A Modified Orthogonal Matching Pursuit for Construction of Sparse Probabilistic Boolean Networks

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Abstract

Probabilistic Boolean Networks play a remarkable role in the modelling and control of gene regulatory networks. In this paper, we consider the inverse problem of constructing a sparse probabilistic Boolean network from the prescribed transition probability matrix. We propose a modified orthogonal matching pursuit for solving the inverse problem. We provide some conditions under which the proposed algorithm can recover a sparse probabilistic Boolean network. We also report some numerical results to illustrate the effectiveness of the proposed algorithm.

Keywords. Probabilistic Boolean network, inverse problem, sparse, modified orthogonal matching pursuit

1 Introduction

1.1 Boolean Networks and probabilistic Boolean networks

Boolean Network (BN) and Probabilistic Boolean Network (PBN) arise in a wide variety of applications. The BN model was originally proposed by Kauffmann in 1969 for exploring dynamical properties of gene regulatory networks [14] (see also [15, 16]). The BN model has been used in different biological systems, including apoptosis, the yeast cell-cycle network, and T Cell Signaling, and so on (see for instance [1, 17, 25, 26]).

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As an extension of the BN, the PBN has gained much attention since it introduces uncertainty principles into a rule-based BN modelling [27, 28, 29]. The PBN model was originally proposed by Shmulevich et al. in 2002 for modelling genetic regulatory networks [29]. The PBN has been used in many applications such as biological systems (see for instance [19, 27]), biomedicine [31], credit defaults [13], and industrial machine systems [23, 24], etc.

In the following, we give the basic framework of BNs and PBNs. As noted in [28, 29], a BN includes a set of nodes (genes) $V = \{v_1, v_2, \ldots, v_n\}$ and a list of Boolean functions F = $\{f_1, f_2, \ldots, f_n\}$. Here, for any $1 \le i \le n, v_i(t) \in \{0, 1\}$ is a binary variable, which means the state (off/on) of gene i at time t, and $f_i: \{0,1\}^n \to \{0,1\}$ is a Boolean function. The state of gene v_i at time t+1 is determined by

$$v_i(t+1) = f_i(v_{i_1}(t), \dots, v_{i_{w(i)}}(t)) \equiv f_i(\mathbf{v}(t)),$$

where w(i) is the number of essential variables of f_i and $\mathbf{v}(t) = (v_1(t), \ldots, v_n(t))^T \in \mathbb{R}^n$. Therefore, there are 2^n possible global states in a BN with n genes.

In a PBN with a set of nodes (genes) $V = \{v_1, v_2, \ldots, v_n\}$, for each gene v_i , there exist l(i) possible functions: $F_i = \{f_1^{(i)}, \ldots, f_{l(i)}^{(i)}\}$, where each $f_p^{(i)}$ is a possible function determining the value of gene v_i . A realization of the PBN consists of N different possible realizations, which is determined by N vector functions $\mathbf{f}_1, \ldots, \mathbf{f}_N$ of the form

$$\mathbf{f}_{j} = (f_{j_{1}}^{(1)}, f_{j_{2}}^{(2)}, \dots, f_{j_{n}}^{(n)})^{T}, \quad j = 1, \dots, N, \quad 1 \le p_{i} \le l(i)$$
(1.1)

where $f_{j_i}^{(i)} \in F_i$ for i = 1, ..., n. Suppose $\mathbf{f} = (f^{(1)}, ..., f^{(n)})^T$ is a random vector with $f^{(i)} \in F_i$. Then, the selection probability of function $f^{(i)} = f_i^{(i)}$ for gene v_i is given by

$$c_j^{(i)} = \operatorname{Prob}\{f^{(i)} = f_j^{(i)}\}$$

for $j = 1, \ldots, l(i)$ and $\sum_{j=1}^{l(i)} c_j^{(i)} = 1$. Assume that the random variables $f^{(1)}, \ldots, f^{(n)}$ are independent. Then, the PBN is called independent. In this case, the probability of choosing the vector function \mathbf{f}_i in the form of (1.1) is given by

$$x_j = \operatorname{Prob}\{\mathbf{f} = \mathbf{f}_j\} = \prod_{i=1}^n \operatorname{Prob}\{f^{(i)} = f_{j_i}^{(i)}\} \equiv \prod_{i=1}^n c_{j_i}^{(i)}$$

Therefore, an independent PBN includes a set of nodes V and a list $\mathcal{F} = \{F_1, \ldots, F_n\}$, which has $N = \prod_{i=1}^{n} l(i)$ possible realizations. We note that the independent PBN still has 2^{n} possible global states and the transition probability from state $\mathbf{a} = (a_1, \ldots, a_n)^T$ to state $\mathbf{b} = (b_1, \ldots, b_n)^T$ is determined by

$$\operatorname{Prob}\{\mathbf{v}(t+1) = \mathbf{b} \mid \mathbf{v}(t) = \mathbf{a}\}$$
$$= \sum_{j=1}^{N} \operatorname{Prob}\{\mathbf{v}(t+1) = \mathbf{b} \mid \mathbf{v}(t) = \mathbf{a}, \text{the } j\text{th vector function (1.1) is selected}\} \cdot x_j.$$

Then we obtain the transition probability matrix $P \in \mathbb{R}^{2^n \times 2^n}$ of the PBN [8]:

$$P = \sum_{j=1}^{N} x_j A_j,$$

where $A_j \in \mathbb{R}^{2^n \times 2^n}$ is the transition probability matrix corresponding to the *j*th constituent vector function \mathbf{f}_j . Here, $\mathbb{R}^{n_1 \times n_2}$ is the set of all $n_1 \times n_2$ real matrices ($\mathbb{R}^n = \mathbb{R}^{n \times 1}$) and each column of A_j has only one nonzero entry and each column adds up to one.

1.2 Construction of probabilistic Boolean network

The inverse problem of constructing a PBN aims to identify all the constituent BNs and corresponding selection probabilities such that the constructed PBN has the prescribed transition probability matrix. Suppose a PBN consists of N possible constituent BNs with the transition probability matrices $\{A_j\}_{j=1}^N$. The inverse problem of constructing a PBN aims to find the probability distribution vector $\mathbf{x} = (x_1, \ldots, x_N)^T$ from the prescribed transition probability matrix P and the constituent BN matrices $\{A_j\}_{j=1}^N$ such that

$$P = \sum_{j=1}^{N} x_j A_j, \quad \mathbf{1}^T \mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0},$$
(1.2)

where **1** is a column vector of an appropriate dimension whose entries are all ones and for any two vectors $\mathbf{f}, \mathbf{g} \in \mathbb{R}^N, \mathbf{g} \ge \mathbf{f}$ means that $g_j \ge f_j$ for $j = 1, \ldots, N$.

One may solve (1.2) by the solution of the following minimization problem:

$$\min_{\mathbf{x}\in\mathbb{R}^{N}} \frac{1}{2} \|P - \sum_{j=1}^{N} x_{j} A_{j}\|_{F}^{2}$$
subject to (s.t.) $\mathbf{1}^{T} \mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0},$

$$(1.3)$$

where $\|\cdot\|_F$ denotes the Frobenius norm. Let

$$A = [\operatorname{vec}(A_1), \operatorname{vec}(A_2), \dots, \operatorname{vec}(A_N)] \in \mathbb{R}^{m \times N} \quad \text{and} \quad \mathbf{b} = \operatorname{vec}(P) \in \mathbb{R}^m, \tag{1.4}$$

where $m = 2^{2n} \ll N$ and $\text{vec}(\cdot)$ generates a column vector from a matrix by stacking its column vectors below one another. Then the minimization problem (1.3) takes the form of

$$\min_{\mathbf{x}\in\mathbb{R}^N} \quad \frac{1}{2} \|A\mathbf{x} - \mathbf{b}\|_2^2
s.t. \quad \mathbf{1}^T \mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0}.$$
(1.5)

where $\|\cdot\|_2$ denotes the Euclidean vector norm or its induced matrix norm.

In general, there are many solutions to the inverse problem. However, in practice, it is desired to find only a few major constituent BNs with associated selection probabilities. That is, a sparse solution to the inverse problem gives a simple approximate PBN, which may provide a good control design for gene regulatory networks. To find a sparse solution to problem (1.5), one may solve the following ℓ_0 regularization problem:

$$\min_{\mathbf{x}\in\mathbb{R}^N} \quad \frac{1}{2} \|A\mathbf{x} - \mathbf{b}\|_2^2 + \lambda \|\mathbf{x}\|_0$$
s.t.
$$\mathbf{1}^T \mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0},$$

$$(1.6)$$

where $\lambda > 0$ is a regularization parameter and $\|\cdot\|_0$ means the number of nonzero entries of a vector. However, this is a NP-hard problem [20]. It is natural to consider the following ℓ_1 -norm relaxed version of problem (1.6):

$$\min_{\mathbf{x}\in\mathbb{R}^{N}} \quad \frac{1}{2} \|A\mathbf{x} - \mathbf{b}\|_{2}^{2} + \lambda \|\mathbf{x}\|_{1}$$

s.t.
$$\mathbf{1}^{T}\mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0},$$
 (1.7)

There is a large literature on the solution of such convex minimization problem. However, it seems invalid to adopt the ℓ_1 regularization for problem (1.5) since the equality constraint $\mathbf{1}^T \mathbf{x} = 1$ is equivalent to the ℓ_1 -norm regularization term $\|\mathbf{x}\|_1 = 1$ due to $\mathbf{x} \ge 0$.

There exists many methods for finding a sparse solution to the inverse problem. For instance, a heuristic algorithm was proposed in [6]. A dominant modified algorithm was proposed in [9]. A maximum entropy rate approach and its modified version were proposed in [4, 5, 7]. A projection-based gradient descent method was presented in [33].

Recently, an alternating direction method of multipliers was given in [18] for solving the following non-convex minimization problem with the $\ell_{1/2}$ regularization:

$$\min_{\mathbf{x}\in\mathbb{R}^N} \quad \frac{1}{2}\mu \|A\mathbf{x} - \mathbf{b}\|_2^2 + \sum_{j=1}^N x_j \log x_j + \lambda \|\mathbf{x}\|_{1/2}^{1/2}$$

s.t.
$$\mathbf{1}^T \mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0},$$

where μ and λ are two positive constants. In [11], a partial proximal-type operator splitting method was proposed for solving the $\ell_{1/2}$ regularization version of problem (1.6):

$$\min_{\mathbf{x} \in \mathbb{R}^N} \quad \frac{1}{2} \|A\mathbf{x} - \mathbf{b}\|_2^2 + \lambda \|\mathbf{x}\|_{1/2}^{1/2}$$
s.t.
$$\mathbf{1}^T \mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0},$$

where $\lambda > 0$ is a constant.

1.3 Our contribution

The orthogonal matching pursuit (OMP) is a greedy algorithm for solving the sparse approximation problem over a redundant dictionary, which was introduced independently in many references (see for instance [3, 10, 22]). The sparse recovery of the OMP was analyzed by Tropp in [32] and was extended to the noise case [2]. The OMP aims to find a sparse solution to an underdetermined linear system of linear equations $\mathbf{y} = \Phi \mathbf{w}$, where Φ is a $q \times Q$ matrix with q < Q. However, the OMP can not be directly applied to finding a sparse solution to problem (1.5) since there exist additional nonnegative constraint $\mathbf{x} \ge \mathbf{0}$ and equality constraint $\mathbf{1}^T \mathbf{x} = 1$. In this paper, we propose a modified orthogonal matching pursuit (MOMP) for finding a sparse solution to problem (1.5). By exploring the properties of the $m \times N$ matrix A and the vector $\mathbf{b} \in \mathbb{R}^m$ defined by (1.4), we give some conditions to guarantee that our method can find a sparse solution to problem (1.5). We also present some numerical examples to illustrate the efficiency of our method for constructing a sparse PBN.

1.4 Organization

The rest of this paper is organized as follows. In Section 2, we review the OMP and then propose a MOMP for constructing a sparse PBN. In Section 3, we discuss the convergence analysis of our method. In Section 4, we present some numerical examples to show the efficiency of the proposed method. Finally, we give some concluding remarks in Section 5.

1.5 Notation

Throughout this paper, we use the following notation. Let I be the identity matrix of an appropriate dimension. Denote by \mathbf{e}_j the *j*-th column of I. The superscripts ".^{*T*}" denotes the transpose of a matrix. For any $A \in \mathbb{R}^{m \times N}$, let $A = [\mathbf{a}_1, \ldots, \mathbf{a}_N]$. For a complex number a, |a| denotes the modulus of a. Let $[N] = \{1, 2, \ldots, N\}$ and for any set $S \subset [N]$, let |S| and $[N] \setminus S$ be the cardinality of S and the complement of S in [N], respectively. For any set $S \subset [N]$, A_S is the submatrix of a matrix A with columns indexed by S. A vector \mathbf{z} is called d-sparse if at most d entries of \mathbf{z} are nonzero. Finally, denote by $\operatorname{supp}(\mathbf{z}) := \{j \in [N] \mid z_j \neq 0\}$ the support of a vector $\mathbf{z} \in \mathbb{R}^N$.

2 A modified orthogonal matching pursuit

In this section, we first recall the OMP for solving underdetermined linear systems. Then we propose a MOMP for solving problem (1.5).

2.1 Orthogonal matching pursuit

The OMP aims to find a sparse solution to the following underdetermined linear system:

$$\mathbf{y} = \Phi \mathbf{w},\tag{2.1}$$

where $\Phi \in \mathbb{R}^{q \times Q}$ is a measurement matrix with q < Q and $\mathbf{y} \in \mathbb{R}^{q}$ is the observation vector. Then the OMP algorithm is stated as in Algorithm 2.1.

We see that the OMP algorithm is simple and easy to implement. For more details on the OMP, one may refer to [3, 10, 22, 32]. In particular, one may refer to [12, Proposition 3.5] for the exact recovery condition for the OMP.

2.2 A modified orthogonal matching pursuit

In this subsection, we propose a MOMP for solving problem (1.5). It is natural to extend the OMP (i.e., Algorithm 2.1) to the solution of problem (1.5). Compared with problem (2.1), we

Algorithm 2.1 OMP for problem (2.1)

Step 0. Choose an initial point $\mathbf{w}^0 = \mathbf{0}$ and $\mathcal{S}^0 = \emptyset$. Let k := 0.

Step 1. Find $j_{k+1} \in [N]$ such that

$$j_{k+1} \in \operatorname*{argmax}_{j \in [N]} |\mathbf{e}_j^T \Phi^T (\mathbf{y} - \Phi \mathbf{w}^k)|.$$

Set $\mathcal{S}^{k+1} = \mathcal{S}^k \cup \{j_{k+1}\}.$

Step 2. Find

$$\mathbf{w}^{k+1} = \operatorname*{argmin}_{\mathbf{w} \in \mathbb{R}^Q} \operatorname*{argmin}_{\mathrm{supp}(\mathbf{x}) \subset \mathcal{S}^{k+1}} \frac{1}{2} \|\mathbf{y} - \Phi \mathbf{w}\|_2^2.$$

Step 3. Replace k by k + 1 and go to Step 1.

have additional equality constraint $\mathbf{1}^T \mathbf{x} = 1$ and nonnegative constraint $\mathbf{x} \ge \mathbf{0}$. Hence, we cannot solve problem (1.5) by the OMP directly. We also note that, for any $1 \le j \le N$, each column of the *j*-th constituent BN matrix $A_j \in \mathbb{R}^{2^n \times 2^n}$ has only one nonzero entry and each column adds up to one. Thus the matrix A defined by (1.4) is entrywise nonnegative, sparse, and satisfies the property

$$\mathbf{1} \ge A\mathbf{x}, \quad \forall \mathbf{x} \in \mathcal{M}, \tag{2.2}$$

where \mathcal{M} is the feasible domain of problem (1.5), which is defined by

$$\mathcal{M} := \left\{ \mathbf{x} \in \mathbb{R}^N \mid \mathbf{1}^T \mathbf{x} = 1, \ \mathbf{x} \ge \mathbf{0} \right\}.$$

In addition, we see that the prescribed transition probability matrix $P \in \mathbb{R}^{2^n \times 2^n}$ is usually sparse. Hence, the vector $\mathbf{b} \in \mathbb{R}^m$ defined by (1.4) satisfies the following property

$$1 \ge \mathbf{b} \ge \mathbf{0}.\tag{2.3}$$

From the above analysis, sparked by the OMP (i.e., Algorithm 2.1), we propose a MOMP for solving problem (1.5). The algorithm is described in Algorithm 2.2.

We point out that the major work of Algorithm 2.2 is to solve a small linear least square problem (2.4), which can be solved via the standard solvers for constrained linear least square problems, e.g., the interior point algorithm or the active-set algorithm (see for instance [21]).

3 Convergence analysis

In this section, we show that Algorithm 2.2 converges in finite steps under some conditions. For the iterate j_{k+1} generated by Algorithm 2.2, we have the following lemma.

Lemma 3.1 Let \mathbf{x}^k be the current iterate generated by Algorithm 2.2 with $k \ge 1$. If

$$A\mathbf{e}_{j_{k+1}} = A\mathbf{x}^k$$

Algorithm 2.2 MOMP for problem (1.5)

Step 0. Choose an initial guess $\mathbf{x}^0 \in \mathcal{M}$ and $\mathcal{S}^0 = \emptyset$. Let k := 0.

Step 1. Find $j_{k+1} \in [N]$ such that

$$j_{k+1} \in \operatorname*{argmax}_{j \in [N]} \mathbf{e}_j^T A^T (\mathbf{b} - A\mathbf{x}^k).$$

Set $\mathcal{S}^{k+1} = \mathcal{S}^k \cup \{j_{k+1}\}.$

Step 2. Find

$$\mathbf{x}^{k+1} = \operatorname*{argmin}_{\mathbf{x}\in\mathcal{M}, \operatorname{supp}(\mathbf{x})\subset\mathcal{S}^{k+1}} \frac{1}{2} \|\mathbf{b} - A\mathbf{x}\|_2^2.$$
(2.4)

Step 3. Replace k by k + 1 and go to Step 1.

then $j_{k+1} \in \mathcal{S}^{k+1}$ is such that $\mathbf{x}^{k+1} \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}^{k+1}) \subset \mathcal{S}^{k+1}$ but

$$\|\mathbf{b} - A\mathbf{x}^{k+1}\|_2 = \|\mathbf{b} - A\mathbf{x}^k\|_2$$

Moreover, if $\mathbf{x}^{k+1} = \mathbf{x}^k$, then $j_{k+1} \in \mathcal{S}^k$.

Proof: We note that $S^{k+1} = S^k \cup \{j_{k+1}\}$, where $S^k \neq \emptyset$ since $k \ge 1$. By hypothesis, $A\mathbf{e}_{j_{k+1}} = A\mathbf{x}^k$. Then, without loss of generality, we have

$$A_{\mathcal{S}^{k+1}} = [A_{\mathcal{S}^k}, A\mathbf{e}_{j_{k+1}}] = [A_{\mathcal{S}^k}, A\mathbf{x}^k] = [A_{\mathcal{S}^k}, A_{\mathcal{S}^k}\mathbf{x}^k_{\mathcal{S}^k}].$$
(3.1)

This means that the last column of $A_{\mathcal{S}^{k+1}}$ is a convex combination of the columns of $A_{\mathcal{S}^k}$. From (3.1) we have for all $\mathbf{x} \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}) \subset \mathcal{S}^{k+1}$,

$$\|\mathbf{b} - A\mathbf{x}\|_{2} = \|\mathbf{b} - A_{\mathcal{S}^{k+1}}\mathbf{x}_{\mathcal{S}^{k+1}}\|_{2} = \|\mathbf{b} - [A_{\mathcal{S}^{k}}, A_{\mathcal{S}^{k}}\mathbf{x}_{\mathcal{S}^{k}}^{k}]\mathbf{x}_{\mathcal{S}^{k+1}}\|_{2}$$

= $\|\mathbf{b} - A_{\mathcal{S}^{k}}(\mathbf{x}_{\mathcal{S}^{k}} + x_{j_{k+1}}\mathbf{x}_{\mathcal{S}^{k}}^{k})\|_{2}.$ (3.2)

For any $\mathbf{x} \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}) \subset \mathcal{S}^{k+1}$, it is easy to see that $\mathbf{x}_{\mathcal{S}^k} + x_{j_{k+1}} \mathbf{x}_{\mathcal{S}^k}^k \ge 0$, $\sum_{i \in \mathcal{S}^k} \left((\mathbf{x}_{\mathcal{S}^k})_i + x_{j_{k+1}} (\mathbf{x}_{\mathcal{S}^k}^k)_i \right) = 1$, and $\operatorname{supp}(\mathbf{x}_{\mathcal{S}^k} + x_{j_{k+1}} \mathbf{x}_{\mathcal{S}^k}^k) \subset \mathcal{S}^k$. Notice

$$\mathbf{x}^{k} = \operatorname*{argmin}_{\mathbf{x} \in \mathcal{M}, \operatorname{supp}(\mathbf{x}) \subset \mathcal{S}^{k}} \frac{1}{2} \|\mathbf{b} - A\mathbf{x}\|_{2}^{2}.$$

It follows from (3.2) that

$$\|\mathbf{b} - A\mathbf{x}^{k+1}\|_{2} = \min_{\mathbf{x}\in\mathcal{M}, \operatorname{supp}(\mathbf{x})\subset\mathcal{S}^{k+1}} \|\mathbf{b} - A\mathbf{x}\|_{2}^{2}$$
$$= \min_{\mathbf{x}\in\mathcal{M}, \operatorname{supp}(\mathbf{x})\subset\mathcal{S}^{k+1}} \|\mathbf{b} - A_{\mathcal{S}^{k}}(\mathbf{x}_{\mathcal{S}^{k}} + x_{j_{k+1}}\mathbf{x}_{\mathcal{S}^{k}}^{k})\|_{2}$$
$$= \|\mathbf{b} - A\mathbf{x}^{k}\|_{2}, \qquad (3.3)$$

where the last equality holds by setting $\mathbf{x}_{\mathcal{S}^k} = (1 - x_{j_{k+1}})\mathbf{x}_{\mathcal{S}^k}^k$ for all $0 \le x_{j_{k+1}} \le 1$. Moreover, it is easy to see that $\mathbf{x}^{k+1} = \mathbf{x}^k$ is a special solution to (3.3). In this case, we have $j_{k+1} \in \mathcal{S}^k$.

The following result shows that the choice of the index j_{k+1} is reasonable in the sense that the residual is nonincreasing.

Theorem 3.2 Let $\{\mathbf{x}^k\}$ be the sequence generated by Algorithm 2.2. Then we have, for all $k \geq 1$,

$$\|\mathbf{b} - A\mathbf{x}^{k+1}\|_{2}^{2} \begin{cases} = \|\mathbf{b} - A\mathbf{x}^{k}\|_{2}^{2}, & \text{if } A\mathbf{e}_{j_{k+1}} = A\mathbf{x}^{k}, \\ \\ \leq \|\mathbf{b} - A\mathbf{x}^{k}\|_{2}^{2} - \frac{\left(\mathbf{e}_{j_{k+1}}^{T}A^{T}(\mathbf{b} - A\mathbf{x}^{k}) - (\mathbf{x}^{k})^{T}A^{T}(\mathbf{b} - A\mathbf{x}^{k})\right)^{2}}{\|A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^{k})\|_{2}^{2}}, & \text{otherwise.} \end{cases}$$

Proof: For any $0 \le t \le 1$, let

$$\check{\mathbf{x}}^k := (1-t)\mathbf{x}^k + t\mathbf{e}_{j_{k+1}}$$

It is easy to verify that $\widetilde{\mathbf{x}}^k \in \mathcal{M}$ and $\operatorname{supp}(\widetilde{\mathbf{x}}^k) \subset \mathcal{S}^{k+1}$. Thus, for any $0 \leq t \leq 1$,

ŝ

$$\begin{aligned} \|\mathbf{b} - A\mathbf{x}^{k+1}\|_{2}^{2} &= \min_{\mathbf{x}\in\mathcal{M}, \, \operatorname{supp}(\mathbf{x})\subset\mathcal{S}^{k+1}} \|\mathbf{b} - A\mathbf{x}\|_{2}^{2} \\ &\leq \|\mathbf{b} - A\widetilde{\mathbf{x}}^{k}\|_{2}^{2} = \|\mathbf{b} - A\big((1-t)\mathbf{x}^{k} + t\mathbf{e}_{j_{k+1}}\big)\|_{2}^{2} \\ &= \|(\mathbf{b} - A\mathbf{x}^{k}) - tA(\mathbf{e}_{j_{k+1}} - \mathbf{x}^{k})\|_{2}^{2} \\ &= \|\mathbf{b} - A\mathbf{x}^{k}\|_{2}^{2} + t^{2}\|A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^{k})\|_{2}^{2} - 2t\langle A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^{k}), \mathbf{b} - A\mathbf{x}^{k}\rangle. \quad (3.4) \end{aligned}$$

If $A\mathbf{e}_{j_{k+1}} = A\mathbf{x}^k$, then using Lemma 3.1 we have

$$\|\mathbf{b} - A\mathbf{x}^{k+1}\|_2 = \|\mathbf{b} - A\mathbf{x}^k\|_2$$

We now assume that $A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^k) \neq \mathbf{0}$. From (3.4) we have

$$\|\mathbf{b} - A\mathbf{x}^{k+1}\|_{2}^{2} \le \|\mathbf{b} - A\mathbf{x}^{k}\|_{2}^{2} + \|A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^{k})\|_{2}^{2} (t^{2} - 2t\sigma_{k}),$$

for all $0 \le t \le 1$, where

$$\sigma_k := \frac{\langle A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^k), \mathbf{b} - A\mathbf{x}^k \rangle}{\|A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^k)\|_2^2} = \frac{\mathbf{e}_{j_{k+1}}^T A^T (\mathbf{b} - A\mathbf{x}^k) - (\mathbf{x}^k)^T A^T (\mathbf{b} - A\mathbf{x}^k)}{\|A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^k)\|_2^2}.$$

Thus,

$$\|\mathbf{b} - A\mathbf{x}^{k+1}\|_{2}^{2} \le \|\mathbf{b} - A\mathbf{x}^{k}\|_{2}^{2} + \|A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^{k})\|_{2}^{2} \min_{0 \le t \le 1} (t^{2} - 2t\sigma_{k}).$$

We now show that $0 \leq \sigma_k \leq 1$. We first derive that $\sigma_k \geq 0$. Using the definition of j_{k+1} and $\mathbf{x}^k \in \mathcal{M}$ and $\operatorname{supp}(\mathbf{x}^k) \subset \mathcal{S}^k$ we have

$$(\mathbf{x}^k)^T A^T (\mathbf{b} - A\mathbf{x}^k) \le \mathbf{e}_{j_{k+1}}^T A^T (\mathbf{b} - A\mathbf{x}^k) \sum_{j \in \mathcal{S}^k} x_j^k = \mathbf{e}_{j_{k+1}}^T A^T (\mathbf{b} - A\mathbf{x}^k)$$

This shows that $\sigma_k \geq 0$. On the other hand, we note that, if $\mathbf{e}_i^T A \mathbf{e}_{j_{k+1}} \neq 0$ for some $1 \leq i \leq m$, then $\mathbf{e}_i^T A \mathbf{e}_{j_{k+1}} = 1$. Thus,

$$\|A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^k)\|_2^2 - \langle A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^k), \mathbf{b} - A\mathbf{x}^k \rangle = \langle A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^k), A\mathbf{e}_{j_{k+1}} - \mathbf{b} \rangle \ge 0,$$

where the last inequality uses the fact that $\mathbf{e}_i^T A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^k) \ge 0$ and $\mathbf{e}_i^T (A\mathbf{e}_{j_{k+1}} - \mathbf{b}) \ge 0$ for all $i \in \operatorname{supp}(A\mathbf{e}_{j_{k+1}})$ and $\mathbf{e}_i^T A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^k) \le 0$ and $\mathbf{e}_i^T (A\mathbf{e}_{j_{k+1}} - \mathbf{b}) \le 0$ for all $i \notin \operatorname{supp}(A\mathbf{e}_{j_{k+1}})$ by using the properties (2.2) and (2.3). Therefore, we have $0 \le \sigma_k \le 1$. Substituting $t = \sigma_k$ yields

$$\begin{aligned} \|\mathbf{b} - A\mathbf{x}^{k+1}\|_{2}^{2} &\leq \|\mathbf{b} - A\mathbf{x}^{k}\|_{2}^{2} - \sigma_{k}^{2} \|A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^{k})\|_{2}^{2} \\ &= \|\mathbf{b} - A\mathbf{x}^{k}\|_{2}^{2} - \frac{\left(\mathbf{e}_{j_{k+1}}^{T} A^{T}(\mathbf{b} - A\mathbf{x}^{k}) - (\mathbf{x}^{k})^{T} A^{T}(\mathbf{b} - A\mathbf{x}^{k})\right)^{2}}{\|A(\mathbf{e}_{j_{k+1}} - \mathbf{x}^{k})\|_{2}^{2}}.\end{aligned}$$

The proof is complete.

On the optimality conditions of problem (2.4), we have the following result from [21, Theorem 16.4].

Lemma 3.3 Let \mathbf{x}^{k+1} be the current iterate of Algorithm 2.2. Then $\mathbf{x}^{k+1} \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}^{k+1}) \subset \mathcal{S}^{k+1}$ is a global solution to problem (2.4) if and only if

$$\left(A_{\mathcal{S}^{k+1}}^{T}(\mathbf{b} - A\mathbf{x}^{k+1})\right)_{l} \begin{cases} = (\mathbf{x}^{k+1})^{T} A^{T}(\mathbf{b} - A\mathbf{x}^{k+1}), & \text{if } l \in \operatorname{supp}(\mathbf{x}^{k+1}), \\ \leq (\mathbf{x}^{k+1})^{T} A^{T}(\mathbf{b} - A\mathbf{x}^{k+1}), & \text{if } l \in \mathcal{S}^{k+1} \setminus \operatorname{supp}(\mathbf{x}^{k+1}). \end{cases}$$

Moreover, if $A_{\mathcal{S}^{k+1}} : \mathcal{Z}_{\mathcal{S}^{k+1}} \to \mathbb{R}^m$ is injective, then $\mathbf{x}^{k+1} \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}^{k+1}) \subset \mathcal{S}^{k+1}$ is the unique global solution to problem (2.4), where $\mathcal{Z}_{\mathcal{S}^{k+1}} := \{\mathbf{z} \in \mathbb{R}^{|\mathcal{S}^{k+1}|} \mid \mathbf{1}^T \mathbf{z} = 1, \mathbf{z} \geq 0\}.$

We now discuss the convergence conditions for the MOMP. We first give some necessary conditions for Algorithm 2.2 to recover a sparse solution to the linear system $\mathbf{b} = A\mathbf{x}$. The proof can be seen as a generalization of [12, Proposition 3.5].

Theorem 3.4 Let $A \in \mathbb{R}^{m \times N}$ and $\mathbf{b} \in \mathbb{R}^m$ be defined by (1.4). Suppose every nonzero vector $\mathbf{x}^* \in \mathcal{M}$ supported on a set S of size d is recovered from $\mathbf{b} = A\mathbf{x}^*$ via Algorithm 2.2 with any fixed starting point $\mathbf{x}^0 \in \mathcal{M}$ after at most d iterations. Then the linear operator $A_S : \mathcal{Z}_S \to \mathbb{R}^m$ is injective,

$$\max_{j\in\mathcal{S}} \left(A^T(\mathbf{b} - A\mathbf{x}^0) \right)_j > \max_{l\in[N]\setminus\mathcal{S}} \left(A^T(\mathbf{b} - A\mathbf{x}^0) \right)_l, \tag{3.5}$$

for all $\mathbf{b} \in \{A\mathbf{x} \mid \mathbf{x} \in \mathcal{M}, \operatorname{supp}(\mathbf{x}) \subset \mathcal{S}\}, where \mathcal{Z}_{\mathcal{S}} := \{\mathbf{z} \in \mathbb{R}^{|\mathcal{S}|} \mid \mathbf{1}^T \mathbf{z} = 1, \ \mathbf{z} \ge 0\}.$

Proof: Suppose Algorithm 2.2 recovers all vectors supported on a set S of size d at most d iterations. Then, for any two vectors $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{M}$ supported on S with $A\mathbf{x}_1 = \mathbf{b} = A\mathbf{x}_2$, we must have $\mathbf{x}_1 = \mathbf{x}_2$. This shows that the linear operator $A_S : \mathcal{Z}_S \to \mathbb{R}^m$ is injective. On the other hand, if there exists a vector $\mathbf{x}^* \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}^*) \subset S$ such that $\mathbf{b} = A\mathbf{x}^*$, then the index j_1 generated by Algorithm 2.2 at the first iteration should not belong to $[N] \setminus S$, i.e., $\max_{j \in S} (A^T(\mathbf{b} - A\mathbf{x}^0))_j > \max_{l \in [N] \setminus S} (A^T(\mathbf{b} - A\mathbf{x}^0))_l$. Therefore, we have $\max_{j \in S} (A^T(\mathbf{b} - A\mathbf{x}^0))_j$.

 $(A\mathbf{x}^0)_j > \max_{l \in [N] \setminus S} (A^T(\mathbf{b} - A\mathbf{x}^0))_l$ for all $\mathbf{b} \in \{A\mathbf{x} \mid \mathbf{x} \in \mathcal{M}, \operatorname{supp}(\mathbf{x}) \subset S\}$. This completes the proof.

Next, we provide some sufficient conditions to guarantee Algorithm 2.2 recovers all sparse solutions of the linear system $\mathbf{b} = A\mathbf{x}$ exactly. The proof can be seen as a generalization of [12, Proposition 3.5].

Theorem 3.5 Let $A \in \mathbb{R}^{m \times N}$ and $\mathbf{b} \in \mathbb{R}^m$ be defined by (1.4). Then every nonzero vector $\mathbf{x}^* \in \mathcal{M}$ supported on a set S of size d is recovered from $\mathbf{b} = A\mathbf{x}^*$ via Algorithm 2.2 with any fixed starting point $\mathbf{x}^0 \in \mathcal{M}$ after at most d iterations if the linear operator $A_S : \mathcal{Z}_S \to \mathbb{R}^m$ is injective,

$$\max_{j \in \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^0) \right)_j > \max_{l \in [N] \setminus \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^0) \right)_l, \tag{3.6}$$

and

$$\max_{j \in \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}) \right)_j > \max_{l \in [N] \setminus \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}) \right)_l, \tag{3.7}$$

for all $\mathbf{x} \in \mathcal{M}_{\mathcal{S}} := {\mathbf{x} \in \mathcal{M} \mid \operatorname{supp}(\mathbf{x}) \subset \mathcal{S} \setminus {\mathbf{x}^*}, \text{ where } \mathcal{Z}_{\mathcal{S}} := {\mathbf{z} \in \mathbb{R}^{|\mathcal{S}|} \mid \mathbf{1}^T \mathbf{z} = 1, \ \mathbf{z} \ge 0}.$

Proof: Suppose the starting point $\mathbf{x}^0 \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}^0) \not\subset \mathcal{S}$ is such that $\mathbf{b} = A\mathbf{x}^0$. This contradicts (3.6). We now assume that $\mathbf{b} \neq A\mathbf{x}^k$ for $k = 1, \ldots, d-1$ (otherwise, we have found the solution). We claim that, for any $1 \leq k \leq d$, $\mathcal{S}^k \subset \mathcal{S}$ is of size k. Therefore $\mathcal{S} = \mathcal{S}^d$ and $\mathbf{x}^* = \mathbf{x}^d$ since the linear operator $A_{\mathcal{S}} : \mathcal{Z}_{\mathcal{S}} \to \mathbb{R}^m$ is injective. In the following, we show the claim by the induction. We first show that, for any $1 \leq k \leq d$, $\mathcal{S}^k \subset \mathcal{S}$ (which implies that $\mathbf{x}^k \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}^k) \subset \mathcal{S}^k$). Using (3.6), we know that the first index j_1 must belong to \mathcal{S} and thus $\mathcal{S}^1 = \mathcal{S}^0 \cup \{j_1\} = \{j_1\} \subset \mathcal{S}$. Now, suppose $\mathcal{S}^k \subset \mathcal{S}$ for some $1 \leq k \leq d-1$. Then, using (3.7) we have the index $j_{k+1} \in \mathcal{S}$ and thus $\mathcal{S}^{k+1} = \mathcal{S}^k \cup \{j_{k+1}\} \subset \mathcal{S}$. By the induction, we have $\mathcal{S}^k \subset \mathcal{S}$ for all $1 \leq k \leq d$. Next, we show that \mathcal{S}^k is of size k for all $1 \leq k \leq d$. For any $1 \leq k \leq d$, using Lemma 3.3 we have

$$\left(A_{\mathcal{S}^{k}}^{T}(\mathbf{b}-A\mathbf{x}^{k})\right)_{l} \begin{cases} = (\mathbf{x}^{k})^{T} A^{T}(\mathbf{b}-A\mathbf{x}^{k}), & \text{if } l \in \operatorname{supp}(\mathbf{x}^{k}), \\ \leq (\mathbf{x}^{k})^{T} A^{T}(\mathbf{b}-A\mathbf{x}^{k}), & \text{if } l \in \mathcal{S}^{k} \setminus \operatorname{supp}(\mathbf{x}^{k}) \end{cases}$$

By definition, $j_{k+1} = \operatorname{argmax}_{j \in [N]} \mathbf{e}_j^T A^T (\mathbf{b} - A\mathbf{x}^k) \notin \mathcal{S}^k$. Otherwise, if $j_{k+1} \in \mathcal{S}^k$, then it follows from (3.7) that

$$\max_{j\in\mathcal{S}^k} \left(A^T(\mathbf{b} - A\mathbf{x}^k) \right)_j = \max_{j\in\mathcal{S}} \left(A^T(\mathbf{b} - A\mathbf{x}^k) \right)_j > \max_{l\in[N]\setminus\mathcal{S}} \left(A^T(\mathbf{b} - A\mathbf{x}^k) \right)_l$$

Thus,

$$\left(A^{T}(\mathbf{b}-A\mathbf{x}^{k})\right)_{l} \begin{cases} = (\mathbf{x}^{k})^{T} A^{T}(\mathbf{b}-A\mathbf{x}^{k}), & \text{if } l \in \operatorname{supp}(\mathbf{x}^{k}), \\ \leq (\mathbf{x}^{k})^{T} A^{T}(\mathbf{b}-A\mathbf{x}^{k}), & \text{if } l \in \mathcal{S}^{k} \setminus \operatorname{supp}(\mathbf{x}^{k}) \\ \leq (\mathbf{x}^{k})^{T} A^{T}(\mathbf{b}-A\mathbf{x}^{k}), & \text{if } l \in \mathcal{S} \setminus \mathcal{S}^{k}, \\ < (\mathbf{x}^{k})^{T} A^{T}(\mathbf{b}-A\mathbf{x}^{k}), & \forall l \in [N] \setminus \mathcal{S}. \end{cases}$$

Using Lemma 3.3 and the injectivity of the linear operator $A_{\mathcal{S}} : \mathcal{Z}_{\mathcal{S}} \to \mathbb{R}^m$, we know that \mathbf{x}^k is the unique global solution to problem (1.5). By assumption, $\mathbf{x}^* \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}^*) \subset \mathcal{S}$ is such that $\mathbf{b} = A\mathbf{x}^*$, which is a global solution to problem (1.5). Thus $\mathbf{x}^* = \mathbf{x}^k$. This is a contradiction. Therefore, \mathcal{S}^k is of size k. The proof is complete.

Remark 3.6 We observe that the necessary conditions in Theorem 3.4 are not equivalent to the sufficient conditions in Theorem 3.5. This may be caused by the additional constraints: $\mathbf{1}^T \mathbf{x} = 1$ and $\mathbf{x} \ge \mathbf{0}$. By assumptions, $\mathbf{b} = A\mathbf{x}^*$ for every exact recovery $\mathbf{x}^* \in \mathcal{M}$ supported on a set \mathcal{S} of size d. Then \mathbf{b} belongs to the set $\{A\mathbf{x} \mid \mathbf{x} \in \mathcal{M}, \operatorname{supp}(\mathbf{x}) \subset \mathcal{S}\}$. While, for any $1 \le k \le d-1$, we have $\mathcal{S}^k \subset \mathcal{S}$ but the residual $\mathbf{r}^k := \mathbf{b} - A\mathbf{x}^k = A(\mathbf{x}^* - \mathbf{x}^k + \mathbf{x}^0) - A\mathbf{x}^0$, where $A(\mathbf{x}^* - \mathbf{x}^k + \mathbf{x}^0)$ is not guaranteed to belong to the set $\{A\mathbf{x} \mid \mathbf{x} \in \mathcal{M}, \operatorname{supp}(\mathbf{x}) \subset \mathcal{S}\}$ since the support of \mathbf{x}^0 is not necessary on \mathcal{S} and the entrywise nonnegativity of the vector $(\mathbf{x}^* - \mathbf{x}^k + \mathbf{x}^0)$ is not guaranteed.

By following the similar proof of Theorem 3.5, we have the following sufficient conditions on the sparse recovery of Algorithm 2.2 for problem (1.5).

Theorem 3.7 Let $A \in \mathbb{R}^{m \times N}$ and $\mathbf{b} \in \mathbb{R}^m$ be defined by (1.4). Then every nonzero vector $\mathbf{x}^* \in \mathcal{M}$ supported on a set S of size d solve problem (1.5) via Algorithm 2.2 after at most d iterations if the linear operator $A_S : \mathcal{Z}_S \to \mathbb{R}^m$ is injective,

$$\max_{j \in \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^0) \right)_j > \max_{l \in [N] \setminus \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^0) \right)_l,$$

and

$$\max_{j \in \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}) \right)_j > \max_{l \in [N] \setminus \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}) \right)_l$$

for all $\mathbf{x} \in \mathcal{M}_{\mathcal{S}}$, where $\mathcal{M}_{\mathcal{S}}$ and $\mathcal{Z}_{\mathcal{S}}$ are defined as in Theorem 3.5.

Remark 3.8 In Theorems 3.4–3.7, we require that the injectivity of the linear operator $A_{\mathcal{S}}$: $\mathcal{Z}_{\mathcal{S}} \to \mathbb{R}^m$, which is guaranteed if $A_{\mathcal{S}} : \mathbb{R}^{|\mathcal{S}|} \to \mathbb{R}^m$ is injective i.e., $A_{\mathcal{S}}$ is full column rank. We note that $\mathcal{Z}_{\mathcal{S}}$ is a closed convex subset of $\mathbb{R}^{|\mathcal{S}|}$. It is easy to see that if $|\mathcal{S}| > m$, then the linear operator $A_{\mathcal{S}} : \mathbb{R}^{|\mathcal{S}|} \to \mathbb{R}^m$ cannot be injective. This shows that, if Algorithm 2.2 generates a sparse solution to problem (1.5), then the sparsity is no more than m.

Based on Theorems 3.5–3.7 and Remark 3.8, for Algorithm 2.2, we have the following results on the recovery with a given support for problem (1.5) exactly or in the least square sense.

Corollary 3.9 Let $A \in \mathbb{R}^{m \times N}$ and $\mathbf{b} \in \mathbb{R}^m$ be defined by (1.4). Let $S \subset [N]$ with d = |S|. Then every nonzero vector $\mathbf{x}^* \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}^*) \subset S$ is recovered from $\mathbf{b} = A\mathbf{x}^*$ via Algorithm 2.2 after at most d iterations if A_S has full column rank and

$$\max_{j \in \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^k) \right)_j > \max_{l \in [N] \setminus \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^k) \right)_l,$$

for $k = 0, 1, \ldots, d - 1$.

Corollary 3.10 Let $A \in \mathbb{R}^{m \times N}$ and $\mathbf{b} \in \mathbb{R}^m$ be defined by (1.4). Let $S \subset [N]$ with d = |S|. Then every nonzero vector $\mathbf{x}^* \in \mathcal{M}$ with $\operatorname{supp}(\mathbf{x}^*) \subset S$ solve problem (1.5) in the least square sense via Algorithm 2.2 after at most d iterations if A_S has full column rank and

$$\max_{j \in \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^k) \right)_j > \max_{l \in [N] \setminus \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^k) \right)_l,$$

for $k = 0, 1, \ldots, d - 1$.

Remark 3.11 If one chooses the starting point $\mathbf{x}^0 = \mathbf{0}$ in Algorithm 2.2, then, in Theorems 3.5–3.7 and Corollaries 3.9–3.10, the condition

$$\max_{j \in \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^0) \right)_j > \max_{l \in [N] \setminus \mathcal{S}} \left(A^T (\mathbf{b} - A\mathbf{x}^0) \right)_l.$$

is replaced by

$$\max_{j\in\mathcal{S}}(A^T\mathbf{b})_j > \max_{l\in[N]\setminus\mathcal{S}}(A^T\mathbf{b})_l$$

From the latter numerical examples, we can see that different sparse solutions to problem (1.5) can be obtained via Algorithm 2.2 with different choices of sparse $\mathbf{x}^0 \in \mathcal{M}$ or $\mathbf{x}^0 = \mathbf{0}$.

4 Numerical experiments

In this section, we present the numerical performance of Algorithm 2.2 for solving problem (1.5). To illustrate the efficiency of our method, we compare the proposed algorithm with the maximum entropy rate approach (MEM) in [4] and the projection-based gradient descent method (PG) in [33]. All numerical tests were carried out using MATLAB R2020a on a personal laptop with an Intel(R) Core(TM) i7–5500U CPU at 2.4 GHz and 8GB of RAM.

In our numerical experiments, the initial point \mathbf{x}^0 is chosen to be (a) $\mathbf{x}^0 = \mathbf{0}$ and (b) $\mathbf{x}^0 \in \mathcal{M}$ is a random sparse *N*-vector with *s* uniformly distributed nonzero entries, where s = 1, 2. The stopping criterion for Algorithm 2.2 is given by

$$\|A_{\operatorname{supp}(\mathbf{x}^k)}^T \mathbf{r}^k - (\mathbf{x}^k)^T A^T \mathbf{r}^k\|_2 + \|\max(A_{[N]\setminus\operatorname{supp}(\mathbf{x}^k)}^T \mathbf{r}^k - (\mathbf{x}^k)^T A^T \mathbf{r}^k, \mathbf{0})\|_2 \le 10^{-7}$$

with $\mathbf{r}^k = \mathbf{b} - A\mathbf{x}^k$ and the largest number of iterations for Algorithm 2.2 is set to be m.

We consider the following numerical examples.

Example 4.1 Consider another example in [5] with two genes (n = 2), where the observed transition probability matrix is given by

$$P_1 = \begin{bmatrix} 0.1 & 0.3 & 0.2 & 0.1 \\ 0.2 & 0.3 & 0.2 & 0.0 \\ 0.0 & 0.0 & 0.6 & 0.4 \\ 0.7 & 0.4 & 0.0 & 0.5 \end{bmatrix}$$

In this PBN, there are N = 81 BNs.

Example 4.2 We consider a network in [33] where the prescribed transition probability matrix of the PBN is given by

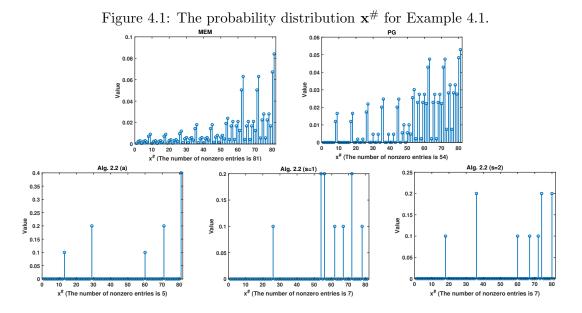
$$P_2 = \left[\begin{array}{cc} P_1 & 0\\ 0 & P_1 \end{array} \right].$$

In this PBN, there are 6561 BNs.

The numerical results for Examples 4.1–4.2 are displayed in Figures 4.1–4.2 and Tables 4.1– 4.2. Here, $\mathbf{x}^{\#}$ denotes the computed solution to problem (1.5) obtained via MEM, PG, and Algorithm 2.2 accordingly, the symbols 'Obj.' and 'CT.' mean the total computing time in seconds and the objective function value $\frac{1}{2} || A \mathbf{x}^{\#} - \mathbf{b} ||_2^2$ at the final iterate of the corresponding algorithm, respectively, ' $\mathbf{sum}(\mathbf{j})$ ' is the sum of the *j* largest components of the computed solution $\mathbf{x}^{\#}$ for different *j* and 'Obj(\mathbf{j})' is the corresponding reconstructed objective function value $\frac{1}{2} || \mathbf{b} - A_{\pi(1:j)} \mathbf{x}^{\#}(\pi(1:j)) ||_2^2$, where $\pi = {\pi(1), \ldots, \pi(N)}$ is a permutation such that

$$x_{\pi(1)}^{\#} \ge x_{\pi(2)}^{\#} \ge \dots \ge x_{\pi(N)}^{\#}$$
 and $\mathbf{x}^{\#}(\pi(1:j)) = (x_{\pi(1)}^{\#}, \dots, x_{\pi(j)}^{\#})^T \in \mathbb{R}^j$.

We observe from Figures 4.1–4.2 that the solution obtained by Algorithm 2.2 are much sparser than MEM and PG. We also see from Tables 4.1–4.2 that the identified major BNs by Algorithm 2.2 with various initial guesses leads to much less residual than MEM and PG.

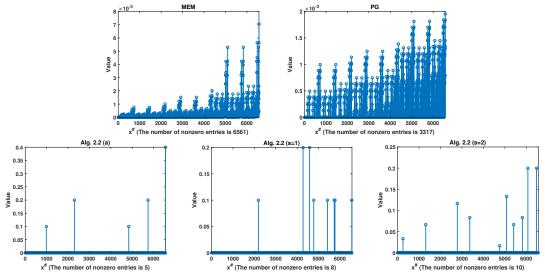


To further illustrate the effectiveness of our method, in the following numerical example, we only compare the performance of our method with that of PG for reconstructing a sparse solution to problem (1.5) in the least square sense since the problem size is very large and the MEM is not so effective as expected.

| | MEM | | PG | | Alg. 2.2 (a) | | Alg. 2.2 $(s=1)$ | | Alg. 2.2 (s=2) | |
|---------------------------|--------------------------|-------------------|-------------------------|-------------------|--------------------------|-------------------|--------------------------|-------------------|--------------------------|-------------------|
| Obj. | 1.9035×10^{-12} | | 2.7759×10^{-8} | | 1.9324×10^{-12} | | 1.1331×10^{-12} | | 1.2651×10^{-13} | |
| CT. | 0.0039 | | 0.0022 | | 0.0274 | | 0.0198 | | 0.0273 | |
| $\ \mathbf{x}^{\#}\ _{0}$ | 81 | | 54 | | 5 | | 7 | | 7 | |
| j | Obj(j) | <pre>sum(j)</pre> | ОЪј(ј) | <pre>sum(j)</pre> | Obj(j) | <pre>sum(j)</pre> | Obj(j) | <pre>sum(j)</pre> | Obj(j) | <pre>sum(j)</pre> |
| 1 | 1.1826×10^{0} | 0.0840 | 1.2323×10^{0} | 0.0528 | 7.8740×10^{-1} | 0.4000 | 1.1045×10^{0} | 0.2000 | 1.0296×10^{0} | 0.2000 |
| 2 | 1.0809×10^{0} | 0.1512 | 1.1578×10^{0} | 0.1011 | 5.4772×10^{-1} | 0.6000 | 8.3666×10^{-1} | 0.4000 | 8.8318×10^{-1} | 0.4000 |
| 3 | 9.8401×10^{-1} | 0.2142 | 1.0837×10^{0} | 0.1486 | 3.1623×10^{-1} | 0.8000 | 5.4772×10^{-1} | 0.6000 | 6.1644×10^{-1} | 0.6000 |
| 4 | 8.8997×10^{-1} | 0.2772 | 1.0108×10^{0} | 0.1960 | 2.0000×10^{-1} | 0.9000 | 4.2426×10^{-1} | 0.7000 | 4.8990×10^{-1} | 0.7000 |
| 5 | 8.1831×10^{-1} | 0.3276 | 9.4840×10^{-1} | 0.2389 | 1.9324×10^{-12} | 1.0000 | 2.8284×10^{-1} | 0.8000 | 3.4641×10^{-1} | 0.8000 |
| 6 | 7.4996×10^{-1} | 0.3780 | 8.8778×10^{-1} | 0.2818 | | | 2.0000×10^{-1} | 0.9000 | 2.0000×10^{-13} | 0.9000 |
| 7 | 7.1145×10^{-1} | 0.4060 | 8.4215×10^{-1} | 0.3146 | | | 1.1331×10^{-12} | 1.0000 | 1.2651×10^{-13} | 1.0000 |
| 8 | 6.7424×10^{-1} | 0.4340 | 7.9794×10^{-1} | 0.3474 | | | | | | |
| 9 | 6.4511×10^{-1} | 0.4580 | 7.6017×10^{-1} | 0.3775 | | | | | | |
| 10 | 6.1692×10^{-1} | 0.4804 | 7.2474×10^{-1} | 0.4057 | | | | | | |
| 11 | 5.8994×10^{-1} | 0.5028 | 6.9094×10^{-1} | 0.4339 | | | | | | |
| 12 | 5.6353×10^{-1} | 0.5238 | 6.5929×10^{-1} | 0.4615 | | | | | | |
| 13 | 5.3828×10^{-1} | 0.5448 | 6.2431×10^{-1} | 0.4889 | | | | | | |
| 14 | 5.1350×10^{-1} | 0.5658 | 5.9108×10^{-1} | 0.5163 | | | | | | |
| 15 | 4.9018×10^{-1} | 0.5868 | 5.5855×10^{-1} | 0.5437 | | | | | | |
| 16 | 4.6415×10^{-1} | 0.6060 | 5.2830×10^{-1} | 0.5711 | | | | | | |

Table 4.1: Numerical results for Example 4.1.

Figure 4.2: The probability distribution $\mathbf{x}^{\#}$ for Example 4.2.



Example 4.3 We consider a network in [13] for modelling credit defaults, where the prescribed transition probability matrix of the PBN is given by

| | 0.57 | 0.00 | 0.10 | 0.00 | 0.00 | 0.04 | 0.00 | ך 0.00 |
|------|----------------|------|------|------|------|------|--|---|
| | 0.14 | 0.31 | 0.00 | 0.50 | 0.13 | 0.13 | 0.33 | 0.06 |
| | 0.00 | 0.08 | 0.40 | 0.25 | 0.25 | 0.00 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | 0.00 |
| D _ | $0.00 \\ 0.00$ | 0.15 | 0.00 | 0.00 | 0.00 | 0.08 | 0.00 | 0.00 |
| 13 — | 0.00 | 0.15 | 0.30 | 0.00 | 0.00 | 0.13 | 0.00 | 0.00 |
| | 0.29 | 0.31 | 0.20 | 0.00 | 0.25 | 0.29 | 0.00 | 0.39 |
| | 0.00 | 0.00 | 0.00 | 0.00 | 0.38 | 0.00 | 0.00 | $\begin{array}{c} 0.00 \\ 0.56 \end{array} \right]$ |
| | 0.00 | 0.00 | 0.00 | 0.25 | 0.00 | 0.33 | 0.00 | 0.56 |

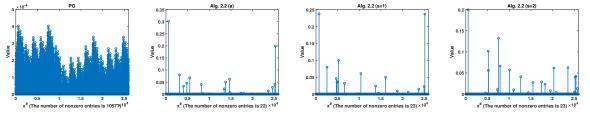
| | MEM | | PG | | Alg. 2.2 (a) | | Alg. 2.2 $(s=1)$ | | Alg. 2.2 (s=2) | |
|---------------------------|-------------------------|-------------------|-------------------------|-------------------|--------------------------|-------------------|--------------------------|-------------------|--------------------------|-------------------|
| Obj. | 3.6129×10^{-9} | | 1.5072×10^{-7} | | 1.6574×10^{-13} | | 1.0598×10^{-13} | | 2.3896×10^{-12} | |
| CT. | 2.3761 | | 1.6465 | | 0.0286 | | 0.0351 | | 0.0407 | |
| $\ \mathbf{x}^{\#}\ _{0}$ | 6561 | | 3317 | | 5 | | 8 | | 10 | |
| j | Obj(j) | <pre>sum(j)</pre> | Obj(j) | <pre>sum(j)</pre> | Obj(j) | <pre>sum(j)</pre> | Obj(j) | <pre>sum(j)</pre> | ОЪј(ј) | <pre>sum(j)</pre> |
| 1 | 1.8489×10^{0} | 0.0071 | 1.8609×10^{0} | 0.0020 | 1.1136×10^{0} | 0.4000 | 1.6248×10^{0} | 0.2000 | 1.4832×10^{0} | 0.2000 |
| 2 | 1.8359×10^{0} | 0.0127 | 1.8566×10^{0} | 0.0038 | 7.7460×10^{-1} | 0.6000 | 1.2166×10^{0} | 0.4000 | 1.1136×10^{0} | 0.4000 |
| 3 | 1.8230×10^{0} | 0.0183 | 1.8524×10^{0} | 0.0056 | 4.4721×10^{-1} | 0.8000 | 1.0198×10^{0} | 0.5000 | 8.6152×10^{-1} | 0.5333 |
| 4 | 1.8108×10^{0} | 0.0236 | 1.8482×10^{0} | 0.0075 | 2.8284×10^{-1} | 0.9000 | 7.8740×10^{-1} | 0.6000 | 6.9121×10^{-1} | 0.6500 |
| 5 | 1.7988×10^{0} | 0.0289 | 1.8440×10^{0} | 0.0093 | 1.6574×10^{-13} | 1.0000 | 6.1644×10^{-1} | 0.7000 | 5.3229×10^{-1} | 0.7333 |
| 6 | 1.7867×10^{0} | 0.0342 | 1.8399×10^{0} | 0.0111 | | | 4.6904×10^{-1} | 0.8000 | 3.8006×10^{-1} | 0.8167 |
| 7 | 1.7746×10^{0} | 0.0395 | 1.8357×10^{0} | 0.0129 | | | 2.8284×10^{-1} | 0.9000 | 2.6667×10^{-1} | 0.8833 |
| 8 | 1.7645×10^{0} | 0.0440 | 1.8318×10^{0} | 0.0146 | | | 1.0598×10^{-13} | 1.0000 | 1.2472×10^{-1} | 0.9500 |
| 9 | 1.7551×10^{0} | 0.0483 | 1.8280×10^{0} | 0.0163 | | | | | 4.7140×10^{-2} | 0.9833 |
| 10 | 1.7456×10^{0} | 0.0525 | 1.8242×10^{0} | 0.0180 | | | | | 2.3896×10^{-12} | 1.0000 |
| 11 | 1.7362×10^{0} | 0.0567 | 1.8204×10^{0} | 0.0197 | | | | | | |
| 12 | 1.7268×10^{0} | 0.0610 | 1.8166×10^{0} | 0.0214 | | | | | | |
| 13 | 1.7174×10^{0} | 0.0652 | 1.8127×10^{0} | 0.0231 | | | | | | |
| 14 | 1.7079×10^{0} | 0.0694 | 1.8089×10^{0} | 0.0248 | | | | | | |
| 15 | 1.6985×10^{0} | 0.0737 | 1.8051×10^{0} | 0.0265 | | | | | | |
| 16 | 1.6891×10^{0} | 0.0779 | $1.8013 	imes 10^0$ | 0.0282 | | | | | | |

Table 4.2: Numerical results for Example 4.2.

In this PBN, there are 25920 BNs.

The numerical results for Example 4.3 are displayed in Figures 4.3 and Table 4.3. Figure 4.3 shows that the least square solution generated by our method is much sparse than PG. We also see from Table 4.3 that the major BNs obtained by Algorithm 2.2 yields much less residual than PG.





5 Concluding remarks

Several numerical methods have been developed for the construction of sparse probabilistic Boolean networks. However, few greedy methods were explored. In this paper, we propose a greedy-type method, a modified orthogonal matching pursuit, for solving the inverse problem. We derive some conditions such that, given the transition probability matrix, our method can recover a sparse probabilistic Boolean network exactly or in the least square sense. Numerical experiments show that our method is very effective in terms of sparse recovery. An interesting question is how to analyze the exact sparse recovery condition in terms of the coherence as in [32]. This needs further study.

| | | | | | - | | - | |
|---------------------------|------------------------|-------------------|-------------------------|-------------------|-------------------------|-------------------|-------------------------|-------------------|
| | \mathbf{PG} | | Alg. 2.2 (a) | | Alg. 2.2 (s | | Alg. $2.2 (s=2)$ | |
| Obj. | $7.6376 	imes 10^{-3}$ | | 7.6376×10^{-3} | | 7.6376×1 | 0^{-3} | 7.6376×10^{-3} | |
| CT. | 2.9839 | | 0.1392 | | 0.2088 | | 0.2310 | |
| $\ \mathbf{x}^{\#}\ _{0}$ | 10577 | | 22 | | 23 | | 23 | |
| j | Obj(j) | <pre>sum(j)</pre> | Obj(j) | <pre>sum(j)</pre> | Obj(j) | <pre>sum(j)</pre> | Obj(j) | <pre>sum(j)</pre> |
| 1 | 1.7007×10^{0} | 0.0004 | 1.1740×10^{0} | 0.3019 | 1.3997×10^{0} | 0.2377 | 1.3595×10^{0} | 0.1998 |
| 2 | 1.6998×10^{0} | 0.0008 | $8.5697 	imes 10^{-1}$ | 0.5019 | 9.4187×10^{-1} | 0.4747 | 1.1870×10^{0} | 0.3319 |
| 3 | 1.6990×10^{0} | 0.0012 | $7.2396 	imes 10^{-1}$ | 0.5819 | 7.7130×10^{-1} | 0.5746 | 1.0009×10^{0} | 0.4338 |
| 4 | 1.6982×10^{0} | 0.0016 | 6.1625×10^{-1} | 0.6497 | 6.2345×10^{-1} | 0.6545 | 8.6691×10^{-1} | 0.5002 |
| 5 | 1.6974×10^{0} | 0.0019 | 5.2749×10^{-1} | 0.7114 | 5.1882×10^{-1} | 0.7155 | 7.5744×10^{-1} | 0.5631 |
| 6 | 1.6966×10^{0} | 0.0023 | 4.3873×10^{-1} | 0.7616 | 4.3079×10^{-1} | 0.7657 | 6.5260×10^{-1} | 0.6248 |
| 7 | 1.6958×10^{0} | 0.0027 | $3.5896 	imes 10^{-1}$ | 0.8067 | 3.4471×10^{-1} | 0.8119 | 5.4269×10^{-1} | 0.6825 |
| 8 | 1.6950×10^{0} | 0.0031 | $2.7739 	imes 10^{-1}$ | 0.8466 | 2.7640×10^{-1} | 0.8490 | 4.4473×10^{-1} | 0.7388 |
| 9 | 1.6943×10^{0} | 0.0034 | 2.1471×10^{-1} | 0.8866 | 2.0859×10^{-1} | 0.8852 | 3.6801×10^{-1} | 0.7810 |
| 10 | 1.6935×10^{0} | 0.0038 | 1.5347×10^{-1} | 0.9194 | 1.5972×10^{-1} | 0.9172 | 3.0392×10^{-1} | 0.8221 |
| 11 | 1.6928×10^{0} | 0.0041 | 1.0387×10^{-1} | 0.9470 | 1.2150×10^{-1} | 0.9414 | 2.3503×10^{-1} | 0.8621 |
| 12 | 1.6920×10^{0} | 0.0045 | $6.6657 	imes 10^{-2}$ | 0.9688 | 7.2729×10^{-2} | 0.9642 | 1.9174×10^{-1} | 0.8910 |
| 13 | 1.6912×10^{0} | 0.0049 | $3.6778 	imes 10^{-2}$ | 0.9825 | 4.4031×10^{-2} | 0.9791 | $1.4679 	imes 10^{-1}$ | 0.9184 |
| 14 | 1.6905×10^{0} | 0.0052 | $2.6746 	imes 10^{-2}$ | 0.9887 | 2.6876×10^{-2} | 0.9885 | 1.0694×10^{-1} | 0.9419 |
| 15 | 1.6898×10^{0} | 0.0056 | 1.8270×10^{-2} | 0.9933 | 1.6651×10^{-2} | 0.9939 | 8.5392×10^{-2} | 0.9550 |
| 16 | 1.6890×10^{0} | 0.0059 | 1.2374×10^{-2} | 0.9968 | 1.1768×10^{-2} | 0.9967 | $7.1039 	imes 10^{-2}$ | 0.9658 |
| 17 | 1.6883×10^{0} | 0.0063 | 8.3336×10^{-3} | 0.9993 | 9.2747×10^{-3} | 0.9985 | 5.1373×10^{-2} | 0.9763 |
| 18 | 1.6876×10^{0} | 0.0066 | 7.8849×10^{-3} | 0.9997 | 8.1940×10^{-3} | 0.9994 | 3.4444×10^{-2} | 0.9841 |
| 19 | 1.6869×10^{0} | 0.0070 | $7.7370 	imes 10^{-3}$ | 0.9999 | 7.9249×10^{-3} | 0.9997 | $2.5720 	imes 10^{-2}$ | 0.9894 |
| 20 | 1.6862×10^{0} | 0.0073 | $7.6775 	imes 10^{-3}$ | 0.99995 | 7.7959×10^{-3} | 0.9998 | 1.8746×10^{-2} | 0.9932 |
| 21 | 1.6855×10^{0} | 0.0076 | $7.6503 	imes 10^{-3}$ | 0.99998 | 7.6777×10^{-3} | 0.9999 | 1.2993×10^{-2} | 0.9967 |
| 22 | 1.6848×10^{0} | 0.0080 | 7.6376×10^{-3} | 1.0000 | 7.6563×10^{-3} | 0.99998 | 8.4447×10^{-3} | 0.9993 |
| 23 | 1.6841×10^{0} | 0.0083 | | | 7.6376×10^{-3} | 1.0000 | 7.6376×10^{-3} | 1.0000 |

Table 4.3: Numerical results for Example 4.3.

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