TRADEOFF - MSNBC DATASET (2/2)



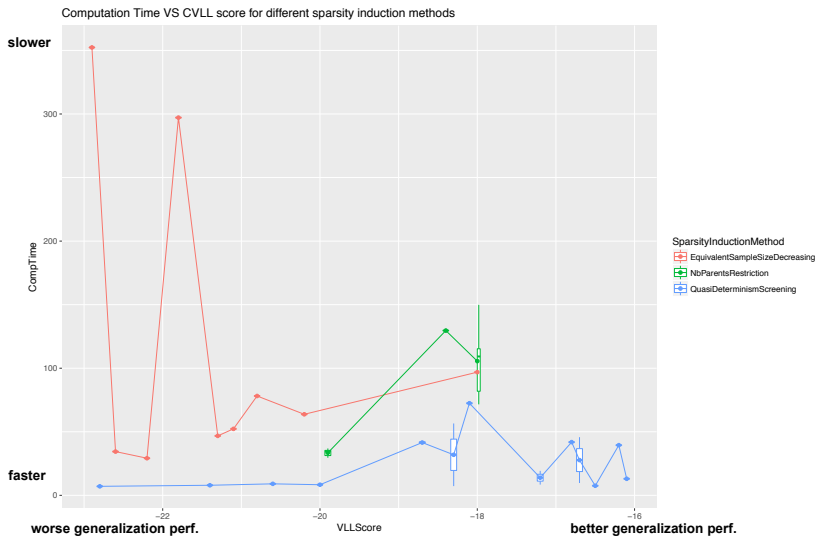
APP 2. PERFORMANCE/TIME TRADEOFF - MSNBC DATASET



APP 3. PERFORMANCE/READABILITY TRADEOFF - PIU DATASET



APP 4. PERFORMANCE/TIME TRADEOFF - PIU DATASET

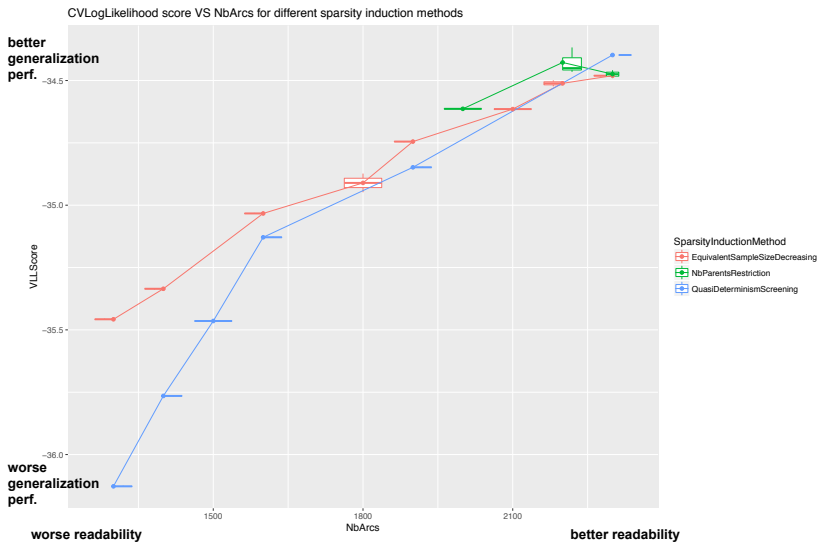


Algorithm 4 Quasi-determinism screening (qds)

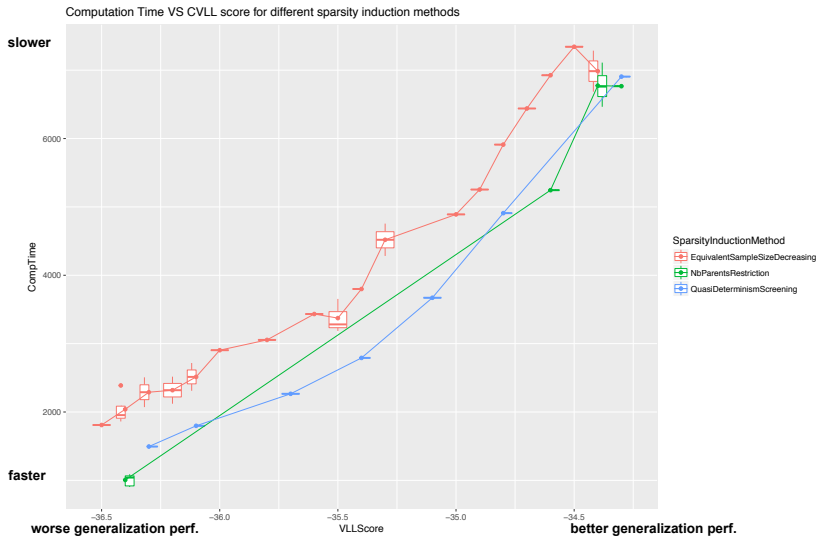
Input: D, ϵ

- 1: Compute empirical cond. entropy matrix $\mathbb{H}^D = (\mathbb{H}^D(X_i|X_j))_{1 \leq i, j \leq n}$
 - 2: **for** $i = 1$ to n **do**
 - 3: compute $\pi_\epsilon(i) = \{j \in \llbracket 1, n \rrbracket \setminus \{i\} \mid \mathbb{H}_{ij}^D \leq \epsilon\}$
 - 4: **for** $i = 1$ to n **do**
 - 5: **if** $\exists j \in \pi_\epsilon(i)$ s.t. $i \in \pi_\epsilon(j)$ **then**
 - 6: **if** $\mathbb{H}_{ij}^D \leq \mathbb{H}_{ji}^D$ **then** $\pi_\epsilon(j) \leftarrow \pi_\epsilon(j) \setminus \{i\}$
 - 7: **else** $\pi_\epsilon(i) \leftarrow \pi_\epsilon(i) \setminus \{j\}$
 - 8: **for** $i = 1$ to n **do**
 - 9: $\pi_\epsilon^*(i) \leftarrow \underset{j \in \pi_\epsilon(i)}{\operatorname{argmin}} |\operatorname{Val}(X_j)|$
 - 10: Compute forest $F_\epsilon = (V_{F_\epsilon}, A_{F_\epsilon})$, where
 - $V_{F_\epsilon} = \llbracket 1, n \rrbracket$
 - $A_{F_\epsilon} = \{(\pi_\epsilon^*(i), i) \mid i \in \llbracket 1, n \rrbracket \text{ s.t. } \pi_\epsilon^*(i) \neq \emptyset\}$
- Output:** F_ϵ

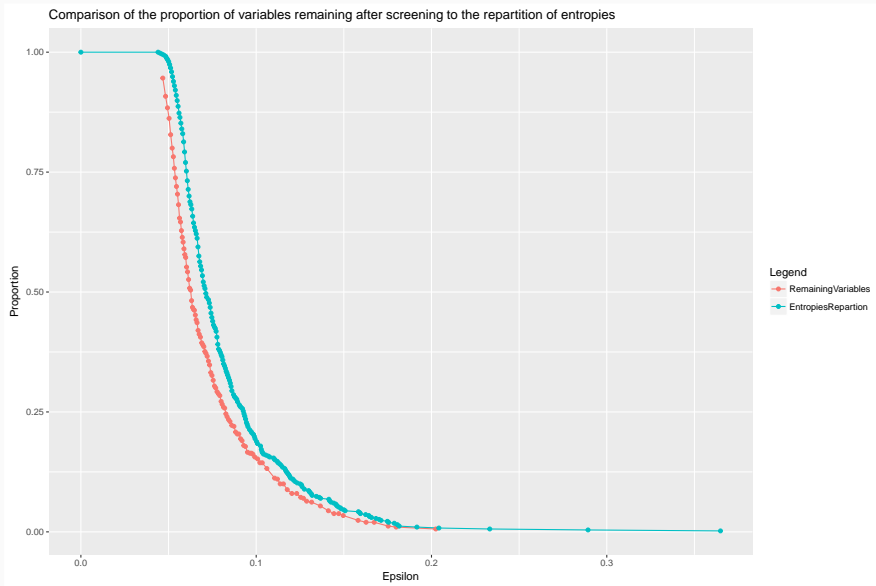
APP 6. PERFORMANCE/READABILITY TRADEOFF - BOOK DATASET



APP 7. PERFORMANCE/COMPUTATION TIME TRADEOFF - BOOK DATASET



APP 8.. CANDIDATE CRITERION FOR CHOICE OF ϵ - BOOK DATASET



Thibaud Rahier, Sylvain Marié, Stéphane Girard, and Florence Forbes. Fast bayesian network structure learning using quasi-determinism screening. In JFRB 2018-9èmes Journées Francophones sur les Réseaux Bayésiens et les Modèles Graphiques Probabilistes, pages 14–24, 2018.