Screening strong pairwise relationships for fast Bayesian network structure learning

Thibaud Rahier, Sylvain Marié, Stéphane Girard, Florence Forbes

SCREENING STRONG PAIRWISE RELATIONSHIPS FOR FAST BAYESIAN NETWORK STRUCTURE LEARNING

IFSS 2018

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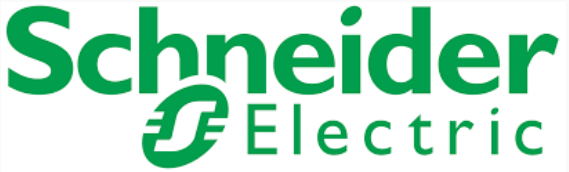
September 7, 2018

INRIA - Schneider Electric



OUTLINE

I - Bayesian network structure learning

II - Determinism and Bayesian networks

III - Structure learning with (quasi-)determinism screening

IV - Experiments

V - Discussion

OUTLINE

Setting

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

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

- $G = (V, A)$: DAG structure with
  - $V = [\![1, n]\!]$ vertices associated to the n variables
  - $A \subset V^2$ set of arcs
  - $\pi(i)$ the set of parents of i in G

    Factorization of the joint distribution:

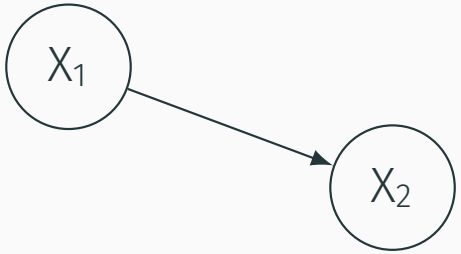
$$P(X_1, \ldots, X_n) = \prod_{i=1}^{n} P(X_i | \mathbf{X}_{\pi(i)})$$

- 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

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



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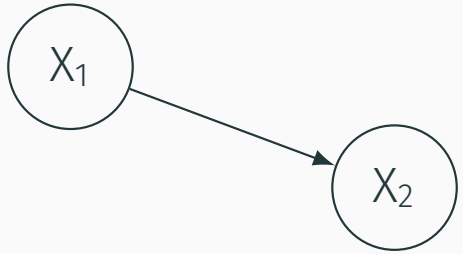

$\Theta = \{\Theta_1, \Theta_2\}$

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

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

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

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

Score&search-based BN structrure learning

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

$$\hat{G} \in \underset{G \in \mathrm{DAG}_V}{\operatorname{argmax}}\, s(G)$$

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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):

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

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As the Bayesian information criterion score (BIC):

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

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As the Bayesian Dirichlet equivalent score (BDe):

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

OUTLINE

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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Linking the entropy with MLL score

The MLL score can be rewritten as

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

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 $\epsilon-$quasi deterministic wrt D iff

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

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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 $T \in \mathrm{DAG}_V$ is a deterministic tree (single-parented DAG) wrt D then T is a solution of $\mathrm{BNSL}_{\mathrm{MLL}}$:

$$s_D^{\mathrm{MLL}}(T) = \max_{G \in \mathrm{DAG}_V} s_D^{\mathrm{MLL}}(G)$$

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Proposition 2: Deterministic forests and the MLL score

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

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

OUTLINE

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

$\rightarrow$ Let's search for deterministic subtrees before solving BNSL!

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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.

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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
$\longrightarrow$ 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 $\mathsf{R}(\mathsf{F}_\epsilon) = \{\mathsf{i} \in [\![1, \mathsf{n}]\!] \mid \pi^{\mathsf{F}_\epsilon}(\mathsf{i}) = \emptyset\}$, the set of F_ϵ's roots.
3: Compute $\mathsf{G}^*_{\mathsf{R}(\mathsf{F}_\epsilon)}$ by running sota-BNSL on $\mathbf{X}_{\mathsf{R}(\mathsf{F}_\epsilon)}$
4: $\mathsf{G}^*_\epsilon \leftarrow \mathsf{F}_\epsilon \cup \mathsf{G}^*_{\mathsf{R}(\mathsf{F}_\epsilon)}$

Output: G^*_ϵ

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

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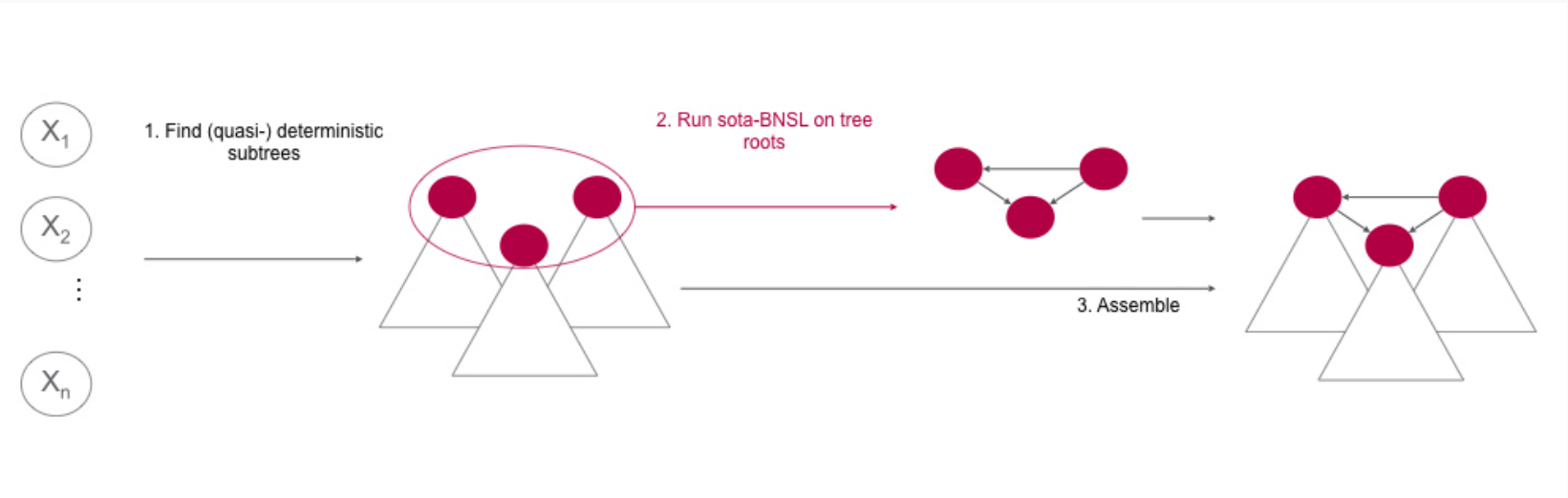
3: Compute $G^*_{R(F_\epsilon)}$ by running sota-BNSL on $\mathbf{X}_{R(F_\epsilon)}$

4: $G^*_\epsilon \leftarrow F_\epsilon \cup G^*_{R(F_\epsilon)}$

Output: G^*_ϵ



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 $\mathbf{X}_{R(F_\epsilon)}$
4: $G^*_\epsilon \leftarrow F_\epsilon \cup G^*_{R(F_\epsilon)}$

Output: G^*_ϵ

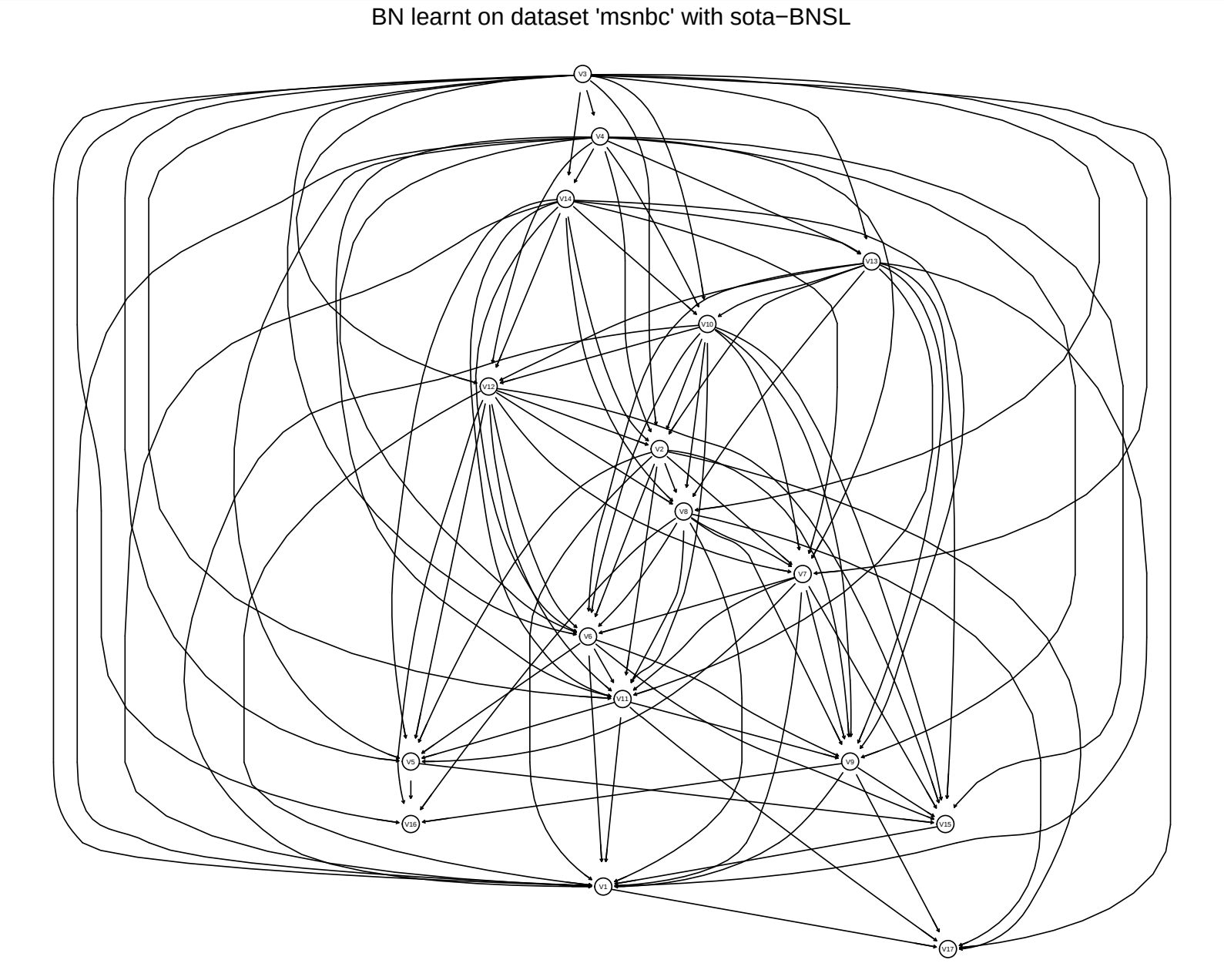
Complexity

- 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)

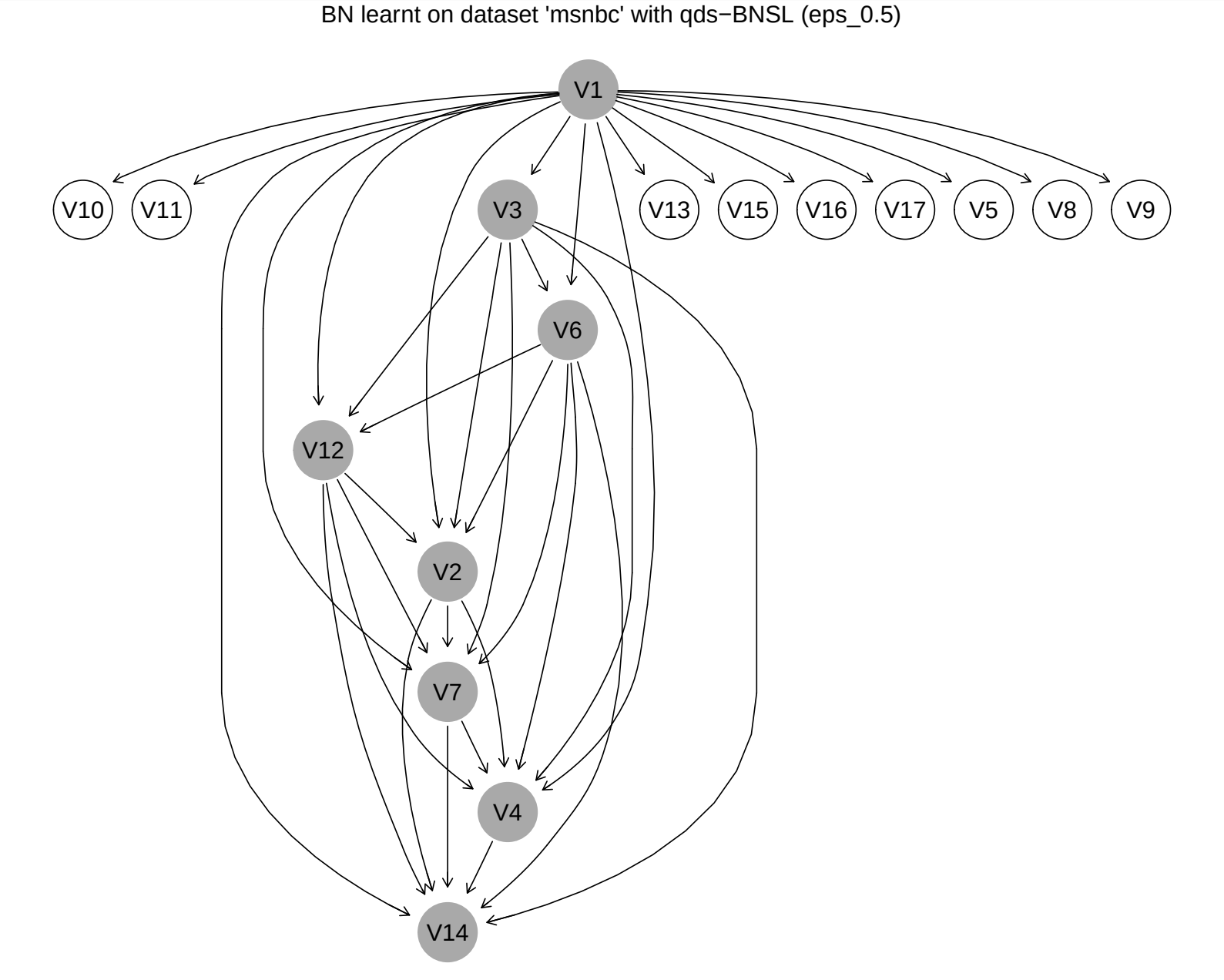
We expect qds-BNSL to be faster than sota-BNSL when $|R(F_\epsilon)| < n$ (Rahier et al., 2018)

OUTLINE

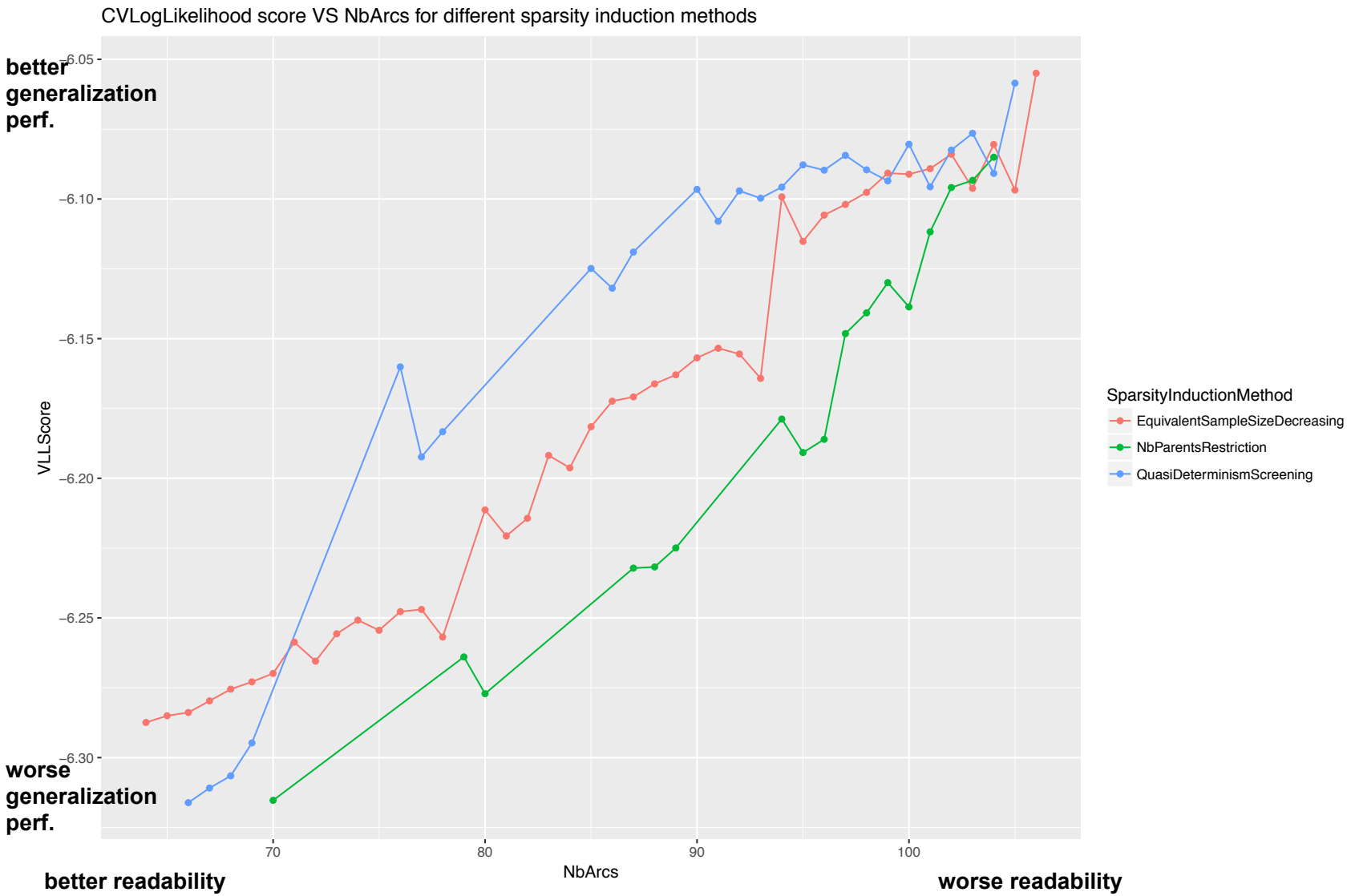
IV-1. BAYESIAN NETWORKS LEARNT ON THE MSNBC DATASET: BASELINE



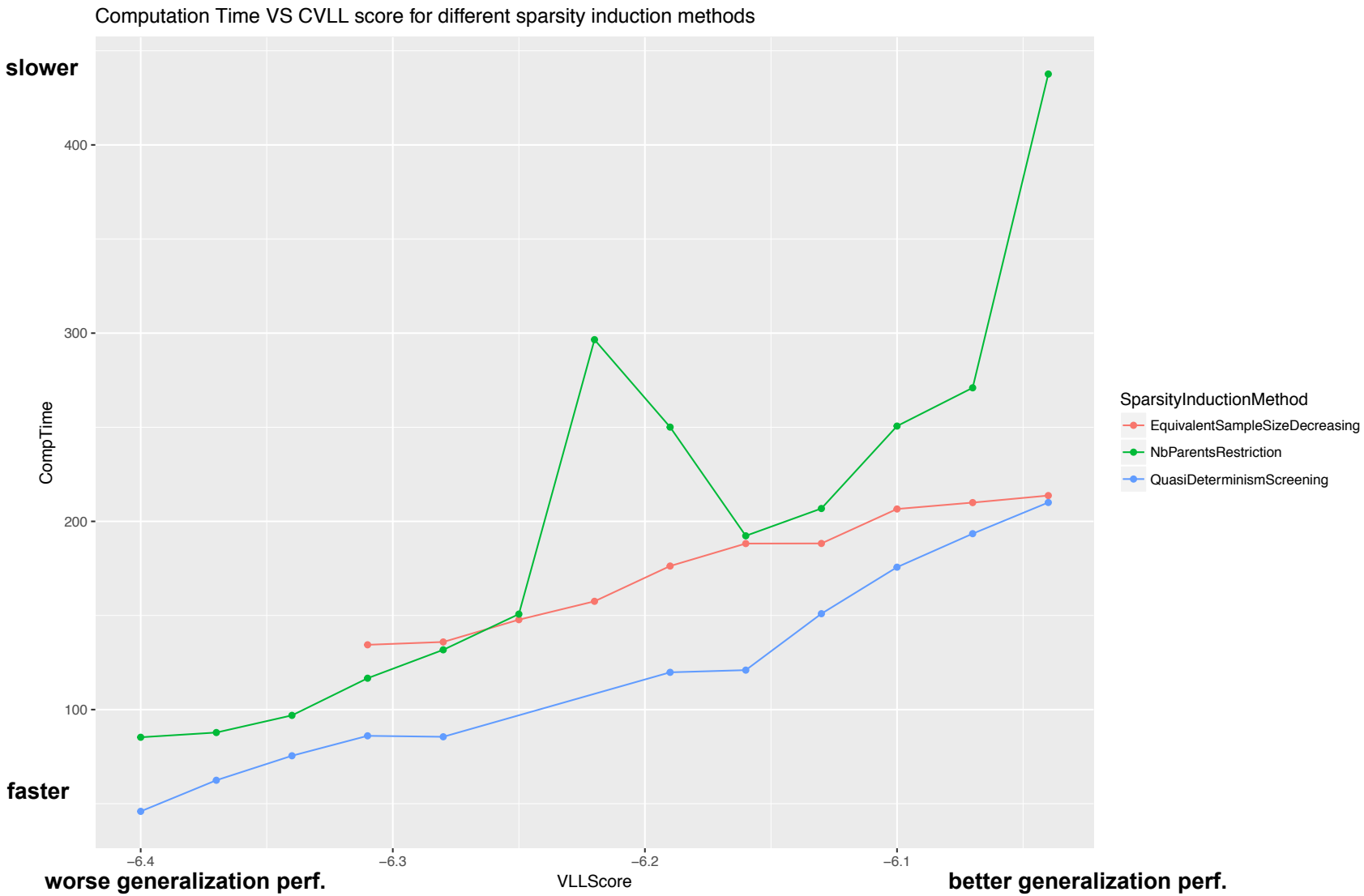
IV-1. BAYESIAN NETWORKS LEARNT ON THE MSNBC DATASET: QDS



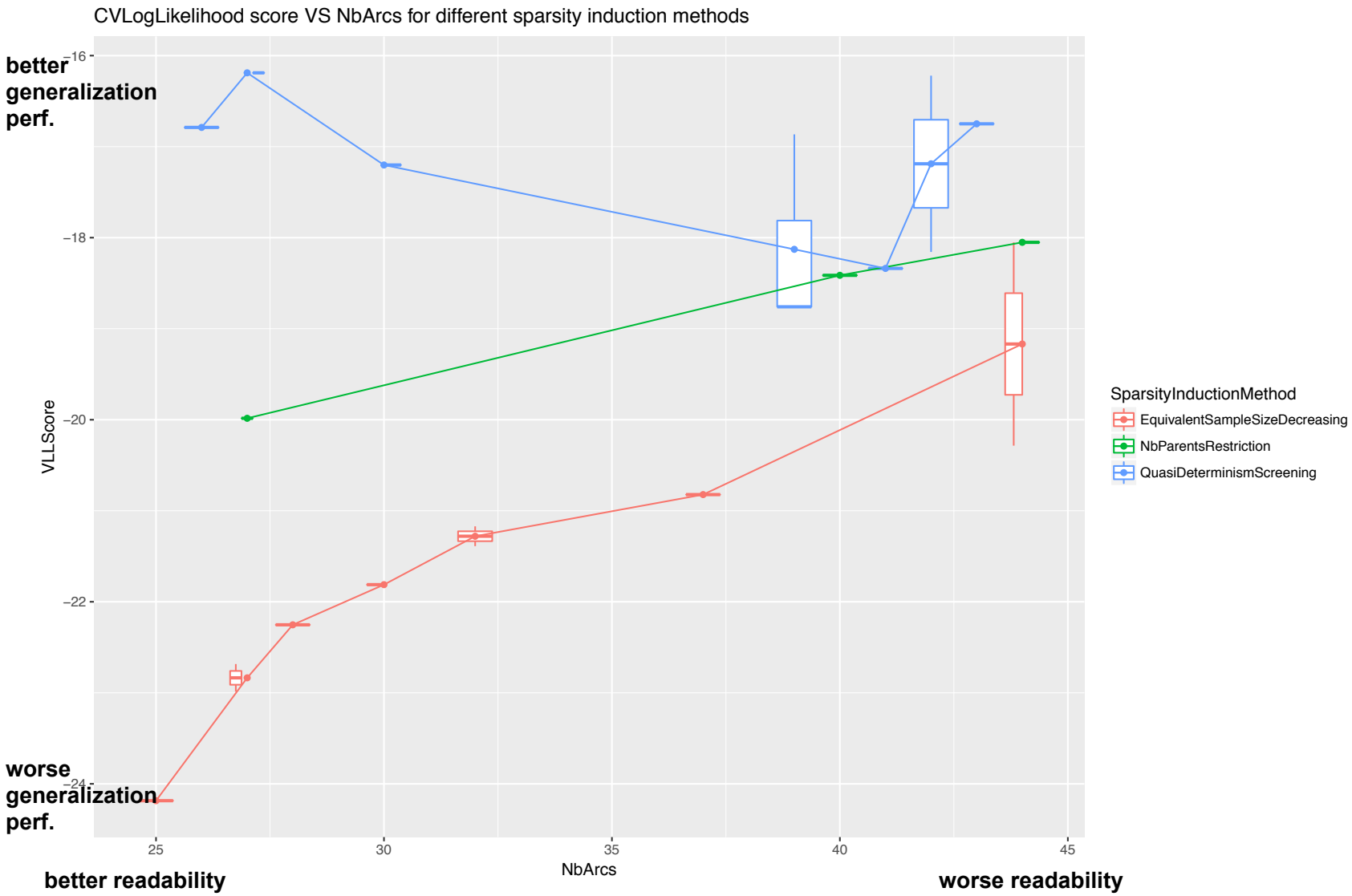
IV-2. PERFORMANCE/READABILITY TRADEOFF - MSNBC DATASET



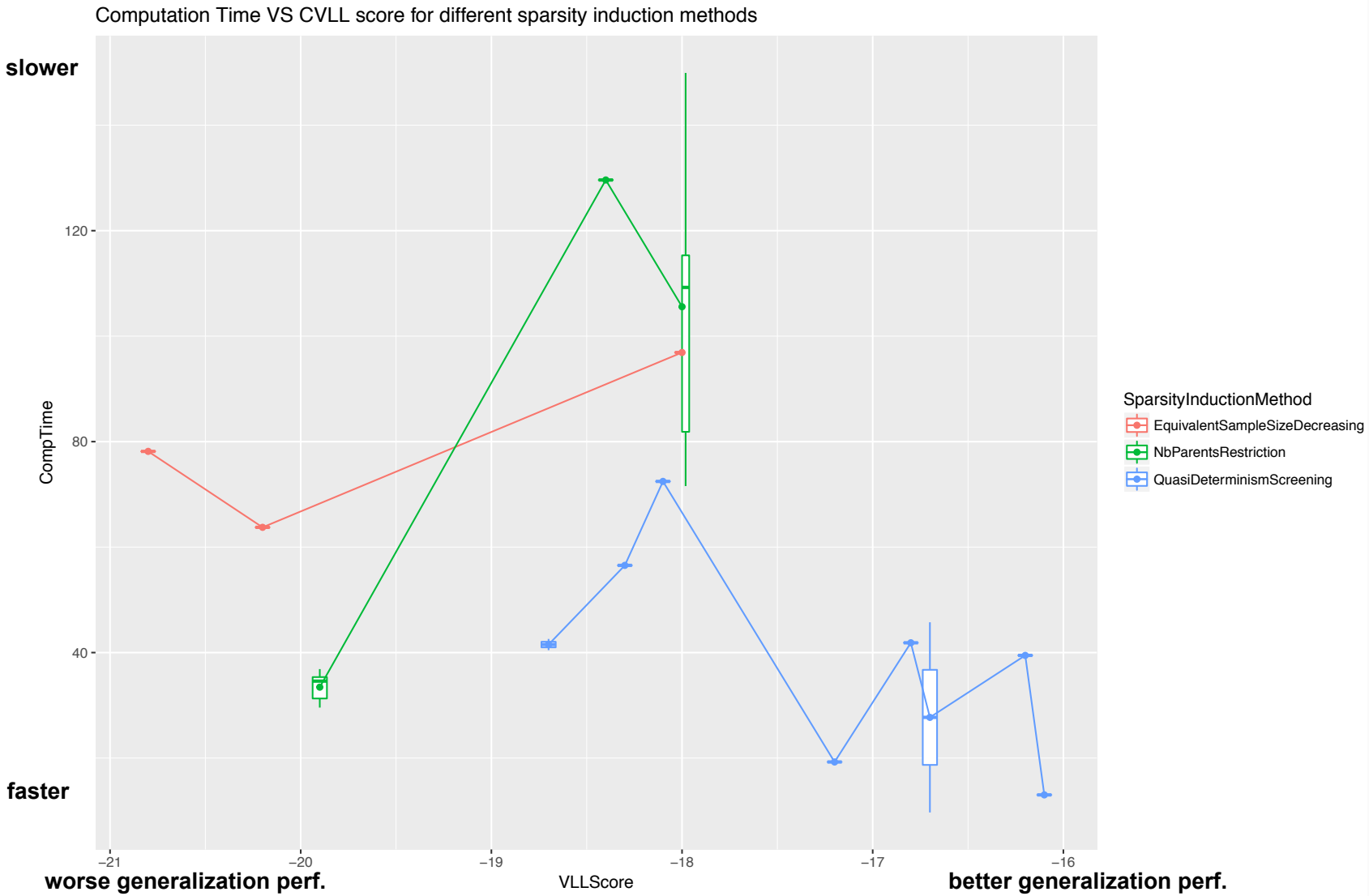
IV-3. PERFORMANCE/COMPUTATION TIME TRADEOFF - MSNBC DATASET



IV-4. PERFORMANCE/READABILITY TRADEOFF - PIU DATASET



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



OUTLINE

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

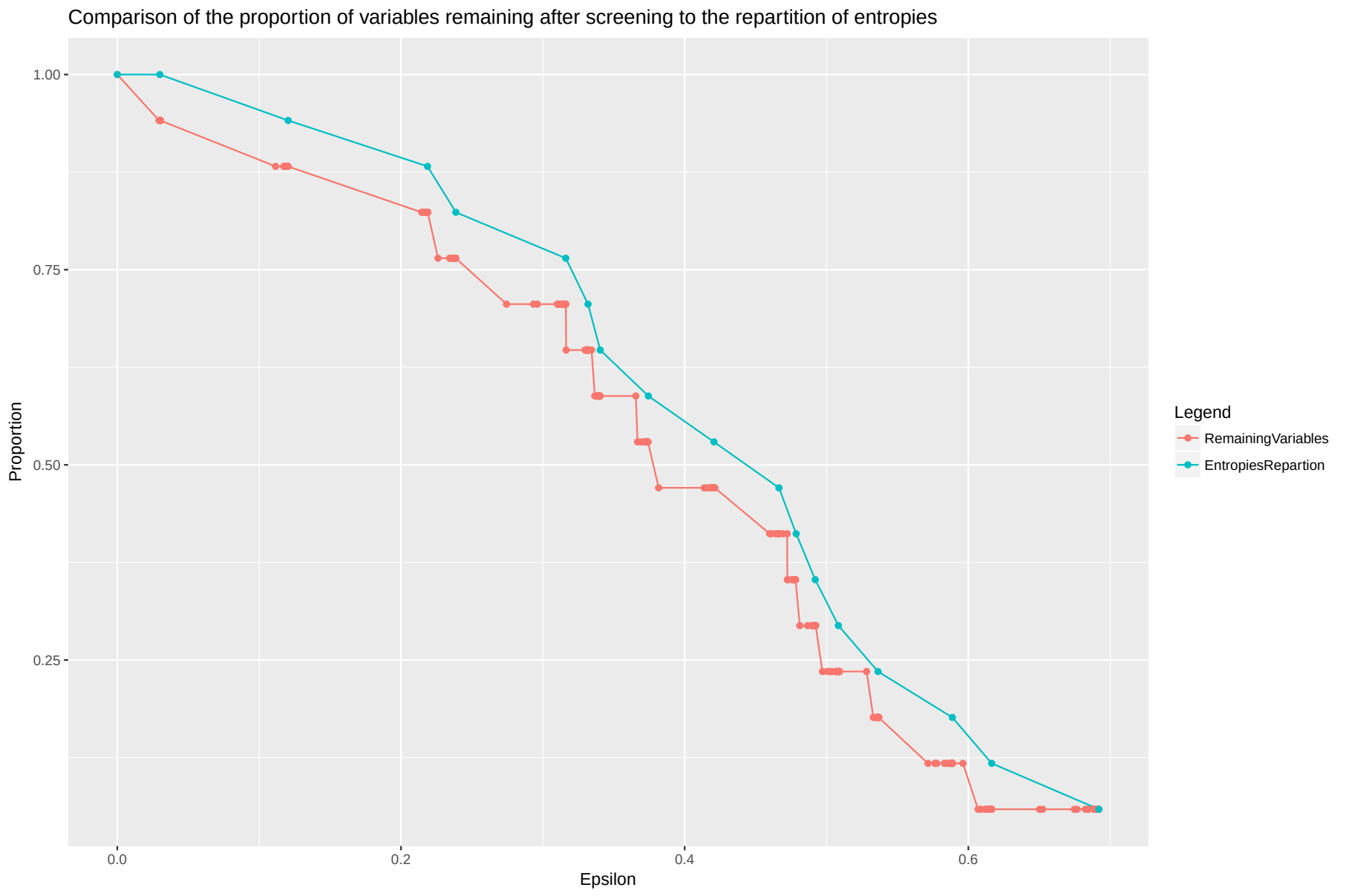
In the future we plan to

- 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



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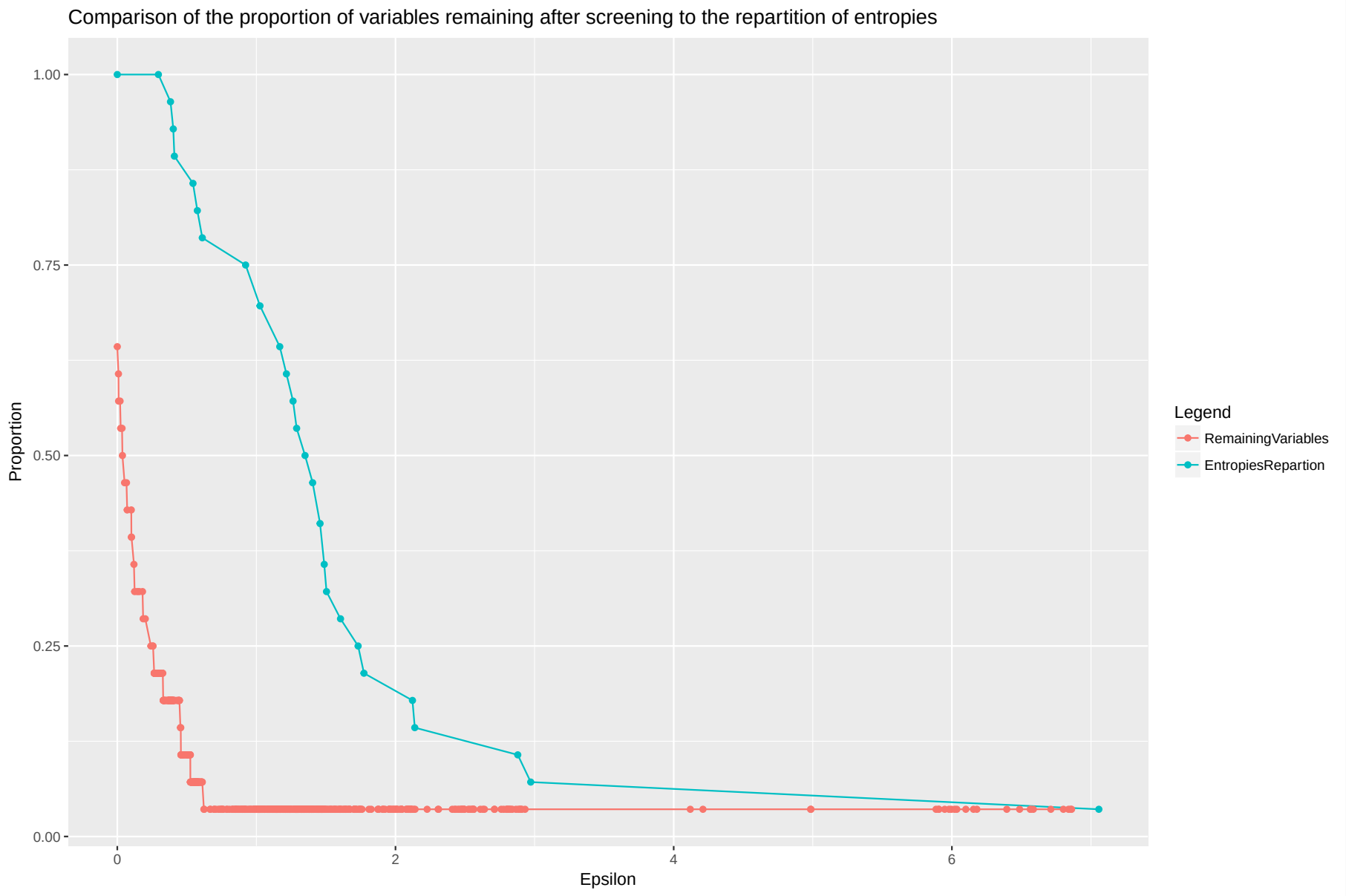
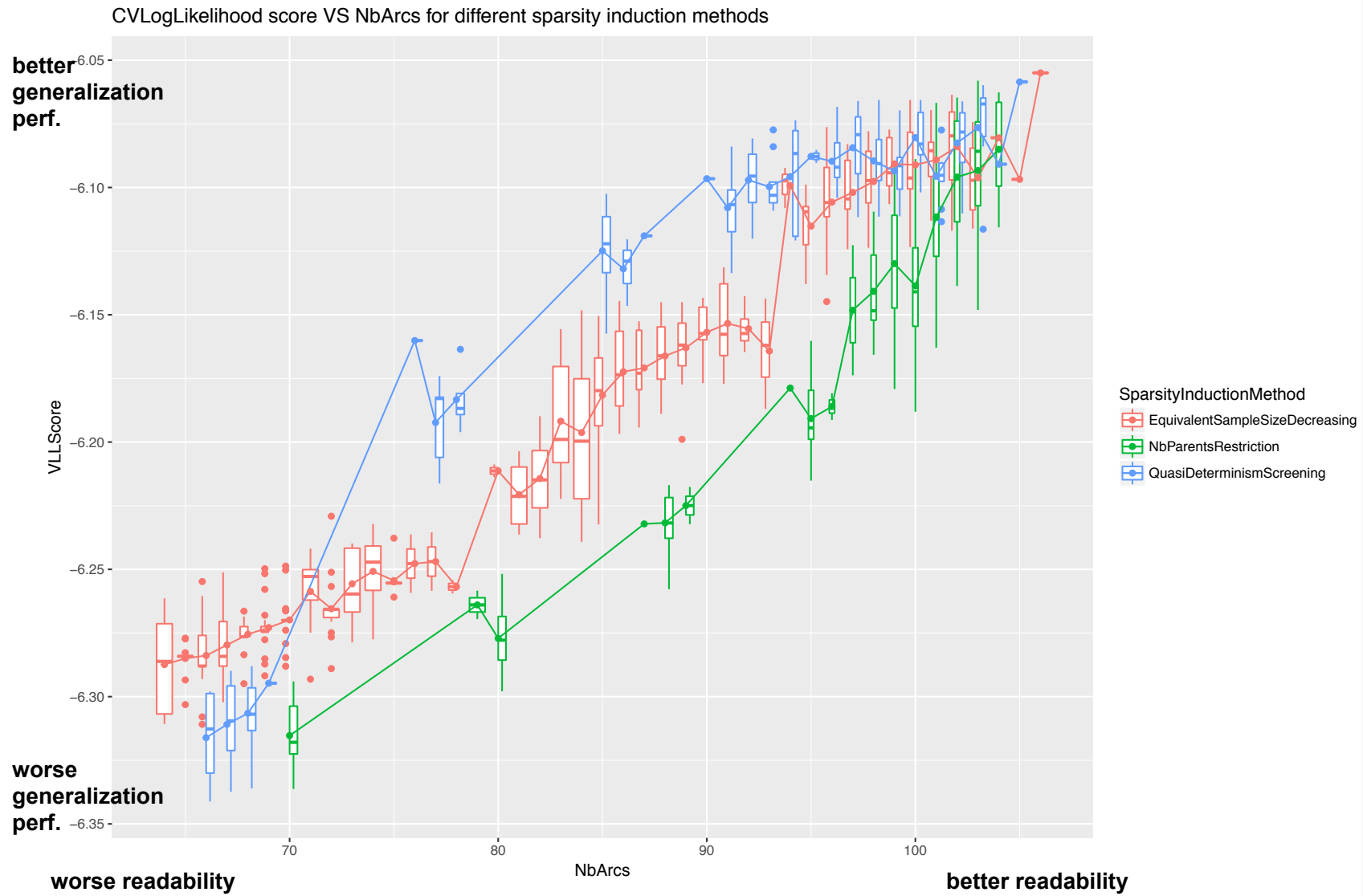
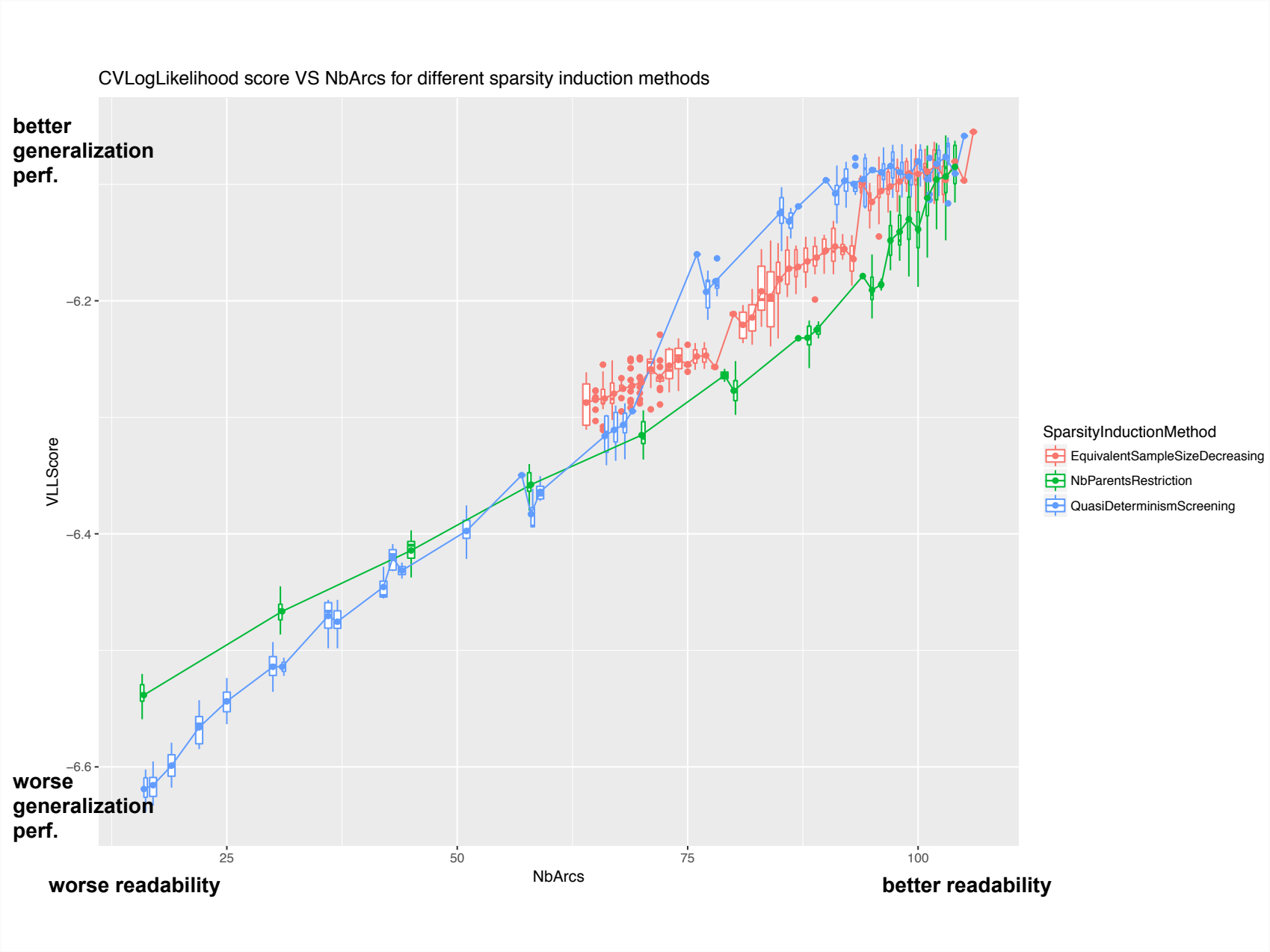


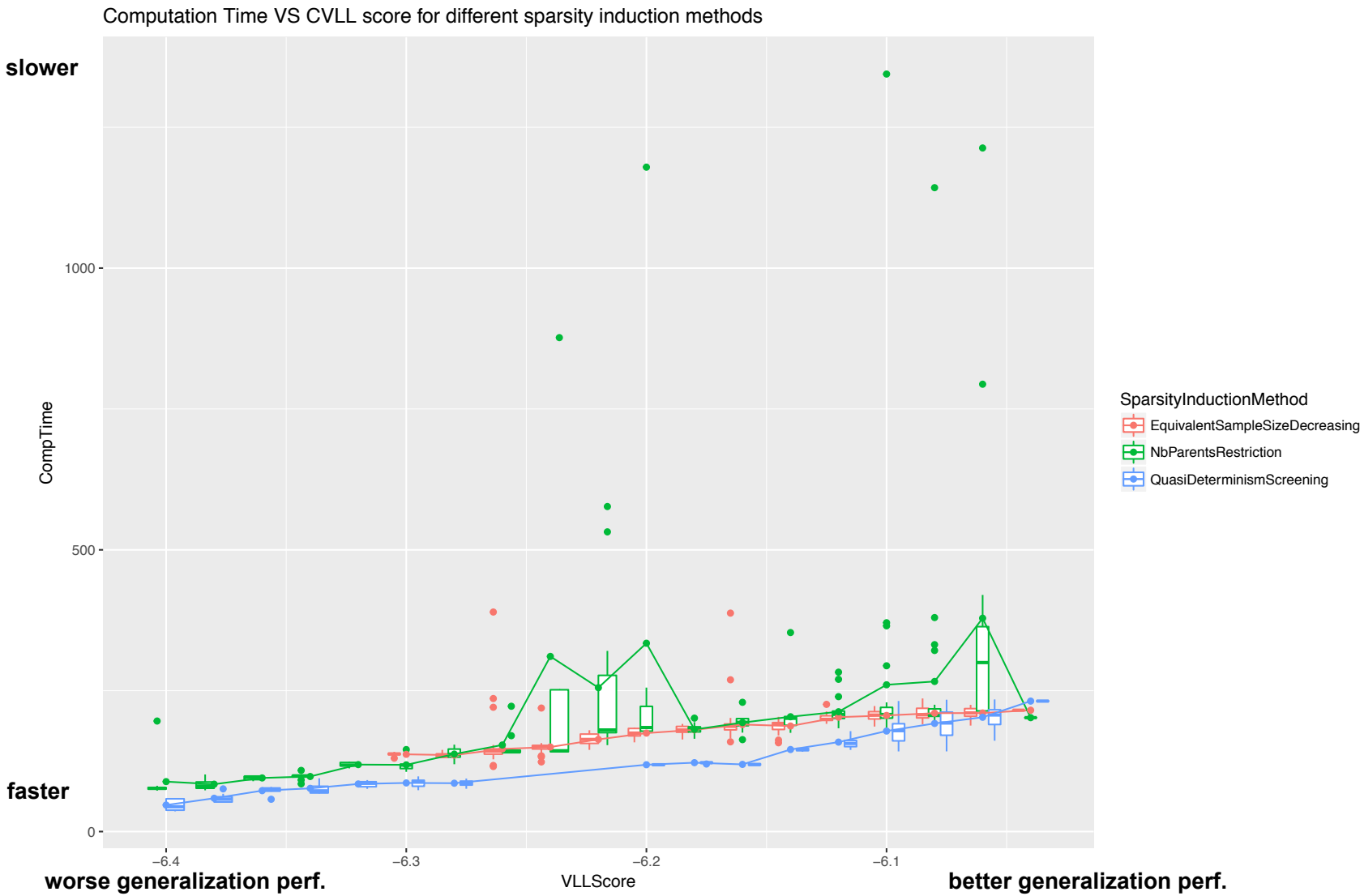
APP 1. PERFORMANCE/READABILITY TRADEOFF - MSNBC DATASET (1/2)



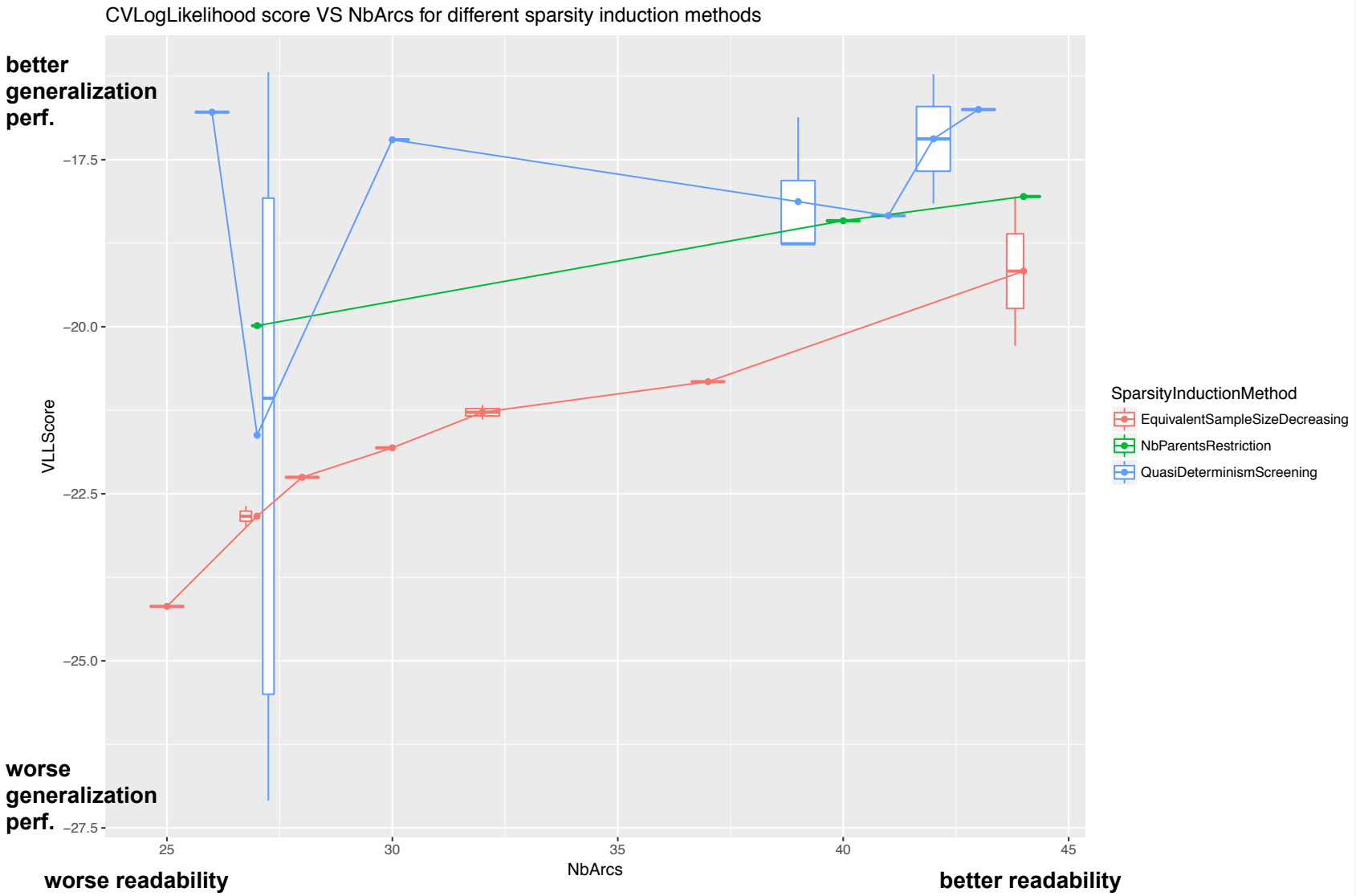
APP 1. PERFORMANCE/READABILITY TRADEOFF - MSNBC DATASET (2/2)



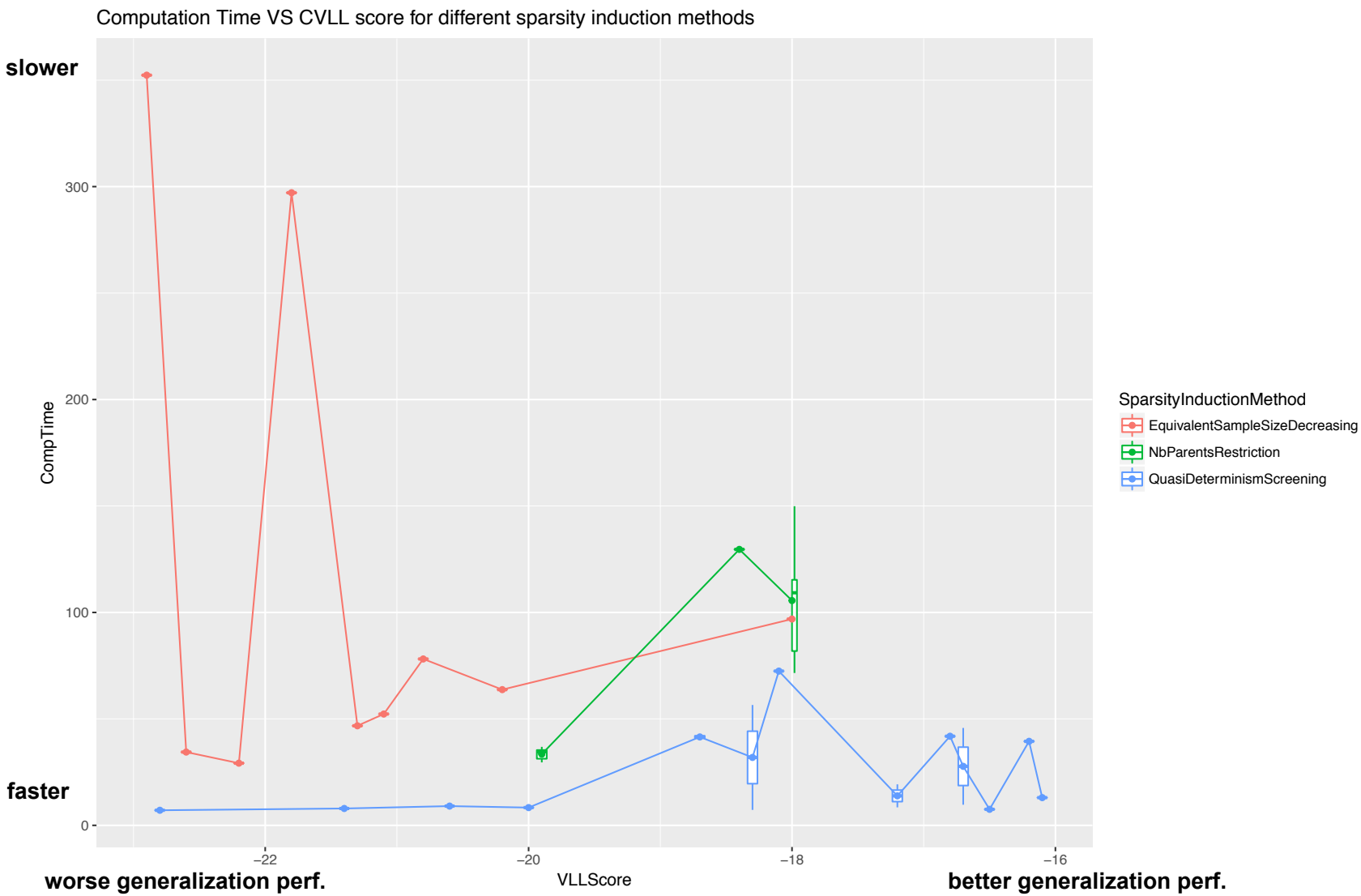
APP 2. PERFORMANCE/TIME TRADEOFF - MSNBC DATASET



APP 3. PERFORMANCE/READABILITY TRADEOFF - PIU DATASET



APP 4. PERFORMANCE/TIME TRADEOFF - PIU DATASET



Algorithm 4 Quasi-determinism screening (qds)

Input: D , ϵ

Compute empirical cond. entropy matrix $\mathbb{H}^D = \left(H^D(X_i|X_j)\right)_{1\leq i,j\leq n}$

for $i = 1$ to n **do**

  compute $\pi_\epsilon(i) = \{j \in [\![1, n]\!] \setminus \{i\} \mid \mathbb{H}^D_{ij} \leq \epsilon\}$

for $i = 1$ to n **do**

  if $\exists j \in \pi_\epsilon(i)$ s.t. $i \in \pi_\epsilon(j)$ **then**

    if $\mathbb{H}^D_{ij} \leq \mathbb{H}^D_{ji}$ **then** $\pi_\epsilon(j) \leftarrow \pi_\epsilon(j) \setminus \{i\}$

    else $\pi_\epsilon(i) \leftarrow \pi_\epsilon(i) \setminus \{j\}$

for $i = 1$ to n **do**

  $\pi^*_\epsilon(i) \leftarrow \underset{j\in\pi_\epsilon(i)}{\operatorname{argmin}} |\mathrm{Val}(X_j)|$

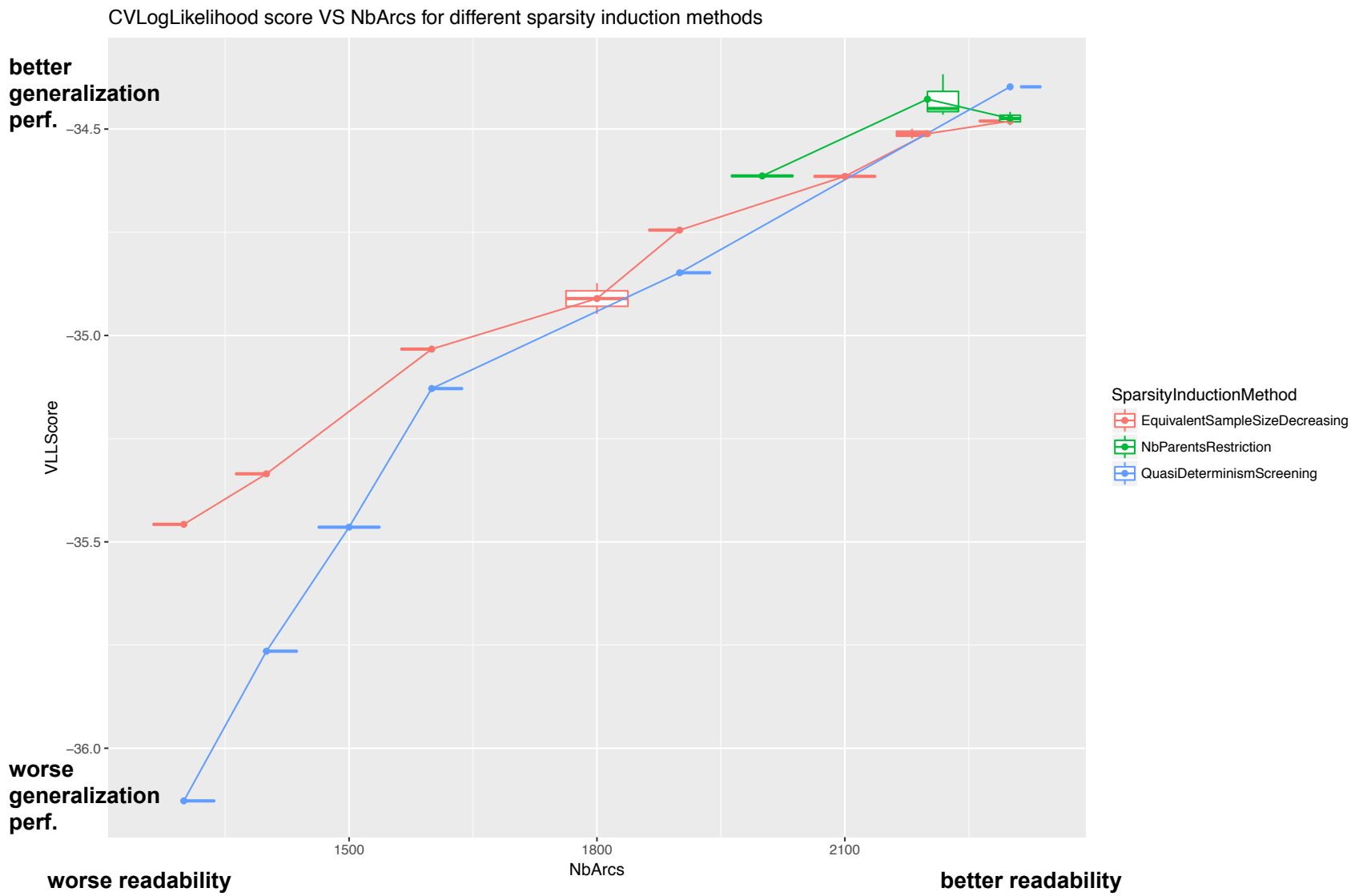
Compute forest $F_\epsilon = (V_{F_\epsilon}, A_{F_\epsilon})$, where

  $V_{F_\epsilon} = [\![1, n]\!]$

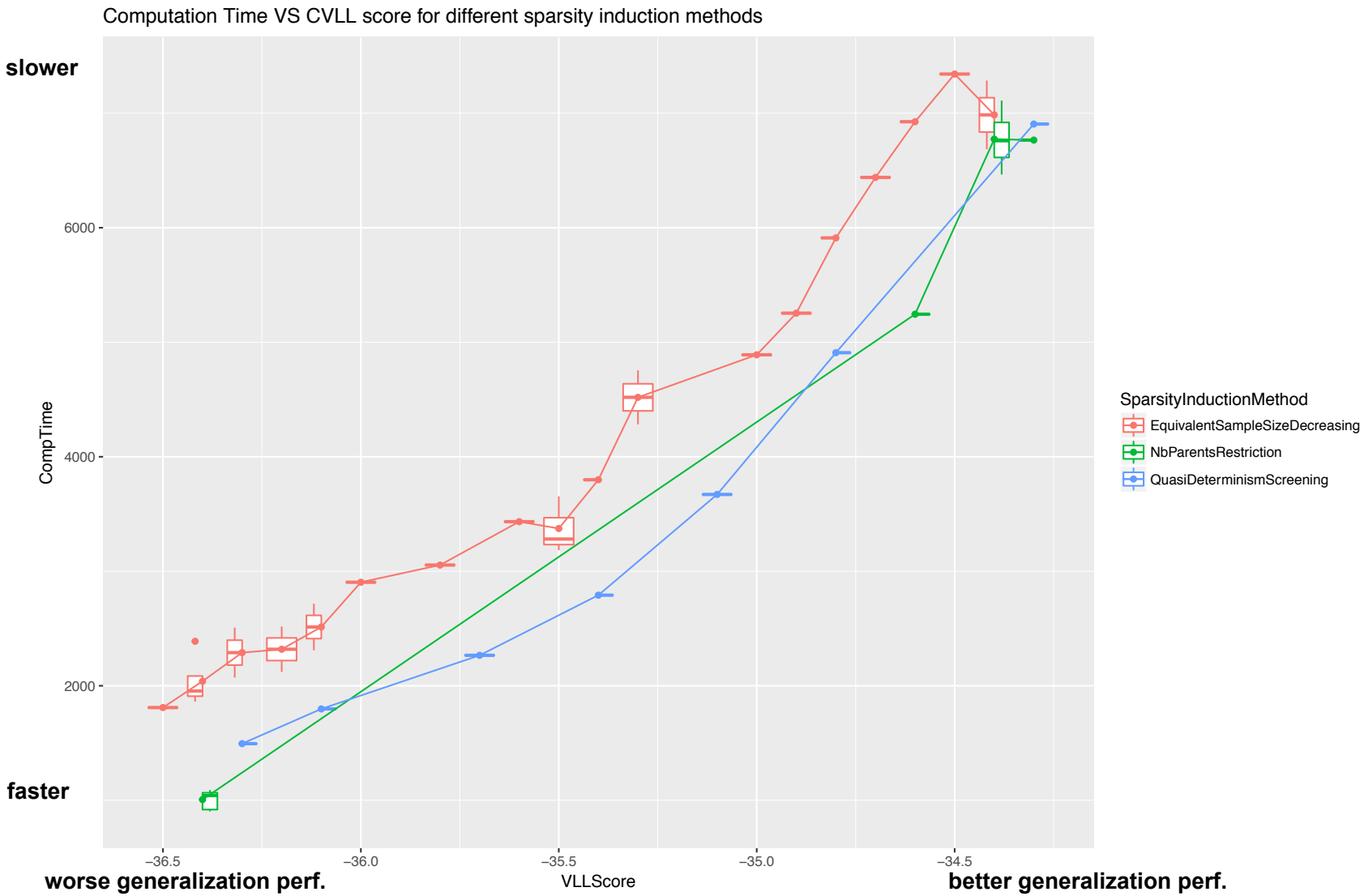
  $A_{F_\epsilon} = \{(\pi^*_\epsilon(i), i) \mid i \in [\![1, n]\!] \text{ s.t. } \pi^*_\epsilon(i) \neq \emptyset\}$

Output: F_ϵ

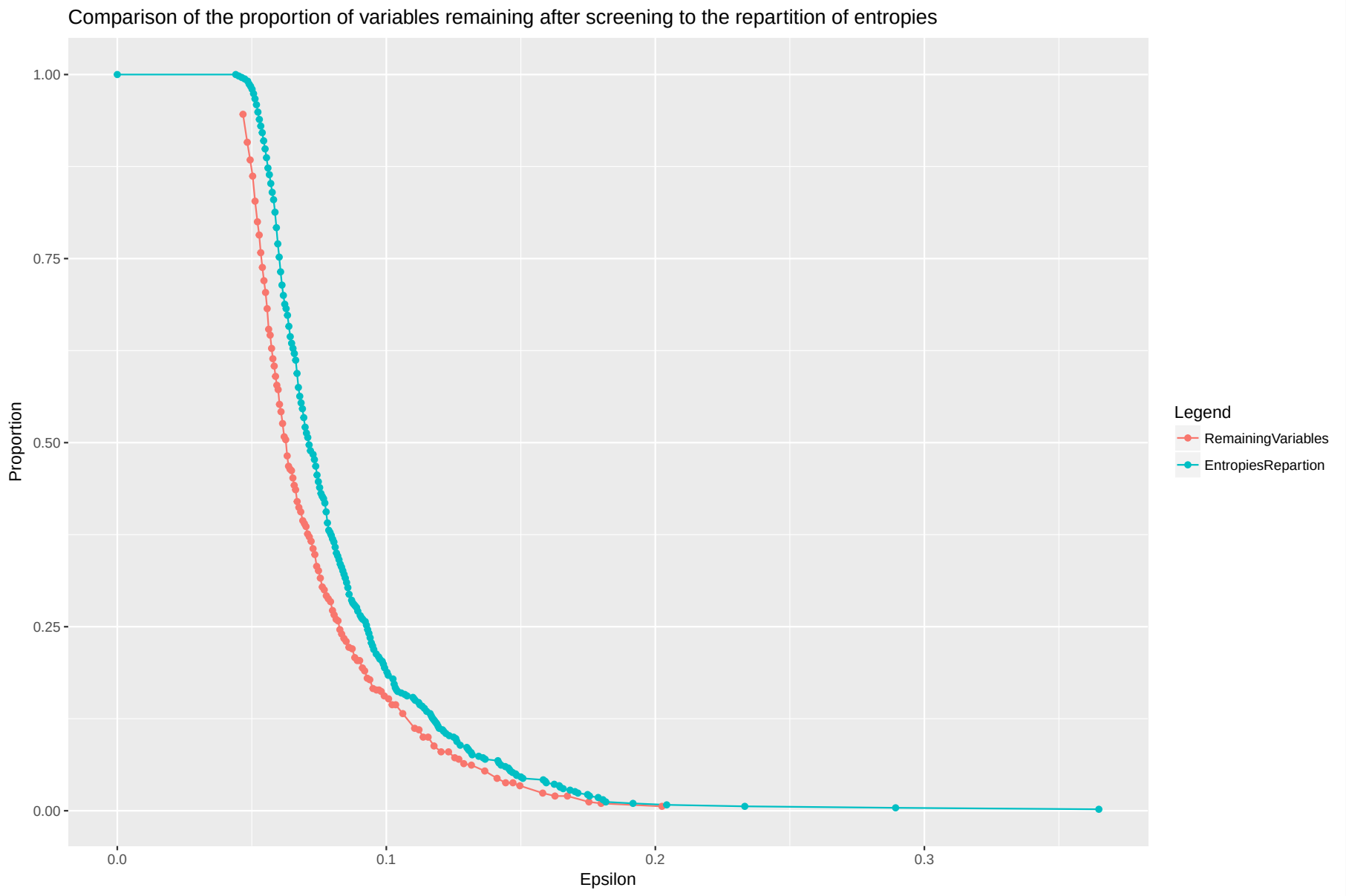
APP 6. PERFORMANCE/READABILITY TRADEOFF - BOOK DATASET



APP 7. PERFORMANCE/COMPUTATION TIME TRADEOFF - BOOK DATASET



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



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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.