A Sparse Structure Learning Algorithm for Bayesian Network Identification from Discrete High-Dimensional Data

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Abstract This paper addresses the problem of learning a sparse structure Bayesian network from high-dimensional discrete data. Compared to continuous Bayesian networks, learning a discrete Bayesian network is a challenging problem due to the large parameter space. Although many approaches have been developed for learning continuous Bayesian networks, few approaches have been proposed for the discrete ones. In this paper, we address learning Bayesian networks as an optimization problem and propose a score function that satisfies the sparsity and the DAG property simultaneously. Besides, we implement a block-wised stochastic coordinate descent algorithm to optimize the score function. Specifically, we use a variance reducing method in our optimization algorithm to make the algorithm work efficiently in high-dimensional data. The proposed approach is applied to synthetic data from well-known benchmark networks. The quality, scalability, and robustness of the constructed network are measured. Compared to some competitive approaches, the results reveal that our algorithm outperforms the others in evaluation metrics.

Keywords Bayesian Network · Structure Learning · Stochastic Gradient Descent · Block-Wised Coordinate Descent

1 Introduction

Bayesian Networks (BNs) are probabilistic graphical models that have been widely used for representing dependencies and independencies among variables of a problem (Zhang et al., 2017; Koller and Friedman, 2009). We can consider a BN as a compact representation of a joint probability distribution function (Margaritis, 2003). A BN consists of a structure which is a Directed Acyclic Graph (DAG), and a parameter set which represents the quantitative information about dependencies among a set of variables. These networks have been widely used in the fields of machine vision (Wu et al., 2020), bioinformatics (Luo et al., 2017), data fusion (Akbar et al., 2018), and decision-making support systems (Cypko et al., 2017). Learning the structure of a BN has attracted a great deal of attention over the last decades. Although many approaches have been developed for learning a continuous BN, there is a lack for the discrete one. The reason is learning a discrete BN is a challenging problem due to the large parameter space and the difficulty in searching for an efficient structure. However, the problem becomes more challenging when we need to learn a sparse BN from high-dimensional discrete data. There is great demand for sparse structures in a broad collection of problems from brain sciences (Hastie et al., 2019) to biological sciences (Cassidy et al., 2014). For example, identifying brain regions interacting in task performance (Li et al., 2008), or modeling the interacting patterns between genes from microarray gene expression data (Rodin and Boerwinkle, 2005) represents high-dimensional data in which the number of samples is equal or less than the number of variables. In addition, many real-world networks, such as gene association networks and brain connectivity networks are sparse (Shuai et al., 2013). Hence, accurately learn-
ing a sparse structure from such datasets is of great importance.

Most methods that have been proposed for BN structure learning fall into three categories: 1) constraint-based methods (Jiang et al., 2018) such as PC (Spirtes et al., 2000), MMPC (Tsamardinos et al., 2006), and FCI (Colombo et al., 2012), 2) score-based methods (Shuai et al., 2013; Adabor et al., 2015), and 3) hybrid methods (Perrier et al., 2008; Dai et al., 2020) such as MMHC (Tsamardinos et al., 2006). With growing tendency toward sparse modeling, score-based methods have attracted more attention since their capability of applying constraints to the score functions.

Score-based methods assign a score to each structure and then search for the structure with the best score. Different score functions such as Bayesian Dirichlet (BD) metric, Bayesian Information Criterion (BIC), Minimum Description Length (MDL), and entropy-based metrics are used in score-based structure learning. After assigning scores, a search algorithm is used to find the optimal structure (with the optimal score). Various search algorithms have been proposed for search step in score-based structure learning methods, such as Hill Climbing (HC), k2 (Cooper and Herskovits, 1992) and Monte Carlo methods (Ninimaki et al., 2016; Zhou, 2011). The most important weakness of score-based methods is that finding an exact structure is an NP-Hard problem (Chickering et al., 2004; Malone, 2015), hence, heuristic search techniques (Scutari et al., 2019), genetic algorithms (Zeng and Ge, 2020; Contaldi et al., 2019) and simulated annealing method (Lee and Kim, 2019) were employed for solving this problem.

BN structure learning can be modeled as an optimization problem. By adding a penalty term to the score function, conditions such as sparsity and DAG property of BN can be modeled in the score function. By optimizing the new score function, we can find the best sparse structure. Sparse Candidate (SC) ( Friedman et al., 2013), L1MB-DAG (Schmidt et al., 2007) which uses LASSO to select a sparse structure, and SBN (Zhang et al., 2017) which proposed for Gaussian data are some examples of this approach. In another research (Shojaie and Michaileidis, 2010), the DAG estimation problem has been formulated as a linear regression. Fu and Zhou (2013) used a maximum likelihood function with a L1 penalty term as score function. Afterward, this algorithm has been expanded to use a concave penalty term (Aragam and Zhou, 2015).

However, most of the research about BNs is concentrated on continuous one. Learning discrete BNs is challenging because of large parameter space and difficulty in searching for a sparse structure. Recently, a block-wised coordinate descent (BCD) method has been proposed for learning discrete BN’s structure (Gu et al., 2019). The proposed algorithm is a deterministic method which uses Newton-Raphson technique to optimize a score function. BCD algorithm employs an L1 regularized likelihood score function and a constraint has been applied to the score function to guarantee the sparsity. The algorithm needs further efforts to ensure the acyclicity constraint. In addition, stochastic methods have shown better performance in high-dimensional problems, but the problem with the stochastic gradient descent (SGD) is that its variance is large, and in particular does not decay to zero with the iteration index. Hence, we have to decay the size to zero step-by-step and hence the convergence rate is slow. Since, new algorithms have to be developed for discrete BN structure learning to accommodate these difficulties.

As a solution, we have proposed a stochastic score-based method called stochastic variance reduction coordinate descent (SVRCD) for discrete BN sparse structure learning in this paper. We have proposed a new penalized log-likelihood score function and developed an optimization algorithm accordingly. To achieve a sparse directed acyclic structure, we have added two penalties to the likelihood term to define the new score function, one for controlling sparsity, and another for achieving a directed acyclic structure (Shuai et al., 2013). The optimization algorithm uses a BCD method in which each coordinate is optimized using SGD. We have utilized a reducing variance method (Johnson and Zhang, 2013) in SGD to accelerate the optimization process. The efficiency, scalability, and robustness of the algorithm are measured. The results show that SVRCD outperforms some of the well-known algorithms in BN structure learning.

The rest of the paper is organized as follows: Section 2 briefly reviewed the BN and required definitions. Section 3 presents our novel score function definition and its components. Section 4 presents the SVRCD algorithm. Section 5 reports the result of the proposed algorithm for simulated networks. Concluding remarks are presented in Section 6.

2 Preliminaries

A BN is a graphical representation for a joint probability distribution function. This graphical model consists of a parameter set and a structure. The structure is a DAG $G = (V, E)$ where $V$ is the set of nodes, and $E$ is the set of edges $E = \{ i \rightarrow j | i, j \in V \}$, where $i$ and $j$ are respectively parent and child. Given $G$, joint probability
distribution function is represented as:

\[ P(X_1 + \ldots + X_p) = \prod_{i=1}^{p} P(X_i \mid \Pi^G_i) \]  

where \( X_i \) is a random variable for \( V_i \), and \( \Pi^G_i \) is parent set of \( X_i \). Because of the big parameter space and the difficulty in finding a sparse structure, BN structure learning is a challenge. The score-based approach is a popular structure learning method. In this approach, the score function assigns a numeric value to each structure showing how the data fits the structure. Given dataset \( D \) and graph \( G \), the score is represented as:

\[ \text{Score}(G \mid D) = P(G \mid D) = \frac{P(D \mid G)P(G)}{P(D)} \]  

We consider the equal probability for all structures, and therefore, just the numerator of the equation \(2 \) need to be optimized. If the structure score is a summation of all variables scores, the score function is called decomposable. Given a variable and its parents, the variable score is:

\[ \text{Score}(G \mid D) = \sum_{i=1}^{n} \text{Score}(X_i \mid \Pi_i, D) \]  

Most score functions have a Penalized Log-Likelihood (PLL) form. We can formulate the constraints by adding a penalty term to Log-Likelihood (LL) function. Given \((D, G)\) an LL function is defined as:

\[ LL(D \mid G) = \sum_{h=1}^{n} \log P(D_h \mid G) = \sum_{i=1}^{p} \sum_{h=1}^{n} \log P(D_{ih} \mid \Pi_{ih}) \]  

where \( D_{ih} \) is the value of \( X_i \) in data row \( h \), and \( \Pi_{ih} \) is the value of \( X_i \)'s parents in data row \( h \). A PLL function is defined as:

\[ PLL(G \mid D) = LL(D \mid G) - \sum_{i=1}^{n} \text{Penalty}(X_i, G, D) \]  

where \( \sum_{i=1}^{n} \text{Penalty}(X_i, G, D) \) is the penalty term that has been added to the score function.

There are different optimization methods for optimizing the score function. A coordinate descent (CD) method is an iterative optimization method which in each iteration optimizes the function given one component. This method decomposes the problem to some reduced dimension sub-problems (Wright 2015). A BCD algorithm is a CD algorithm but optimizes the score function using a subset of all components in each iteration.

Algorithm 1: CD Algorithm

1. set \( k \leftarrow 0 \), choose \( x^0 \in \mathbb{R}, \gamma > 0 \);
2. while termination test not satisfied do
   3. choose a random \( i \in \{1, \ldots, n\} \);
   4. \( x^{k+1} \leftarrow x^k - \gamma (\nabla h_i(x)) \);
3. end

Algorithm 1 is a CD algorithm which has two steps: choosing a component of the score function, and optimizing the score function with regard to the selected component using a gradient descent (GD) method. Using SGD method in the second step, we could have better performance in high-dimensional datasets. This method optimizes the score function using just a mini batch of data which is selected stochastically.

A convex function has just one global and no local optimum. Convex functions are very important in optimization problems, since formulating a problem as a convex function could help to find the global optimum. Commonly, a quadratic optimization method such as Newton-Raphson is used for optimizing convex functions. Quadratic methods need calculating the Hessian of the function that is impossible or too complex in most problems. Instead of quadratic methods we can use GD and SGD with an appropriate learning rate \( \gamma \). GD and SGD could find global optimum in a convex function. In addition, these methods use the first derivative of a function that is simply calculable.

3 The Proposed Score Function

Structure learning could be modelled as an optimization problem by defining an appropriate score function, and hence, it could be solved using an optimization algorithm. We have proposed a PLL score function with two penalty terms to control structure acyclicity and sparsity simultaneously. Consider \( X_i \) as a discrete variable of a BN which its domain has \( n_i \) value \( 1, 2, \ldots, n_i \). \( \Pi^G_i \) is \( X_i \)'s parents that has \( \pi_k \) value \( 1, 2, \ldots, \pi_k \) in its domain. The parameter set of a BN is:

\[ \Theta = \{ \Theta_{ijk} \geq 0 : \Theta_{ijk} = P(X_i = j|\Pi^G_i = \pi_k) \} \]  

The number of parameters is:

\[ N(\Theta) = \sum_{i=1}^{p} n_i \prod_{j \in \Pi^G_i} n_j \]  

If \( n_i = O(n) \) for all \( X_i \), the number of parameters is:

\[ N(\Theta) = O(\sum_{i=1}^{p} n^{1+|\Pi^G_i|}) \]
We use a multi-logit model (Gu et al., 2019) to decrease the number of parameters. Using this model the likelihood function is:

\[
P(X_i = \ell | \Pi_i^G) = \frac{\exp(x_i^T \beta_{i.\ell})}{\sum_{m=1}^{p} \exp(x_i^T \beta_{i.m})} \triangleq p_{i.\ell}(x)
\]

where we code each \(X_i\) using \(d_i = n_i - 1\) dummy variables as a vector \(x_i = (x_{i1}, x_{i2}, \ldots, x_{id_i}) \in \{0,1\}^{d_i}\); if \(X_i = \ell\) then \(x_{i\ell} = 1\) and \(x_{i,j} = 0\), and if \(X_i = 0\) then we say \(X_i\) has the reference value.

\[
\beta_{i.0} = [\beta_{i.0_1}, \beta_{i.0_1}, \ldots, \beta_{i.0_p}] \in \mathbb{R}^d
\]

is a coefficient vector for predicting how probable \(X_i = \ell\) is. If \(j \notin \Pi_i^G\) then \(\beta_{i.j} = 0\). We use a symmetric multi-logit model and add two constraints to the model since the model is identifiable (Friedman et al., 2010):

\[
\beta_{1.0} = 0, \quad \sum_{m=1}^{p} \beta_{i.m} = 0, \quad \forall i, j = 1, \ldots, p
\]

The number of parameters in this model is:

\[
N(\beta) = \sum_{i=1}^{p} \left[(n_i - 1) + n_i \sum_{j \notin \Pi_i^G} d_j\right] = \sum_{i=1}^{p} \left[(n_i - 1) + n_i \sum_{j \notin \Pi_i^G} d_j\right]
\]

(11)

Consider \(n_i = O(n)\) for all \(i\), then:

\[
N(\beta) = O(n^2)|E| + O(np)
\]

(12)

Multi-logit model is an appropriate estimation of the product multinomial model. In this model, the number of parameters increases linearly with the number of edges. This model is much more efficient than the product multinomial model which grows exponentially as the size of the parent set increases. We consider dataset \(D = (d_{hi})_{n \times p}\) that has been sampled from \(G\), where \(d_{hi}\) is the value of \(X_i\) in data row \(h\). Using multi-logit model, \(LL(\beta)\) could be defined as:

\[
LL(\beta) = \sum_{i=1}^{p} \sum_{k \in G_i} \log[P(d_{hi} | x_{h,i}, j \in \Pi_i^G)]
\]

\[
= \sum_{i=1}^{p} \sum_{k \in G_i} \left[ \sum_{\ell=1}^{r_i} \prod_{m=1}^{r_i} \frac{y_{hi,\ell} x_i^T \beta_{i.\ell}}{\sum_{m=1}^{r_i} \exp(x_i^T \beta_{i.m})} \right] - \log \sum_{m=1}^{r_i} \exp(x_i^T \beta_{i.m})
\]

(13)

where \(y_{hi,\ell} = I(d_{hi} = \ell)\) is index variable, and \(\beta_{i.\ell k} = 0\) for all \(k \notin \Pi_i^G\). The score function controls the structure sparsity using a penalty term. We use a group norm penalty term that penalizes all components of the score function at the same. Let \(G\) be a graph that is learned from parameter set \(\beta\). The sparsity penalty term is defined as:

\[
\text{Sparsity Penalty} = \lambda_1 \sum_{i=1}^{p} \sum_{j=1}^{p} ||\beta_{i,j}||_2
\]

(14)

We use a different penalty term that causes the structure to not have any directed cycles. Let us consider \(A^G\) and \(PATH^G \in \{0,1\}^{p \times p}\) are adjacency and path matrices, respectively. Path matrix \(PATH^G = (k_{ij})_{p \times p}\) would be defined as:

\[
k_{ij} = \begin{cases} 
1 & \text{if there is a path between } i \text{ and } j \\
0 & \text{else} 
\end{cases}
\]

(15)

Using a BFS algorithm and an adjacency matrix, we can check the existence of a path between every two nodes. **Lemma** A sufficient and necessary condition for existing no path between any pair of nodes is:

\[
||\beta_{i,j} \times P_{ji}||_2 = 0
\]

(16)

**Proof** Consider \(G\) is a DAG. First, imagine for every \(X_i\) and \(X_j\), \(\beta_{i,j} \times P_{ji} \neq 0\). Hence, there is a directed edge between \(X_i\) and \(X_j\), and at least there is a directed path between \(X_j\) and \(X_i\). It means that there is a directed cycle in graph, which is a contradiction to our presumption that \(G\) is a DAG. On the other side, suppose that for every pair of \(X_i\) and \(X_j\), \(\beta_{i,j} \times P_{ji} = 0\). If \(G\) is not a DAG, there is at least one directed cycle in \(G\). Hence, there are two nodes \(X_i\) and \(X_j\) that there is a path from \(X_i\) to \(X_j\). This is a contradiction to our presumption that \(\beta_{i,j} \times P_{ji} = 0\).

Hence, the lemma proved (Shuai et al., 2013).

Regarding the lemma, we can define the following penalty term that guarantees the obtained structure is a DAG.

\[
\text{DAG Penalty} = \lambda_2 \sum_{j \in X_i} ||\beta_{i,j} \times P_{ji}||_2
\]

(17)

Hence, the score function is:

\[
f_\lambda(\beta) = -LL(\beta) + \lambda_1 \sum_{i=1}^{p} \sum_{j=1}^{p} ||\beta_{i,j}|| + \lambda_2 \sum_{j \in X_i} ||\beta_{i,j} \times P_{ji}||_2
\]

(18)

where \(\lambda_1\) and \(\lambda_2\) are regulation parameters. The greater \(\lambda_1\), the more sparse structure and the less accuracy. On the other side, selecting a large \(\lambda_1\), we would have a more sparse structure, but we might miss some edges.

4 The Proposed Optimization Algorithm

In our algorithm, all the weights are updated at the same time. It means, we update \(\beta_{i,j}\) instead of just one component of the vector. In each iteration, one weight vector is selected, then using SGD method, the
score function is updated regarding the selected weight vector. SGD has lower convergence time in comparison to GD algorithm. Therefore, SGD works efficiently in high-dimensional datasets.

SGD calculates gradient using just one or a part of the data, not all the data, and it causes big variance in estimations. Selecting an inappropriate data could mislead the optimization. We need a small \( \gamma \) since a large \( \gamma \) causes big variances and hence the algorithm does not converge correctly. SGD uses smaller \( \gamma \) to solve the data, not all the data, and it causes big variance problem exists.

There are some methods and solutions that reduce the estimation variance. Using these solutions, we can select a larger \( \gamma \). One practical issue for SGD is that in order to ensure the convergence the learning rate has to decay to zero. This leads to slower convergence. The need for a small learning rate is due to the variance of SGD. Using variance reduction method in SGD, the learning rate for SGD does not have to decay, which leads to faster convergence as one can use a relatively large \( \gamma \) (Johnson and Zhang, 2013). We use a variance reduced SGD in the optimization step in our proposed algorithm.

To optimize \( f_x(\beta) \) with regard to \( \beta_{i,j} \), \( f_{\lambda,i}(\beta_{i,.}) \) would be defined as:

\[
f_{\lambda,i}(\beta_{i,.}) = -\sum_{h \in O_i} \left( \sum_{\ell=1}^{r_i} y_{hi\ell} x_i^T \beta_{i,\ell \cdot} \log \sum_{m=1}^{r_i} (x_i^T \beta_{i,m}) \right) + \lambda_1 \sum_{j=1}^{P} \|\beta_{i,j}\|_2 + \lambda_2 \sum_{j \in \mathcal{X}/i} \|\beta_{i,j} \times P_{j,i}\|_2 \tag{19}
\]

where \( \beta_{i,.} = (\beta_{i,0}, \beta_{i,1}, ..., \beta_{i,P}) \). We use an SGD method to optimize equation (19) hence in each iteration, SGD picks a data row randomly and then optimizes (19) regarding the selected data. The cost function for data \( h \) is:

\[
f_{\lambda,i}(\beta_{i,.}) = \sum_{\ell=1}^{r_i} y_{hi\ell} x_i^T \beta_{i,\ell \cdot} \log \sum_{m=1}^{r_i} (x_i^T \beta_{i,m}) + \lambda_1 \sum_{j=1}^{P} \|\beta_{i,j}\|_2 + \lambda_2 \sum_{j \in \mathcal{X}/i} \|\beta_{i,j} \times P_{j,i}\|_2 \tag{20}
\]

Gradient of the cost function is:

\[
\nabla LL_{ih}(\beta_{i,.}^{(t)}) = \begin{bmatrix}
(y_{hi1} - p^{(t)}_{h1}(x_h))x_{h,j_1} \\
\vdots \\
(y_{hirm} - p^{(t)}_{h,m}(x_h))x_{h,j_m}
\end{bmatrix} \tag{21}
\]

To reduce the estimation variance, we have used SVRG (Johnson and Zhang, 2013) method. SVRG saves \( \hat{\beta}_{i,j} \) after each \( m \) iteration and then calculates \( \nabla f_{\lambda,i}(\hat{\beta}_{i,j}) \) and \( \hat{\mu} \) for \( \hat{\beta}_{i,j} \).

\[
\hat{\mu} = \frac{1}{n} \sum_{h=1}^{n} \nabla f_{\lambda,i}(\hat{\beta}_{i,j}) \tag{22}
\]

Weight vectors are updated as follow:

\[
\beta_{i,j}^{(t)} = \beta_{i,j}^{(t-1)} - \gamma (\nabla f_{\lambda,i}(\beta_{i,j}^{(t-1)}) - \nabla f_{\lambda,i}(\hat{\beta}_{i,j}) + \hat{\mu}) \tag{23}
\]

where \( E[\nabla f_{\lambda,i}(\hat{\beta}_{i,j}) - \hat{\mu}] = 0 \), hence:

\[
E \left[ \beta_{i,j}^{(t)} | \beta_{i,j}^{(t-1)} \right] = \beta_{i,j}^{(t-1)} - \gamma \nabla f_{\lambda,i}(\beta_{i,j}^{(t-1)}) \tag{24}
\]

It means this algorithm averagely is equal to ordinary GD.

Our proposed algorithm SVRCD is a BCD algorithm that selects a weight vector in each iteration and then optimizes the cost function. The pseudocode is shown in Algorithm 2. SVRCD needs determined regulation parameters \( \lambda_1, \lambda_2 \), and also learning rate \( \gamma \).

### Algorithm 2: SVRCD Algorithm

1. Initialize \( \beta, \hat{\beta}_{i,j} \);
2. while stop criterion is not met do
   3. for each \((i,j)\) in \([1,...,P]\) and \(i \neq j \) do
      4. for \(s=1,...,m \) do
         5. \( \beta_{i,j} = \hat{\beta}_{i,j}^{(s-1)} \);
         6. \( \hat{\mu} = \frac{1}{n} \sum_{h=1}^{n} \nabla f_{\lambda,i} \hat{\beta}_{i,j}^{(s)} \);
         7. \( \beta_{i,j}^{(s)} = \beta_{i,j}^{(s-1)} + \hat{\mu} \);
   8. end
   9. end
10. end
11. end

In this section, we evaluate the proposed algorithm. At first, we tested the algorithm with different parameter settings to find the best values for \( \lambda_1, \lambda_2 \), and \( \gamma \). Then we compare SVRCD with other known algorithms such as HC, PC, MMHC, and a new competitive algorithm CD (Gu et al., 2019). PC and MMHC are respectively constraint based and hybrid methods proposed for BN structure learning while the other methods are score-based BN structure learning methods. At the end of this section, the algorithm scalability and noise robustness are evaluated.
We have generated simulated datasets using bipartite, scale-free, and random graphs. To produce bipartite, and scale-free graphs, we have used the igraph package \cite{csardi2006igraph} in the R environment. Bipartite graphs have 0.2p upper and 0.8p lower nodes where p is the number of all nodes in the graph, and s0 = p directed edges from upper nodes to lower ones. Scale-free networks are produced using the Barabási-Albert model which has s0 = p − 1 edges. We have set s = −3 and m = 1, which are two needed parameters for producing scale-free networks in the igraph package. Random graphs have been generated using sparsebnUtils package in R. There are s0p edges in our random graphs.

We have run HC and MMHC algorithms using bnlearn package \cite{scutari2009learning}, and PC algorithm using Pcalg package in R. For CD algorithm, we have used its implementation in discretedAlgorithm package \cite{aragam2019discreted} in R. We have set CD parameters to their default values. All variables in graphs are considered to be binary in all implementations. Weight vectors βi,j = (βi,j, βj,i) have been initialized randomly with a value in range (0,1). We have considered different values for the number of data rows and variables (n, p) in evaluations. The goal is to evaluate SVRCD using high dimensional discrete data; hence we have set n ≥ p in data generation process. Different evaluation metrics are used in this paper that are introduced in Table 1. All results are averages over 20 datasets for each (n, p) setting.

In the first step of evaluations, we measure the impact of λ1 on evaluation metrics. We have reported the results in Table 2. As shown in the table, in λ1 = 0.9, P has the greatest value, since λ1 determines how sparse the structure can be. We should set λ1 to a proper value that controls sparsity but does not decrease other metrics such as E. SVRCD has the best SHD and JI in λ1 = 1 for (n, p) = (50, 50). In addition, our proposed algorithm has a greater P in λ1 = 0.9, but a greater FP, FDR, SHD, and a lower JI as well. Also, SVRCD estimates a sparser structure using λ1 = 1.3 but E has a low value in this setting.

Table 2: SVRCD evaluation with changes

| λ1 | P | E   | R   | M   | FP  | TPR | FDR  | SHD  | JI  |
|----|---|-----|-----|-----|-----|-----|------|------|-----|
| 0.9| 45| 26.4| 9.6 | 14  | 10.4| 0.53| 0.43 | 34   | 0.38|
| 1  | 36.8| 26.6| 6.4 | 17  | 3.8 | 0.53| 0.28 | 27.2 | 0.44|
| 1.1| 26.6| 22  | 3.8 | 24.2| 0.8 | 0.44| 0.17 | 28.8 | 0.4 |
| 1.2| 27.6| 16.8| 5.2 | 28  | 5.6 | 0.34| 0.39 | 38.8 | 0.28|
| 1.3| 22.4| 14.8| 3.6 | 31.6| 4   | 0  | 0.34 | 39.2 | 0.26|

Table 3: SVRCD evaluation with λ2 changes

| λ2 | P | E   | R   | M   | FP  | TPR | FDR  | SHD  | JI  |
|----|---|-----|-----|-----|-----|-----|------|------|-----|
| 0.1| 38.8| 24.2| 9   | 16.8| 5.6  | 0.48| 0.37 | 31.4 | 0.37|
| 0.2| 36.8| 26.6| 6.4 | 17  | 3.8  | 0.53| 0.28 | 27.2 | 0.44|
| 0.3| 32.6| 24.2| 7.4 | 18.4| 3.8  | 0.48| 0.31 | 29.6 | 0.4 |
| 0.4| 31.4| 21.2| 6.6 | 22.2| 3.6  | 0.42| 0.33 | 32.4 | 0.35|
| 0.5| 31.4| 18.2| 8.8 | 23  | 4.4  | 0.36| 0.42 | 36.2 | 0.29|

Table 4: SVRCD evaluation with γ changes

| γ  | P | E   | R   | M   | FP  | TPR | FDR  | SHD  | JI  |
|----|---|-----|-----|-----|-----|-----|------|------|-----|
| 0.001| 36.8| 26.6| 6.4 | 17  | 3.8 | 0.53| 0.53 | 27.2 | 0.44|
| 0.002| 38.2| 24.2| 8.6 | 17.2| 5.4 | 0.48| 0.48 | 31.2 | 0.38|
| 0.004| 40.8| 25.8| 9.4 | 14.8| 5.6 | 0.52| 0.52 | 29.8 | 0.4 |
| 0.006| 43.4| 27  | 7.4 | 15.6| 9  | 0.54| 0.54 | 32  | 0.41|
| 0.008| 49  | 24  | 12  | 14  | 13 | 0.48| 0.48 | 39  | 0.32|

Table 1: Evaluation metrics

| Description                                      | Metric          | Abbreviation |
|-------------------------------------------------|-----------------|--------------|
| Number of estimated edges                        | Predicted       | P            |
| Number of edges which are in skeleton and have right direction | Expected       | E            |
| Number of edges which are in skeleton but have wrong direction | Reverse        | R            |
| Number of edges which are not recognized         | Missing         | M = s0 − E − R |
| Right edges learning rate                        | False Positive  | FP = P − E − R |
| Wrong edges learning rate                        | True Positive Rate | TPR = E/F  |
| Distance between estimated and original BN       | False Discovery Rate | FDR = E/R + M + FP |
| Similarity of estimated and original BN          | Structural Hamming Distance | SHD = R + M + FP |
|                                                  | Jaccard Index   | JI = E/R + M + FP |

In the first step of evaluations, we measure the impact of λ1 on evaluation metrics. We have reported the results in Table 2. As shown in the table, in λ1 = 0.9, P has the greatest value, since λ1 determines how sparse the structure can be. We should set λ1 to a proper value that controls sparsity but does not decrease other metrics such as E. SVRCD has the best SHD and JI in λ1 = 1 for (n, p) = (50, 50). In addition, our proposed algorithm has a greater P in λ1 = 0.9, but a greater FP, FDR, SHD, and a lower JI as well. Also, SVRCD estimates a sparser structure using λ1 = 1.3 but E has a low value in this setting.

Table 4 shows the results for different values of λ2. This parameter puts a constraint on the structure to be a DAG. Also, λ2 has a small effect on sparsity, hence selecting a proper value for this parameter is crucial. A large value of λ2 causes a large FP and a low TP, and a low value of λ2 causes the structure not to be a DAG. The results show that with our generated dataset, the best value for this parameter is 0.2. Although SVRCD has the lowest FP in λ2 = 0.4, E, TPR, FDR, SHD, and JI have the best values in λ2 = 0.2. Hence one will observe a better overall performance in λ2 = 0.2.

Table 2 reports measurement metrics with regard to different values for learning rate γ. A large value for γ results in a wrong learnt structure and a large FDR and FP. Furthermore, a low γ increases the runtime. We have found γ = 0.001 the best setting in our evaluations. SVRCD has a better TPR in γ = 0.006, but a larger
Table 5 Comparison among SVRCD and other algorithms on bipartite graph data

| Graph       | Method   | P     | E     | R     | M     | FP    | TPR   | FDR   | SHD   | JI    |
|-------------|----------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Bipartite   | SVRCD    | 105   | 73    | 16.67 | 111.33| 16.33 | 0.37  | 0.29  | 143.33| 0.32  |
|             | BCD      | 84    | 51.95 | 18.65 | 129.4 | 13.4  | 0.26  | 0.37  | 161.45| 0.22  |
|             | PC       | 75.7  | 26.9  | 34.2  | 138.9 | 14.6  | 0.13  | 0.64  | 187.7 | 0.18  |
|             | HC       | 378.1 | 111.5 | 32.9  | 55.6  | 233.8 | 0.56  | 0.71  | 322.4 | 0.24  |
|             | MMHC     | 175.4 | 72.2  | 20.4  | 107.4 | 82.8  | 0.36  | 0.59  | 210.1 | 0.24  |
| Random DAG  | SVRCD    | 95.5  | 67.95 | 18.3  | 113.7 | 9.45  | 0.34  | 0.29  | 141.50| 0.30  |
|             | BCD      | 85.75 | 56    | 18.6  | 125.4 | 11.15 | 0.28  | 0.34  | 155.15| 0.24  |
|             | PC       | 97.3  | 47.1  | 37.0  | 138.9 | 14.6  | 0.13  | 0.52  | 169.7 | 0.19  |
|             | HC       | 376.3 | 96.3  | 52.1  | 55.6  | 227.8 | 0.48  | 0.74  | 335.1 | 0.20  |
|             | MMHC     | 179.8 | 86.4  | 31.1  | 107.4 | 62.4  | 0.45  | 0.52  | 179.6 | 0.29  |
| Scale-free  | SVRCD    | 73.35 | 50.25 | 16.70 | 132.05| 6.40  | 0.50  | 0.31  | 155.15| 0.23  |
|             | BCD      | 80.10 | 45.80 | 23.45 | 129.75| 10.85 | 0.23  | 0.42  | 164.05| 0.20  |
|             | PC       | 99.50 | 46.50 | 23.10 | 138.9 | 30.00 | 0.23  | 0.53  | 182.50| 0.19  |
|             | HC       | 377.80| 121.00| 52.8  | 55.6  | 228.80| 0.61  | 0.68  | 306.90| 0.27  |
|             | MMHC     | 176.80| 93.20 | 16.10 | 107.4 | 67.50 | 0.47  | 0.47  | 173.20| 0.33  |

Table 6 Scalability of SVRCD on bipartite graph data

| (n,p) | P     | E     | R     | M     | FP    | TPR   | FDR   | SHD   | JI    |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| (50,50)| 36.2  | 25    | 4.8   | 20.2  | 6.4   | 0.5   | 0.3   | 31.4  | 0.41  |
| (50,100)| 51.6  | 37.4  | 7.6   | 55    | 8.6   | 0.37  | 0.3   | 71.2  | 0.32  |
| (100,100)| 65.2  | 45.2  | 13.2  | 41.6  | 6.8   | 0.45  | 0.31  | 61.6  | 0.38  |
| (50,200)| 105   | 73    | 16.67 | 111.33| 16.33 | 0.37  | 0.29  | 143.33| 0.32  |

SHD, SHD and JI specify the quality of the estimated structure. Hence, $\gamma = 0.001$ is the best setting in our evaluations.

The second step of evaluations compares SVRCD with some known algorithms. First, the datasets are sampled from a bipartite graph with $(n, p) = (50, 200)$ setting. As shown in Table 5, our proposed algorithm outperforms BCD, PC, HC, and MMHC algorithms regarding FDR, SHD, and JI metrics. Although HC demonstrates better TPR and E than SVRCD, it estimates 387.1 edges for a BN with 200 edges. Hence, the estimated structure is not sparse and has more edges than the original structure. SVRCD estimated two more FP edges than the PC algorithm. The reason is that the PC has estimated fewer edges, and has a lower E. SVRCD with $E = 73$ has defeated PC with $E = 26.9$.

In addition, SVRCD has better FDR, TPR, SHD, and JI than PC. Hence, SVRCD generally outperformed PC. BCD is one of the recently proposed algorithms for estimating sparse BN using high-dimensional discrete data. We compared SVRCD to this algorithm as well. Our proposed algorithm leads to much better SHD, JI, FDR, TPR, and E than BCD, but BCD has estimated a sparser structure and has a lower FP. However, SHD and JI are two important metrics that show the overall performance of a structure learning algorithm. We have also repeated our evaluations with data sampled from random graphs, and scale-free networks. The results are reported in Table 6.

The next set of evaluations examines the scalability of SVRCD with respect to $(n, p)$. The results have been reported in Table 6. The greater $p$ and the lower $n$ are, the more sophisticated problem is. We obtain from Table 6 that SVRCD is more efficient for $(n, p) = (100, 100)$ than $(n, p) = (50, 100)$. On the other hand, comparing $(n, p) = (50, 100)$ to $(n, p) = (50, 200)$, we observe that SVRCD achieves the same TPR, FDR, and JI. It means that increasing the number of variables does not have a significant negative effect on the TPR, FDR, and JI. SVRCD can obtain admissible results on high-dimensional data.

In the fourth step of evaluations, we have tested SVRCD using datasets with $(n, p) = (50, 200)$ settings generated from bipartite graphs, random graphs, and scale-free networks to measure the performance of our proposed algorithm in estimating each graph. For each test, we generated 20 datasets from each graph. Figure 1 represents the means and variances of E, FP, TPR, FDR, and SHD while estimating each graph using 20 datasets.

Table 7 SVRCD robustness against noise on bipartite graph data

| Noise% | P     | E     | R     | M     | FP    | TPR   | FDR   | SHD   | JI    |
|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0      | 86.4  | 64    | 14.2  | 121.8 | 8.2   | 0.32  | 0.26  | 144.2 | 0.29  |
| 1      | 79.2  | 58.2  | 14    | 127.8 | 7     | 0.29  | 0.26  | 148.8 | 0.26  |
| 2      | 72.6  | 55    | 10.2  | 134.8 | 7.4   | 0.28  | 0.24  | 152.4 | 0.25  |
| 3      | 66.8  | 46    | 10.2  | 138.9 | 7.2   | 0.23  | 0.24  | 154.2 | 0.24  |
| 4      | 64.6  | 46    | 10.2  | 140.4 | 5     | 0.23  | 0.29  | 159   | 0.21  |
| 5      | 58.8  | 42    | 10.6  | 147.4 | 6.2   | 0.21  | 0.29  | 164.2 | 0.19  |
bipartite graph, random graph, and scale-free network, respectively.

The final part of evaluations calculates the algorithm robustness against noise. We have sampled data from a bipartite graph with \((n, p) = (50, 200)\). Then we have swapped a specific portion of data to their complement values. The results are reported in Table 7 and Figure 3. From Figure 3, we observe that increasing the noise causes an increase in E and TPR errors. But, FDR increases at first and then decreases, since increasing the noise causes the algorithm to predict fewer edges (smaller P).
6 Conclusion

In this paper, we proposed a novel BN structure learning algorithm, SVRCD, for learning BN structures from discrete high-dimensional data. Also, we proposed a score function consisting of three parts: likelihood, sparsity penalty term, and DAG penalty term. SVRCD is a BCD algorithm that uses a variance reduction method in the optimization step, which is an SGD method. Variance reduction method is used to prevent large variances in estimations and hence, increases the convergence speed. As shown in the previous section, our algorithm outperforms some known algorithms in BN structure learning. SVRCD shows significant results in learning BN structure from discrete high-dimensional data. One of the advantages of SVRCD is that more data rows causes a lower algorithm runtime. Because it uses an SGD method and when the data rows increase, the algorithm iterations should be set on a lower value to prevent the algorithm overfitting. Obtained results show that SVRCD dominates the recently proposed BCD algorithm in SHD and JI metrics.

In future work, we will investigate and prove the algorithm convergence for different discrete data distributions. Furthermore, this algorithm is proposed for learning discrete BN, but the same formulation may be adopted for Gaussian BN. In addition, since BNs have many applications in medical studies, SVRCD may help medical problems such as constructing gene networks. Another potential future work can be finding tuning parameters causing the algorithm to converge to the optimum point.

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