## Causal Discovery in Linear Models with Unobserved Variables and Measurement Error

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## Abstract

The presence of unobserved common causes and the presence of measurement error are two of the most limiting challenges in the task of causal structure learning. Ignoring either of the two challenges can lead to detecting spurious causal links among variables of interest. In this paper, we study the problem of causal discovery in systems where these two challenges can be present simultaneously. We consider linear models which include four types of variables: variables that are directly observed, variables that are not directly observed but are measured with error, the corresponding measurements, and variables that are neither observed nor measured. We characterize the extent of identifiability of such model under separability condition (i.e., the matrix indicating the independent exogenous noise terms pertaining to the observed variables is identifiable) together with two versions of faithfulness assumptions and propose a notion of observational equivalence. We provide graphical characterization of the models that are equivalent and present a recovery algorithm that could return models equivalent to the ground truth.

## 1 Introduction

Causal structure learning, also known as causal discovery, from observational data has been studied extensively in the literature. The majority of work assume that there are no unobserved variables in the system that can affect more than one other variable, i.e., no unobserved common causes, and that variables are measured without error. This leads to identification of the underlying structure up to Markov equivalence class in general [15, 3], and complete identification of the structure under further model assumptions such as assuming a linear non-Gaussian model (LiNGAM, [12, 13]). However, in majority of real-world settings, the researcher will not be able to observe all the relevant variables and hence cannot rule out the presence of unobserved common causes, and further many of the variables may have been measured with error. This necessitates approaches for causal discovery capable of dealing with these two important challenges.

In this work, we study the problem of causal discovery from observational data in the presence of both aforementioned challenges, i.e., in settings with both unobserved common causes and measurement error. We consider a special type of linear structural equation model (SEM) as the underlying data generating process which includes four types of variables: variables that are directly observed (called *observed variables*), variables that are not directly observed but are measured with error (called *measured variables*), the corresponding *measurement variables*, and variables that are neither

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Figure 1: Left: Diagram of an LV-SEM-ME (see Appendix B.2 for more details). We observe  $Y_3$  and  $(X_1, X_2)$ , which are noisy measurements of  $(Z_1, Z_2)$ . Right: Diagram of the corresponding canonical model:  $Z_2$  is an mleaf variable; H is an unobserved variable;  $Z_1$ ,  $Y_3$  are cogent variables.

directly observed nor measured (called *unobserved variables*). We refer to this model as *linear latent variable SEM with measurement error* (linear LV-SEM-ME). We study the identifiability of linear LV-SEM-MEs in a setup where the independent exogenous noise terms that causally (directly or indirectly) affect each observed variable can be distinguished from each other. That is, the mixing matrix of the linear system that transforms exogenous noise terms to observed variables is recoverable up to permutation and scaling of the columns. This can be satisfied, for example, if all independent exogenous noise terms are non-Gaussian. We note that measurement error challenge is essentially a special case of unobserved variable challenge, in which we observe a measurement of an underlying unobserved variable of interest. Yet, the observed measurement variable usually have special properties (such as not being affected by other variables) that can be leveraged to improve the identification power. Hence, our point of view in this work is to allow for coexistence of the challenges of unobserved common causes and measurement error, while leveraging the properties of the measurement variables to improve identification.

We study the identifiability of linear LV-SEM-ME under two faithfulness assumptions. The first assumption prevents existence of zero total causal effects of a variable on its descendants, which we refer to as *conventional faithfulness assumption* as it is widely assumed in the literature. The second assumption prevents additional parameter cancellation or proportionality among specific edges, which we refer to as LV-SEM-ME faithfulness assumption. Both assumptions are mild in that their violations are zero-probability events. We show that under conventional faithfulness assumption, the model can be identified up to an equivalence class characterized by an ordered grouping of the variables which we call ancestral ordered grouping (AOG). Further, under LV-SEM-ME faithfulness assumption, the model can be learned up to an equivalence class characterized by a more refined ordered grouping which we call *direct ordered grouping* (DOG). We provide a graphical characterization of the elements of the equivalence class in which the induced graph on each ordered group includes a star structure where any member (variable) of the group is a potential center of the star. Specifically, every element in the equivalence class corresponds to distinct assignments of the centers of the star graphs, yet it possesses the same ordered grouping of variables and the same unlabelled structure on each group as the rest of the elements in the equivalence class. Models in the same AOG equivalence class are consistent with the same set of causal orders among groups, and models in the same DOG equivalence class share the same unlabeled graph structure, i.e., the causal diagrams are isomorphic. Lastly, we provide a recovery algorithm that could return all models in the AOG and DOG equivalence classes. Previous work presented in [19] only considered confounders and measurement error separately. Moreover, a different definition for AOG and DOG was used.

## 2 Model description

We start with a formal definition of the model that we consider in this work.

**Definition 1 (General linear LV-SEM-ME)** A general linear LV-SEM-ME consists of two sets of variables  $\mathcal{V}$  and  $\mathcal{X}$ . Variables in  $\mathcal{V}$  can be arranged in a causal order, and each variable  $V_i \in \mathcal{V}$  is generated as a linear combination of a subset  $Pa(V_i) \subset \mathcal{V}$  (called its direct parents), plus an exogenous noise term  $N_{V_i}$ , where  $\{N_{V_i}\}_{V_i \in \mathcal{V}}$  are jointly independent. Further,  $\mathcal{V}$  can be partitioned into three sets  $\mathcal{Y}$ ,  $\mathcal{Z}$  and  $\mathcal{H}$ . Variables in  $\mathcal{Y}$  are observed (without error). Variables in  $\mathcal{Z}$  are measured with error, where each variable  $X_i \in \mathcal{X}$  is a noisy measurement of one corresponding variable  $Z_i \in \mathcal{Z}$  plus an exogenous noise term  $N_{X_i}$  (which we call measurement error of  $Z_i$ ). Variables

in  $\mathcal{H}$  are neither observed nor measured with error. We refer to variables in  $\mathcal{H}$ ,  $\mathcal{Y}$ ,  $\mathcal{Z}$ , and  $\mathcal{X}$  as unobserved variables, observed variables, measured variables, and measurements, respectively.

We define a measured leaf variable (mleaf variable) as a measured variable in Z that has no other children besides its noisy measurement. We define a *cogent variable* as a variable in  $Z \cup Y$  that is not an mleaf. As mentioned earlier, we study the problem of recovering the linear LV-SEM-ME from observations of (Y, X). We focus on recovering the subset of linear LV-SEM-ME, called *canonical LV-SEM-ME*, defined as follows. We add two restrictions on the model for the sake of model identifiability based on observational data, where both have been considered in literature [6, 20, 19]. See Appendix B.1 for detailed discussion about the restrictions on the canonical form.

**Definition 2 (Canonical linear LV-SEM-ME)** A canonical LV-SEM-ME is an LV-SEM-ME where variables in  $\mathcal{H}$  are roots and confounders, and mleaf variables do not have exogenous noise terms.

The matrix form of the canonical LV-SEM-ME can be written as

$$H = N_H, (1a)$$

$$\begin{vmatrix} Z^{L} \\ Z^{C} \\ Y \end{vmatrix} = \mathbf{B}H + \begin{bmatrix} \mathbf{D} \\ \mathbf{C}_{Z} \\ \mathbf{C}_{Y} \end{bmatrix} \begin{bmatrix} Z^{C} \\ Y \end{bmatrix} + \begin{bmatrix} \mathbf{0} \\ N_{Z^{C}} \\ N_{Y} \end{bmatrix},$$
(1b)

$$X = \begin{bmatrix} Z^L \\ Z^C \end{bmatrix} + \begin{bmatrix} N_{X^L} \\ N_{X^C} \end{bmatrix},$$
(1c)

where H, Y, X represent the vector of unobserved variables, observed variables, measurements, respectively.  $Z^L$  represent the vector of mleaf variables, and  $Z^C$  represent the vector of measured variables that are not mleaf variables.  $N_H$ ,  $N_Y$ ,  $N_{Z^C}$  are the noise vectors corresponding to H, Y,  $Z^C$ , respectively.  $N_{X^L}$  (resp.  $N_{X^C}$ ) represent the measurement error of the variables in  $Z^L$  (resp.  $Z^C$ ). B represent the causal connections from unobserved variables H to  $[Z^L; Z^C; Y]$ , C represent the causal connections among cogent variables, which is partitioned into  $[\mathbf{C}_Z; \mathbf{C}_Y]$  according to  $[Z^C; Y]$ . D represent the causal connections from cogent variables to mleaf variables. Note that the right hand side of Equation (1b) is not a function of  $Z^L$  since variables on the left hand side do not have mleaf variables as their parents.

We define the causal diagram of a linear LV-SEM-ME as a directed graph, where the nodes are all variables in  $\mathcal{V} \cup \mathcal{X}$ . For any two variables  $W_1, W_2 \in \mathcal{V} \cup \mathcal{X}$ , there is a directed edge from  $W_1$  to  $W_2$  if and only if  $W_1 \in Pa(W_2)$ . Due to the causal order of  $\mathcal{V} \cup \mathcal{X}$ , the causal diagram is acyclic.

**Problem description** We consider a setting with known *observability indicators*, that is, we know whether each variable is observed without error (i.e., belongs to Y) or measured with error (i.e., belongs to X). Suppose we have n i.i.d. observations of the variables  $\{X, Y\}$ . The task is to recover all linear LV-SEM-MEs which have the same observational distribution up to the noise distributions.

#### **3** Identification analysis

In this section we study identification for our model of interest. We first consider the problem for two special submodels in Section 3.2: 1) If  $\mathcal{H} = \emptyset$ , i.e., all unobserved variables have noisy measurements, then the model is linear SEM-ME. 2) If  $\mathcal{Z} = \emptyset$ , i.e., all unobserved variables are roots and confounders, then the model is linear LV-SEM. Identification analysis for these two special cases have been studied in [19], yet different technique was used in that work for the linear LV-SEM. We then study the general form in Section 3.3 where both challenges can be present in the system simultaneously, which is our main identification result. In both subsections, we study identification under two faithfulness assumptions where, as will be discussed shortly, the first one, referred to as the conventional faithfulness, is a weaker assumption.

#### 3.1 Separability and faithfulness assumptions

In the following we present two assumptions for the identifiability of SEM-ME and LV-SEM, namely *separability assumption* and *faithfulness assumption*. Note that for the identifiability of LV-SEM-ME, we need one extra assumption which we will present in Section 3.3.

**Separability assumption.** We first deduce the mixing matrix that transforms independent exogenous noise terms to the observed variables [X; Y]. Denote  $V^C = [Z^C; Y]$  as the vector of cogent variables. We can write variables in  $[Z^L; V^C]$  as linear combinations of the exogenous noise terms:

$$\begin{bmatrix} Z^L \\ V^C \end{bmatrix} = \mathbf{W}^* \begin{bmatrix} N_H \\ N_{V^C} \end{bmatrix}, \quad \text{where} \quad \mathbf{W}^* = \begin{bmatrix} \mathbf{B}^L + \mathbf{D}(\mathbf{I} - \mathbf{C})^{-1} \mathbf{B}^C & \mathbf{D}(\mathbf{I} - \mathbf{C})^{-1} \\ (\mathbf{I} - \mathbf{C})^{-1} \mathbf{B}^C & (\mathbf{I} - \mathbf{C})^{-1} \end{bmatrix}.$$
(2)

**B** is partitioned into  $[\mathbf{B}^L; \mathbf{B}^C]$  according to  $[Z^L; V^C]$ ,  $N_{V^C} = [N_{Z^C}; N_Y]$ , and **I** represents the identity matrix. Combined with Equation (1c), the overall mixing matrix **W** can be written as

$$\begin{bmatrix} X \\ Y \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{W}^* & \mathbf{I} \\ \mathbf{W} \end{bmatrix}}_{\mathbf{W}} \begin{bmatrix} N_H \\ N_{V^C} \\ N_{X^L} \\ N_{X^C} \end{bmatrix}.$$
 (3)

We note that because mleaf variables have no exogenous noise, each column in  $W^*$  either has at least two non-zero entries, or has one non-zero entry where the non-zero entry is not in X.

**Assumption 1 (Separability)** The mixing matrix W in Equation (3) can be recovered from observations of [X; Y] up to permutation and scaling of its columns.

Separability assumption states that the independent exogenous noise terms pertaining to this mixture can be separated. An example of a setting where this assumption holds is when all exogenous noises are non-Gaussian. Further, given the recovered matrix W, the matrix  $W^*$  can be recovered by removing the one-hot column vectors in W where the non-zero entry is in a row corresponding to a variable in  $\mathcal{X}$ . Please refer to Appendix C.1 for more details.

**Faithfulness assumption.** For each variable  $V_i$ , define possible parent set of  $V_i$ ,  $PP(V_i)$ , as the union of  $An(V_i) \setminus \mathcal{H}$  and the set of mleaf variables whose parent sets are subsets of  $An(V_i)$ . We provide two versions of faithfulness assumption that will be used in our identification results.

**Assumption 2 (Conventional faithfulness)** The total causal effect of any variable  $V_i \in \mathcal{V}$  on its descendant  $V_j \in \mathcal{V}$  is not zero.

**Assumption 3 (LV-SEM-ME faithfulness)** For each variable  $V_i \in \mathbb{Z} \cup \mathcal{Y}$  and any pair of subsets  $(J, K) \subseteq (\mathcal{H} \cup \mathcal{V}^C) \times \mathbb{Z} \cup \mathcal{Y}$  that satisfies at least one of the conditions below, the rank of the submatrix  $\mathbf{W}_{K \cup \{V_i\}, J}$  is equal to the size of the smallest set that blocks all directed paths from J to  $K \cup \{V_i\}$ :

- (a)  $J \subseteq An(V_i), K \subseteq PP(V_i);$
- (b)  $J \subseteq An(V_i) \setminus \{V_j\}, K \subseteq PP(V_j)$ , when  $V_i$  is a mleaf variable and  $V_j$  is a parent of  $V_i$ .

Assumption 2 is widely assumed in the literature, and hence we refer to it as the conventional faithfulness. It requires that when multiple causal paths exist from any (observed or unobserved) variable to its descendants, their combined effect (i.e., sum of products of path coefficients) is not equal to zero. Assumption 3 provides a stronger notion of faithfulness. The intuition of Assumption 3 is as follows. The structure of the causal diagram in the data generating process implies proportionality in the corresponding entries in the mixing matrix. For example, in the structure  $V_1 \rightarrow V_2 \rightarrow V_3$ , the mixing matrix with rows corresponding to  $\{V_2, V_3\}$  and columns corresponding to  $\{V_1, V_2\}$  is of rank 1. However, there may exists extra proportionality among the entries in the mixing matrix that are not enforced by the graph. This extra proportionality may result in the data distribution corresponding to an alternative model that does not always happen. Note that both assumptions are violated with probability zero. Please refer to Appendix C.2 for more discussion about both faithfulness assumptions.

#### 3.2 Identifiability of SEM-ME and LV-SEM

In this subsection, we summarize the identification results of SEM-ME and LV-SEM under faithfulness and separability assumptions, where the extent of identifiability can be described by two graphical characterizations of equivalence, namely Ancestral ordered grouping (AOG) equivalence and Direct ordered grouping (DOG) equivalence. See Appendix D for more detailed analysis.



Figure 2: Considered models in simulation: NCO, Front-Door, IV, and Union Model.

**Definition 3 (Ancestral/direct ordered grouping)** The AOG/DOG of a linear SEM-ME (resp. LV-SEM) is a partition of  $\mathcal{Z}^L \cup \mathcal{V}^C$  (resp.  $\mathcal{H} \cup \mathcal{V}^C$ ) into distinct sets, described as follows:

- (1) Assign each cogent variable in  $\mathcal{V}^C$  to a distinct group.
- (2) (i) **SEM-ME**: For each mleaf variable  $Z_j \in \mathcal{Z}^L$ , assign  $Z_j$  to the same ordered group as  $Z_i$  if certain graphical condition is satisfied. Otherwise, assign  $Z_j$  to a separate group.
  - (ii) **LV-SEM**: For each unobserved variable  $H_j \in \mathcal{H}$ , assign  $H_j$  to the same ordered group as  $V_i$  if certain graphical condition is satisfied. Otherwise, assign  $H_j$  to a separate group.

**Definition 4 (AOG/DOG equivalence class)** The AOG/DOG equivalence class of a linear SEM-ME (resp. LV-SEM) is a set of models where the elements of this set all have the same mixing matrix (up to permutation and scaling) and same ancestral/direct ordered groups.

The definitions of AOG and DOG only differs in the graphical condition. It was shown in [19] that all models in the AOG equivalence class are consistent with the same set of causal orders among the groups (i.e., if a causal order on the groups is consistent with one model in the class, it is consistent with all the models in the class), but not necessarily all the same edges across the groups.<sup>2</sup> That is, based on AOG, the set of causal orders among groups are identifiable but not the edges across groups.

**Proposition 1** (a) Models in the same DOG equivalence class of a SEM-ME have the same unlabeled graph structure, i.e., the causal diagrams of these models are isomorphic.

(b) Models in the same DOG equivalence class of an LV-SEM have the same graph structure.

For a SEM-ME, according to Definition 3, there is at most one cogent variable in each ancestral ordered group. Furthermore, each observed cogent variable belongs to a separate group. Each mleaf node  $Z_j$  is assigned to the ancestral ordered group of at most one of its parents. Hence, if a group has more than one variable, then there must be exactly one measured cogent variable, and the rest of the nodes are mleaf nodes which are children of this node. This concludes that the induced structure on each ancestral ordered group is a star graph. Similar property holds for LV-SEM. Define the center of the ancestral ordered group as the cogent variable, or the mleaf variable (resp. unobserved variable) if the group does not include a cogent variable. [19] showed that fixing the center of the ancestral ordered groups as well as the choice of scaling and permutation of the columns of **B** for LV-SEM, leads to unique identification of the models. Therefore, by considering all the candidates for the center, models in the same AOG equivalence class of a SEM-ME can be enumerated by switching the center of each group with other nodes that are in the same group. Models in the same AOG equivalence class of a SEM-ME can be enumerated by switching the center of each group with the noise of other nodes in the same group.

As for DOG, we can see from graphical condition in Definition 8 that DOG is a more refined partition compared with AOG. Therefore, similar to AOG equivalence class, models in the DOG equivalence class are also consistent with the same set of causal orders among the groups, and the induced structure on each direct ordered group is also a star graph. Further, models in the same DOG equivalence class of a SEM-ME and an LV-SEM can also be enumerated by switching the center of each group, and switching the exogenous noise of the center of each group with the noise of other nodes in the same group, respectively. For the properties that only hold for DOG, it was shown in [19] that models in the same DOG equivalence class have the same edges across the groups. Combined with the star structure within each group, the following proposition provides a graphical characterization of the DOG equivalence class for SEM-ME and LV-SEM.

<sup>&</sup>lt;sup>2</sup>The identification results in Theorem 1 implies that AOG is the finest partitioning that satisfy this property under Assumption 2, and DOG is the finest partitioning under Assumption 3.

**Proposition 2** (a) Models in the same DOG equivalence class of a SEM-ME have the same unlabeled graph structure, i.e., the causal diagrams of these models are isomorphic.

(b) Models in the same DOG equivalence class of an LV-SEM have the same graph structure.

We provide the identification results for SEM-ME and LV-SEM below. Please refer to Appendix D for detailed discussion about these results.

**Theorem 1** We have the following results regarding the identification of SEM-ME and LV-SEM:

- (a) Under Assumptions 1 and 2, the linear SEM-ME (resp. LV-SEM) can be identified up to its AOG equivalence class.
- (b) Under Assumptions 1 and 3, the linear SEM-ME (resp. LV-SEM) can be identified up to its DOG equivalence class with probability one.

#### 3.3 Identifiability of LV-SEM-ME

In this subsection, we provide identification results for a system in which both unobserved confounders and measurement errors can co-exist. For this case, we need an extra *minimality assumption*.

**Assumption 4 (Minimality)** We assume the linear LV-SEM-ME M is minimal, that is, there does not exist any other linear LV-SEM-ME M' such that M' has strictly fewer unobserved variables than M, the same observability indicators of the variables, and the same mixing matrix as M up to permutation and scaling of the columns.

Minimality assumption asserts that the ground-truth model has fewer (or equal) unobserved variables than any other models that has the same mixing matrix and observability indicator. This assumption is required since we cannot infer the number of unobserved variables without prior knowledge of the system. See Appendix C.3 for more discussion and an equivalent graphical characterization. Equipped with minimality assumption, we are ready to present our main identification result.

**Definition 5 (AOG and DOG of LV-SEM-ME)** *The DOG (resp. AOG) of an LV-SEM-ME consists of a partition of the variables in*  $\mathcal{H} \cup \mathcal{Z}^L \cup \mathcal{V}^C$  *described as follows:* 

- (1) Assign each cogent variable  $V_i \in \mathcal{V}^C$  to a distinct group.
- (2) Assign the mleaf variables in  $Z^L$  to the groups of measured cogent variables or a separate group following the same condition for DOG (resp. AOG) in SEM-ME (i.e., (2)(i) in Def. 3).
- (3) Assign the unobserved variables in H to the groups of cogent variables or a separate group following the same condition for DOG (resp. AOG) in LV-SEM (i.e., (2)(ii) in Def. 3).

Using Definition 5, the AOG and DOG equivalence classes of an LV-SEM-ME are defined as in Definition 4. Similar to Section 3.2, models in the same AOG and DOG equivalence classes are consistent with the different sets of causal orders among the groups, and models in the same DOG equivalence class have isomorphic graph structure, summarized below.

**Proposition 3** Models in the same DOG equivalence class of an LV-SEM-ME have the same unlabeled graph structure, i.e., the causal diagrams of these models are isomorphic.

However, unlike the results in Section 3.2, the induced structure on each group may not be a star graph if there is an edge from the unobserved variables to the mleaf variables in the same group. We extend our approach by defining the center of a group as the cogent variable in that group (if it exists), or the only mleaf or unobserved variable in the group. In this case, all members in the equivalence classes can be enumerated by either switching the center with any mleaf variables in the group, and/or switching the exogenous noises of the center with the noises of any unobserved variables in the group. For example, a group with one measured cogent variable, one mleaf variable and one unobserved variable has three equivalents (switching the cogent with the mleaf, switching the noise of the cogent with the noise of the unobserved confounder, and both). Below, we show that the introduced notion of equivalnece, is indeed the extent of identification in the generalized LV-SEM-ME.

**Theorem 2** We have the following results regarding the identification in LV-SEM-ME:

	DOGEC (ours)			GRICA [16]			lvLiNGAM[11]			Cross-Moment[7]		
	Mean	20%	80%	Mean	20%	80%	Mean	20%	80%	Mean	20%	80%
NCO	0.08	0.06	0.11	0.38	0.30	0.43	1.15	0.88	1.49	0.08	0.04	0.10
Front	0.02	0.01	0.02	0.46	0.35	0.57	0.84	0.60	0.93	0.23	0.03	0.23
IV	0.19	0.02	0.36	0.50	0.37	0.59	0.84	0.69	0.99	1.33	0.49	1.21
Union	0.11	0.08	0.14	0.39	0.30	0.42	0.73	0.28	0.89	0.30	0.23	0.38

Table 1: Performance of the algorithms on estimating the causal effect in four different models. Mean, 20%, 80% stand for the average, 20% and 80% percentiles of the estimation error, respectively.

- (a) Under Assumptions 1, 2 and 4, the linear LV-SEM-ME can be identified up to its AOG equivalence class.
- (b) Under Assumptions 1, 3 and 4, the linear LV-SEM-ME can be identified up to its DOG equivalence class with probability one.

## 4 Recovery algorithm and numerical experiments

We first describe the recovery algorithm for the introduced LV-SEM-ME model. The algorithm includes two main parts. The first part, namely AOG recovery algorithm (Algorithm 1), returns the ancestral ordered grouping of the underlying model given mixing matrix and observability indicator. The second part is to return all members in the AOG and DOG equivalence class (Algorithm 2). As described above, given the recovered AOG, members in the AOG equivalence class can be enumerated by switching the center with any mleaf variables in the group and/or switching the exogenous noises of the center with the noises of any unobserved variables in the group. For recovering the members in the DOG equivalence class, we show that members in the AOG equivalence class of the ground-truth but not DOG equivalence class has strictly more edges than the ground truth (Proposition 7). Therefore, members in the DOG equivalence class can be recovered by finding the models in the AOG equivalence class that has the fewest number of edges. See Appendix E for more details.

We evaluated the performance of our algorithm on synthetic data. We consider the following four models, all with three observed variables and one unobserved variable: (1) Negative Control Outcome (NCO) model; (2) Front-door model; (3) Instrumental Variable (IV) model; (4) A union model that can be considered as a generalization of all three models. See Figure 2 for causal diagrams of four models. Our theoretical results imply that all four models are uniquely identifiable, i.e., the DOG equivalence class only includes the ground truth. The edge weights are randomly generated from [0.5, 0.9], and the noises are sampled from uniform distribution. The task is to estimate the edge weight from  $Y_2$  to  $Y_3$ . We use Reconstruction ICA (RICA) [9] to recover the mixing matrix.

We compare our recovery algorithm with lvLiNGAM algorithm [11], Graphical RICA (GRICA) algorithm [16] and cross-moment approach [7] on 10 randomly generated models. We note that both GRICA and cross-moment assume that the causal graph is known. However, this is not given as input in our algorithm. We calculate the relative error between the true value and the estimated value, and report the average error, as well as the 20% and 80% percentile of the errors in Table 1. The results show that our method significantly outperforms the baselines even without knowing the true causal graph, which aligns with our theoretical results.

## 5 Conclusion

We studied causal discovery in the presence of unobserved variables and measurement error by defining the linear LV-SEM-ME model. We characterized its identifiability under separability and two faithfulness assumptions, and showed that it can be identified up to AOG and DOG equivalence classes respectively. We provided graphical characterization of the models that are equivalent and presented a recovery algorithm that could return models equivalent to the ground truth. A remaining challenge in our proposed methodology is its reliance on the accuracy of the provided estimate of the mixing matrix of the underlying model. Hence, devising accurate approaches for estimating the mixing matrix is an important direction of future research.

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## A Related work

The two aforementioned challenges have been addressed in several work in the literature. Regarding the challenge of unobserved common causes, constraint-based algorithms such as the Fast Causal Inference (FCI) algorithm has been widely used [15]. However, these approaches are often unable to identify the direction of the majority of causal connections in the recovered graph. In the presence of the unobserved common causes, methods based on linearity and non-Gausianity also in general are not able to learn the structure uniquely. Proposed methods such as latent variable LiNGAM [6, 11] and partially observed LiNGAM [1] provide graphical conditions for unique identifiability of the model. These conditions are usually non-trivial, which demonstrates the difficulty of the task of causal discovery in the presence of unobserved common causes.

There are fewer work focusing on the challenge of causal discovery in the presence of measurement error. Majority of the work [14, 8, 17, 18] assume that each unobserved (but measured) variable has at least two measurements. This assumption facilitates the task of discovery and usually leads to unique identifiability of the model, yet may not hold in many settings.<sup>3</sup> Without this assumption, [5] consider the model where the measured variables are binary, and [10] consider the case where the relations among measured variables are nonlinear, and the measurement errors are Gaussian. In linear models, [20] provide conditions for unique identifiability of linear Gaussian and non-Gaussian models. None of the aforementioned work on measurement error considered the case when the model is not uniquely identifiable (i.e., there are other models that are observationally equivalent to the true model). Hence, characterization of observational equivalence for measurement error models is missing in the literature.

### **B** Detailed description of LV-SEM-ME model

#### B.1 Additional restriction on canonical LV-SEM-ME model

We add the following two restrictions on the model for the sake of model identifiability based on observational data.

- Firstly, as discussed in [20, 19], for any mleaf variable  $Z_i$ , the exogenous noise term  $N_{Z_i}$  is not distinguishable from its measurement error  $N_{X_i}$ . Specifically, for any two models that only differ in  $Z_i$  and  $X_i$  for some mleaf variable  $Z_i$  but have the same sum  $N_{Z_i} + N_{X_i}$ , they have the same observational distribution. This follows because  $Z_i$  is not observed, and  $N_{Z_i}$ only influences its noisy measurement  $X_i$  and no other observed variables in  $\mathcal{Y}$ . Therefore, we consider the model where  $N_{Z_i} = 0$  for all mleaf variables for model identifiability, i.e., we assume that mleaf variables are deterministically generated from its direct parents.
- Secondly, we assume that variables in  $\mathcal{H}$  are all root variables (i.e., have no direct parents) and confounders (i.e., have at least two children). This is because for any linear latent variable model with a non-root latent variable, there exists an equivalent latent variable

<sup>&</sup>lt;sup>3</sup>As seen in Section 2, we avoid positing this assumption in our work.

model where the latent variables are all roots, such that both models have the same joint distribution across observed variables and total causal effect between any pair of observed variables [6].

Due to the aforementioned restrictions, we focus on recovering the subset of linear LV-SEM-ME, called *canonical LV-SEM-ME*, defined as in Definition 2.

## **B.2** Example of a linear LV-SEM-ME

**Example 1** Figure 1 shows an example of a causal diagram including unobserved variable H, observed variable  $\{Y_3\}$ , measured variables  $\{Z_1, Z_2\}$  and their corresponding measurements  $\{X_1, X_2\}$ . The generating model is as follows.

$$\begin{split} H &= N_H, \\ Z_1 &= N_{Z_1}, \\ Z_2 &= b_2 H + a_{21} Z_1 + N_{Z_2}, \\ Y_3 &= b_3 H + N_{Z_3}, \\ X_1 &= Z_1 + N_{X_1}, \\ X_2 &= Z_2 + N_{X_2}. \end{split}$$

We note that  $Z_2$  is an mleaf variable; it has no other children except for  $X_2$ .  $\{Z_1, Y_3\}$  are cogent variables. Therefore, in the canonical form, the exogenous noise of  $Z_2$  is 0, and the measurement error of  $Z_2$  is  $N_{Z_2} + N_{X_2}$ . In the matrix form of Equation (1b), we have  $Z^L = [Z_2], Z^C = [Z_1], Y = [Y_3], \mathbf{B} = [b_2, 0, b_3]^\top, \mathbf{D} = [a_{21}, 0], \mathbf{C}_Z = \mathbf{C}_Y = [0, 0].$ 

The mixing matrix  $\mathbf{W}$  in this example can be written as

$$\begin{bmatrix} X_2 \\ X_1 \\ Y_3 \end{bmatrix} = \begin{bmatrix} b_2 & a_{21} & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ b_3 & 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} N_H \\ N_{Z_1} \\ N_{Y_3} \\ N_{X_2} \\ N_{X_1} \end{bmatrix}.$$

The leftmost three columns correspond to  $\mathbf{W}^*$ , and  $\mathbf{I}$  is of dimension  $2 \times 2$ .

#### **C** Detailed discussion on the identification assumptions

#### C.1 Separability assumption

Separability assumption states that the independent exogenous noise terms pertaining to the mixture in Equation (3) can be separated, i.e., the mixing matrix can be recovered up to permutation and scaling of its columns. An example of a setting where this assumption holds is when all exogenous noises are non-Gaussian. In this case, if the model satisfies the requirement in [4, Theorem 1], then overcomplete Independent Component Analysis (ICA) can be used to recover the mixing matrix up to permutation and scaling of its columns. Another example where separability assumption is satisfied is the setup in which the noise terms are piecewise constant functionals satisfying a set of mild conditions [2]. On the other hand, an example where this assumption is violated is when all exogenous noise terms have Gaussian distributions. In this case, the mixing matrix can only be recovered up to an orthogonal transformation.

We note that under separability assumption, the matrix  $\mathbf{W}^*$  can also be recovered up to permutation and scaling of its columns. Suppose the recovered mixing matrix is  $\hat{\mathbf{W}}$ , and we also have the information whether each variable is observed (i.e., belongs to  $\mathcal{Y}$ ) or measured with error (i.e., belongs to  $\mathcal{X}$ ). Then the matrix  $\mathbf{W}^*$  can be recovered by removing the one-hot column vectors in  $\hat{\mathbf{W}}$ where the non-zero entry is in a row corresponding to a variable in  $\mathcal{X}$ .

The justification of the above approach is as follows: If a variable  $X_i$  is measured with error, then there must exist one column in  $\hat{\mathbf{W}}$  that corresponds to the measurement error  $N_{X_i}$  (or  $N_{X_i} + N_{Z_i}$  for mleaf variables in the original form). This column has only one non-zero entry in the row corresponding to the measurement  $X_i$ . The columns that we remove in the procedure above correspond to such

measurement errors. We note that by removing these columns from  $\hat{\mathbf{W}}$  we are not losing any information. This is due to the fact that we can simply recover a matrix (permutationally) equivalent to  $\hat{\mathbf{W}}$  from  $\mathbf{W}^*$ : Since we know which variables are measured with error, we can simply add the corresponding one-hot column vectors back to the matrix. The order of adding these is irrelevant (no information) since it is arbitrary in the original  $\hat{\mathbf{W}}$  as well (recall that  $\mathbf{W}$  is identifiable up to permutation and scaling of the columns).

#### C.2 Faithfulness assumption

For each variable  $V_i \in \mathcal{V}$ , define the ancestor set,  $An(V_i)$  as the set of variables that has a direct path to  $V_i$  (excluding  $V_i$ ). Define the cogent ancestor set  $An_V(V_i)$  as  $An(V_i) \setminus \mathcal{H}$ . Define the possible parent set of  $V_i$ ,  $PP(V_i)$ , as the union of  $An_V(V_i)$  and the set of mleaf variables whose parent sets are subsets of  $An(V_i)$  (excluding  $V_i$  itself if  $V_i$  is an mleaf). For two sets of variables  $J \subseteq \mathcal{H} \cup \mathcal{V}^C$ and  $K \subseteq \mathcal{Z} \cup \mathcal{Y}$ , define the matrix  $\mathbf{W}_K^J$  as the submatrix of  $\mathbf{W}^*$  where the rows correspond to the variables in K, and the columns correspond to the exogenous noise terms of variables in  $\mathcal{J}$ . A set of variables  $\mathcal{B}$  is said to be a bottleneck from J to K if for every directed path from a variable in J to a variable in K, at least one variable on this path (including the start and end nodes) is in  $\mathcal{B}$ .  $\mathcal{B}$  is said to be a minimal bottleneck from J to K if no other bottlenecks from J to K have fewer number of variables.

Assumption 2 is widely assumed in the literature, and hence we refer to it as the conventional faithfulness. It requires that when multiple causal paths exist from any (observed or unobserved) variable to its descendants, their combined effect (i.e., sum of products of path coefficients) is not equal to zero. Note that Assumption 2 is a special case of Assumption 3(a) with  $K = \emptyset$  and J being singleton set of any ancestor of  $V_i$ . The intuition of Assumption 3 is as follows. The structure of the causal diagram in the data generating process implies proportionality in the corresponding entries in the mixing matrix. For example, in the structure  $V_1 \rightarrow V_2 \rightarrow V_3$ , the mixing matrix with rows corresponding to  $\{V_2, V_3\}$  and columns corresponding to  $\{V_1, V_2\}$  is of rank 1. However, there may exists extra proportionality among the entries in the mixing matrix that are not enforced by the graph. This extra proportionality may result in the data distribution corresponding to an alternative model that does not always happen. Faithfulness assumption prevents such extra proportionality in the generating model. A similar bottleneck faithfulness has been proposed in [1], where they consider any pair of subset (J, K). Assumption 2 is strictly weaker than that assumption.

**Remark 1** Both Assumptions 2 and 3 are violated with probability zero if all model coefficients are drawn randomly and independently from continuous distributions. However, Assumption 2 is only focused on marginal independencies and requires that an ancestor of a variable should not be independent of it due to parameter cancellation. In practice, due to sample size limitations, an approximate cancellation may be perceived as an actual cancellation. Therefore, although Assumptions 2 and 3 both rule out measure-zero subsets of the model, and may be perceived equally weak assumptions mathematically, in practice, Assumption 2 may be preferred. Due to this reason, in the following, we provide results under Assumption 2 and Assumption 3 separately.

#### C.3 Minimality assumption

Minimality assumption asserts that the ground-truth model has fewer (or equal) unobserved variables than any other models that has the same mixing matrix and observability indicator. This assumption is required since we cannot infer the number of unobserved variables without prior knowledge of the system. Recall from Equation (2) that the number of columns of  $W^*$  is the sum of the number of cogent variables and unobserved variables. However, the number of each type of variable is not known apriori under only separability assumption.

Minimality assumption is always required when unobserved variables are present in the system. Specifically, it is often assumed that the ground-truth model either has the fewest number of edges [1], or the fewest number of unobserved variables [11]. Our minimality condition falls into the latter case, and in Proposition 4 below, we show that the minimality assumption has a equivalent graphical characterization.

**Proposition 4 (Minimality)** Under Assumption 2, a linear LV-SEM-ME is not minimal if and only if there exists an unobserved variable  $H_i$  and a mleaf child  $Z_j$  of  $H_i$ , such that for any other child

 $V_k$  of  $H_i$ ,  $An(Z_j) \subseteq An(V_k)^4$ . This is equivalent to the following. Any (observed or unobserved) parent of  $Z_j$  is also an ancestor of  $V_k$ .

We note that there is a similarity between the condition in Proposition 4 and the condition in the definition of AOG in Definition 6. The reason for this similarity is that both intend to characterize the situation in which the location of an exogenous source is unknown. The former condition considers the case where this source belongs to a unobserved variable, while the latter considers the case where this source belongs to a measured cogent variable.

## D Identifiability results of SEM-ME and LV-SEM

#### D.1 AOG for SEM-ME and LV-SEM

We present the formal definition of Ancestral ordered grouping (AOG) and AOG equivalence class below.

**Definition 6 (Ancestral ordered grouping (AOG))** *The AOG of a SEM-ME (resp. LV-SEM) is a partition of*  $Z^L \cup \mathcal{V}^C$  (resp.  $\mathcal{H} \cup \mathcal{V}^C$ ) into distinct sets. This partition is described as follows:

- (1) Assign each cogent variable in  $\mathcal{V}^C$  to a distinct group.
- (2) (i) **SEM-ME**: For each mleaf variable  $Z_j \in \mathcal{Z}^L$ , if it has one measured parent  $Z_i \in \mathcal{Z} \cap \mathcal{V}^C$  such that  $Z_j$  has no other parents, or all other parents of  $Z_j$  are also ancestors of  $Z_i$ , assign  $Z_j$  to the same group as  $Z_i$ . Otherwise, assign  $Z_j$  to a separate group (with no cogent variable).

(ii) **LV-SEM**: For each unobserved variable  $H_j \in \mathcal{H}$ , if it has one cogent child  $V_i \in \mathcal{V}^C$  such that all other children of  $H_j$  are also descendants of  $V_i$ , assign  $H_j$  to the same group as  $V_i$ . Otherwise, assign  $H_j$  to a separate group (with no cogent variable).

**Definition 7 (AOG equivalence class)** The AOG equivalence class of a linear SEM-ME (resp. LV-SEM) is a set of models where the elements of this set all have the same mixing matrix (up to permutation and scaling) and same ancestral ordered groups.

#### D.2 Identification Under LV-SEM-ME Faithfulness

We first present a graphical condition that is used to characterize DOG equivalence class, and then formally show that this notion of equivalence is the extent of identifiability as in Theorem 1(b). Lastly, we add some discussion about the difference between the different extents of identifiable, and provide an example to show the difference.

**Condition 1 (SEM-ME edge identifiability)** For a given edge from a measured cogent variable  $Z_i$ to an mleaf variable  $Z_l$ , at least one of the following two conditions is satisfied: (a)  $Pa(Z_l) \setminus \{Z_i\}$ is not a subset of  $Pa(Z_i)$ . That is, there exists another parent  $V_j$  of  $Z_l$ , which is not a parent of  $Z_i$ . (b)  $Pa(Z_l)$  is not a subset of  $\cap_{V_k \in Ch(Z_i) \setminus \{Z_l\}} Pa(V_k)$ . That is, there exists a child  $V_k$  of  $Z_i$  and a parent  $V_j$  of  $Z_l$  such that  $V_j$  is not a parent of  $V_k$ .

**Condition 2 (LV-SEM edge identifiability)** For a given edge from an unobserved variable  $H_i$  to a cogent variable  $V_i$ , there exists another cogent child  $V_j$  of  $H_i$ , such that at least one of the following two conditions is satisfied: (a)  $V_i$  is not a direct parent of  $V_j$ . (b)  $Pa(V_i)$  is not a subset of  $Pa(V_j)$ . That is, there exists an observed (or unobserved) parent  $V_k$  (or  $H_k$ ) of  $V_i$  that is not a parent of  $V_j$ .

**Definition 8 (Direct ordered grouping (DOG))** The DOG of a linear SEM-ME (resp. LV-SEM) is a partition of  $\mathcal{Z}^L \cup \mathcal{V}^C$  (resp.  $\mathcal{H} \cup \mathcal{V}^C$ ) into distinct sets. This partition is described as follows:

- (1) Assign each cogent variable in  $\mathcal{V}^C$  to a distinct group.
- (2) (i) **SEM-ME**: For each mleaf variable  $Z_j \in \mathcal{Z}^L$ , if it has one measured parent  $Z_i \in \mathcal{Z} \cap \mathcal{V}^C$  such that the edge from  $Z_i$  to  $Z_j$  violates Condition 1, assign  $Z_j$  to the same ordered group as  $Z_i$ . Otherwise, assign  $Z_j$  to a separate ordered group (with no cogent variable).

<sup>&</sup>lt;sup>4</sup>Note that we do not include Z itself in An(Z).



Figure 3: Left: Diagram of the SEM-ME and the corresponding AOG considered in Example 2. Right: DOG of the SEM-ME.

(ii) **LV-SEM**: For each unobserved variable  $H_j \in \mathcal{H}$ , if it has one cogent child  $V_i \in \mathcal{V}^C$  such that the edge from  $H_j$  to  $V_i$  violates Condition 2, assign  $H_j$  to the same ordered group as  $V_i$ . Otherwise, assign  $H_j$  to a separate ordered group (with no cogent variable).

**Definition 9 (DOG equivalence class)** The DOG equivalence class of a linear SEM-ME (resp. LV-SEM) is a set of models where the elements of this set all have the same mixing matrix (up to permutation and scaling) and same direct ordered groups.

**Theorem 3** Under Assumptions 1 and 3, the linear SEM-ME (resp. LV-SEM) can be identified up to its DOG equivalence class with probability one.

DOG equivalence class provides a much more distinctive characterization of the causal relations among the variables compared to the characterization given for AOG equivalence class. This is the benefit achieved by extending the faithfulness assumption from Assumption 2 to Assumption 3. We re-emphasize that, as explained in Remark 1, both these two assumptions are violated with probability zero, but Assumption 2 may be easier to be incorporated in practice. Therefore, in light of Theorem 1(b), we see the trade-off between the Assumptions 2 and 3.

Lastly, as shown in Theorem 1(b), for an LV-SEM, the only undetermined part in the DOG equivalence class pertains to the assignment of the exogenous noises and coefficients, but the structure is the same. Consequently, if only the identification of the structure without weights is of interest, Assumptions 1 and 3 are sufficient.

**Remark 2** The definition for AOG and DOG of a SEM-ME in this work is different from previous work [19]. In that work, mleaf variables are either assigned to the groups of their (observed or measured) parents or a separate group. In contrast, in this work, mleaf variables cannot be assigned to the groups of their observed parents. This change is based on using the information about which cogent variables are measured and which ones are directly observed. Specifically, models in the same equivalence class defined in [19] may have different labeling of  $\mathcal{Y}$  and  $\mathcal{Z}$  among variables, while in this work, models in the same equivalence class have the same mixing matrix, AOG/DOG and the same labeling of  $\mathcal{Y}$  and  $\mathcal{Z}$ . Therefore, this change leads to smaller equivalence classes and hence more identification power.

**Example 2** Figure 3 shows an example of a causal diagram of an LVSEM-ME with 10 measured variables.  $(Z_1, Z_3, Z_7)$  are cogent variables, and the remaining are mleaf variables.

The AOG of the model is shown on the left, and the DOG of the model is shown on the right. We note that  $Z_{10}$  belongs to the same ancestral ordered group as  $Z_7$  since all other parents of  $Z_{10}$  are also parents of  $Z_7$ . However,  $Z_{10}$  does not belong to the same direct ordered group as  $Z_7$ . This is because  $Z_8$  is a child of  $Z_7$ ,  $Z_1$  is a parent of  $Z_{10}$ , but  $Z_1$  is not a parent of  $Z_8$ . Therefore the edge  $Z_7 \rightarrow Z_{10}$  violates the Condition I(b).

## **E** Detailed description of the algorithm

In this section, we present recovery algorithms for the introduced LV-SEM-ME model. We first present AOG recovery algorithm (Algorithm 1) in Section E.1. The algorithm returns the AOG of the underlying model, and it is used in both AOG equivalence class and DOG equivalence class recovery algorithms. We then show how to recover all models in the AOG and DOG equivalence classes in Section E.2 based on the recovered AOG (Algorithm 2).

Both Algorithm 1 and 2 are based on the mixing matrix  $W^*$  defined in Equation (2). Therefore,  $W^*$  will be the input to both algorithms. We note that  $W^*$  can be recovered from the observational data by first recovering the overall mixing matrix W (cf. (3)) using methods such as overcomplete ICA [4] when the exogenous noises are assumed to be non-Gaussian. Then,  $W^*$  can be deduced from W by removing certain columns as described in Section 3.1.

#### E.1 AOG Recovery

The following property can be implied from the definition of AOG, which shows that under conventional faithfulness assumption, we can identify the AOG of the model only based on the support of the mixing matrix  $W^*$ .

#### Proposition 5 Under Assumptions 2 and 4,

- (a) One mleaf variable and one measured cogent variable belong to the same ancestral ordered group if and only if the two rows in  $\mathbf{W}^*$  corresponding to these variables have the same support. Further, for any cogent variable  $V_i$  and its descendant  $V_j$ , the row support of  $V_i$  must be a subset of the row support of  $V_j$ .
- (b) One unobserved variable and one cogent variable belong to the same ancestral ordered group if and only if the two columns in  $\mathbf{W}^*$  corresponding to the exogenous noise terms of these variables have the same support. Further, for any cogent variable  $V_i$  and its ancestor  $V_j$ , the column support of  $N_{V_i}$  must be a subset of the column support of  $N_{V_i}$ .

The proof of Proposition 5 directly follow from the definition of AOG, and hence are omitted.

Equipped with Proposition 5, we propose an iterative algorithm for recovering the AOG in Definition 5 from  $\mathbf{W}^*$ . The pseudo-code of the proposed method is presented in Algorithm 1. In the first iteration, the Algorithm randomly chooses a row in  $\mathbf{W}^*$  with the fewest number of non-zero entries and finds all other rows with the same support. Denote the selected rows as  $\mathcal{Z}_{\mathcal{J}}$ , and columns corresponding to these non-zero entries as  $\mathcal{N}_I$ . Each of the selected row may either correspond to a cogent variable or an mleaf variable, and each of the column in  $\mathcal{N}_I$  may either correspond to the exogenous noise of an cogent variable or an unobserved confounder. The task is to decide whether there exists a cogent variable (and its associated exogenous noise). We first select the columns in  $\mathcal{N}_I$  with the fewest number of non-zero entries in  $\mathbf{W}^*$ . Denote this subset as  $\mathcal{N}_J$ . Then noises in  $\mathcal{N}_I \setminus \mathcal{N}_J$  must correspond to unobserved variables and are assigned to separate groups in  $\mathcal{C}_{unobserved}$ .

We check whether any of the rows in  $\mathcal{Z}_{\mathcal{J}}$  can be a cogent variable. If there is one observed variable in  $\mathcal{Z}_J$  then it must correspond to the cogent variable. If all variables are unobserved, then we look at the submatrix  $\mathbf{W}_0$  of  $\mathbf{W}^*$  with the rows corresponding to the (column) support of any variable in  $\mathcal{N}_{\mathcal{J}}$ , and columns corresponding to the (row) support of  $\mathcal{Z}_{\mathcal{J}}$ . If  $\mathcal{Z}_{\mathcal{J}}$  includes a cogent variable, then its corresponding exogenous noise must be in  $\mathcal{N}_{\mathcal{J}}$ , and the remaining noises are unobserved confounders. Since all noises in  $\mathcal{N}_{\mathcal{J}}$  have the same number of non-zero entries, they must have the same support. Further, any row that includes this exogenous noise must be a descendant of the cogent variable, and must include all the non-zero columns of the cogent variable under Assumption 2. This implies that  $\mathbf{W}_0$  does not include any non zero entry. Therefore, if  $\mathbf{W}_0$  includes any zero entry, then none of the rows in  $\mathcal{Z}_{\mathcal{J}}$  would correspond to a cogent variable. The rows in  $\mathcal{Z}_{\mathcal{J}}$  and the columns in  $\mathcal{N}_{\mathcal{J}}$  all belong to separate groups in  $\mathcal{C}_{mleaf}$  and  $\mathcal{C}_{unobserved}$  as they correspond to mleaf variables and unobserved variables. If  $\mathbf{W}_0$  does not include any zero entry, then under minimality assumption, one of the rows in  $\mathcal{Z}_{\mathcal{J}}$  correspond to a cogent variable. Therefore all noises in  $\mathcal{N}_J$  and all rows in  $\mathcal{Z}_{\mathcal{J}}$  belong to a single ancestral ordered group in  $\mathcal{C}_{cogent}$ . The algorithm then removes the rows in  $\mathcal{N}_J$  and columns in  $\mathcal{N}_J$ . Denote the remaining matrix as  $\tilde{\mathbf{W}}$ . In the second iteration, the Algorithm again chooses the rows w with the fewest number of non-zero entry in  $\tilde{\mathbf{W}}$ . However, we note that the row with the fewest number of non-zero entry in  $\mathbf{W}^*$  is not a cogent variable if some non-zero entries are removed in the first iteration. Therefore, among these columns, we select one column with the fewest number of non-zero entries in the large matrix  $\mathbf{W}^*$ . Then, it selects all other rows in  $\tilde{\mathbf{W}}$  with the same support as w. Denote the selected rows as  $\mathcal{Z}_{\mathcal{I}}$ . Rows in  $\mathcal{Z}_{\mathcal{I}}$  that has more non-zero entries than w in the large matrix  $\mathbf{W}^*$  must be mleaf variables (otherwise Assumption 2) is violated) and are assigned to separate groups in  $\mathcal{C}_{mleaf}$ . Rows that has the same number of non-zero entries as w may either correspond to a cogent variable or an mleaf variable, and we can use the same procedure as in the first iteration to distinguish between them. Finally, this procedure is repeated until all variables and noises are assigned to ordered groups.

The explanation above implies the identifiability result of Algorithm 1, summarized as follows.

**Proposition 6** Under Assumptions 2 and 4, the concatenation of the outputs  $(C_{unobserved}, C_{cogent}, C_{mleaf})$  of Algorithm 1 is the AOG of the LV-SEM-ME corresponding to the input  $W^*$  in a causal order consistent with the AOG equivalence class of the LV-SEM-ME.

**Computational complexity** Algorithm 1 includes  $p_c$  steps of iteration, where  $p_c$  is the number of cogent variables. Each iteration requires O(mn) calculation and needs O(mn) space, where m, n are the dimensions of the mixing matrix  $\mathbf{W}^*$ . Recall that  $m = p_c + p_{ml}$ , and  $n = p_c + p_H$ , where  $p_{ml}$  and  $p_H$  stand for the number of mleaf and unobserved variables. Therefore, the total time complexity of the algorithm is  $O(p_cmn)$ , and the space complexity is O(mn).

#### E.2 Model Recovery in the AOG and DOG Equivalence Class

In this section, we present our algorithm for recovering the models in the equivalence class using  $W^*$ . The psuedo-code of the algorithm is presented in Algorithm 2.

**AOG Equivalence class.** Recall from Section 3.3 that all members in the AOG equivalence class can be enumerated by switching the center with any mleaf variables in the group and/or switching the exogenous noises of the center with the noises of any unobserved variables in the group. Therefore, given the mixing matrix  $\mathbf{W}^*$ , Algorithm 2 first recovers the AOG of the true model using Algorithm 1. Then, it enumerates all possible choices of centers and the noises for each group. Note that groups with only mleaf variables or noises of unonserbed variables (i.e., in  $C_{mleaf}$  or  $C_{unobserved}$ ) only have one choice. Therefore, we only need to consider all the groups that include cogent variables (i.e., in  $C_{cogent}$ ). Denote each single selection of the centers in these groups as row, and the noises as col. The next step is to recover the model parameters  $\mathbf{B}$ ,  $\mathbf{C}$ ,  $\mathbf{D}$  based on  $\mathbf{W}^*$  and the selected row and col following Equation (2). Denote the variables not in row as  $row^C$ , and the noises not in col as  $col^C$ . The selected centers in row correspond to  $V^C$ , and the selected noises in colcorrespond to  $N_{VC}$  in (2). Similarly, variables in  $row^C$  and noises in  $col^C$  correspond to  $Z^L$  and  $N_H$ , respectively. Therefore  $\mathbf{C}$ ,  $\mathbf{B}^C$ ,  $\mathbf{D}$ ,  $\mathbf{B}^L$  can be calculated following lines 6-9 in Algorithm 2. Finding model parameters  $\mathbf{B}$ ,  $\mathbf{C}$ ,  $\mathbf{D}$  for all possible choices of row and col gives us all models in the AOG equivalence class.

**DOG Equivalence class.** Proposition 7 can be leveraged to recover models in the DOG equivalence class of the ground-truth given AOG, which states that the ground-truth model has strictly fewer edges than any model in the AOG equivalence class but does not belong to the DOG equivalence class.

**Proposition 7** Suppose an LV-SEM-ME satisfies Assumptions 1 and 3. Any model that belongs to the same AOG equivalence class but does not belong to the same DOG equivalence class has strictly more edges than any member in the DOG equivalence class.

Recall from Section 3.3 that models in the same DOG equivalence class all have the same unlabeled graph structure, hence the same number of edges. Therefore, using Proposition 7 given the members of the AOG equivalence class of the true model, members in the DOG equivalence class can be found by finding all models in the AOG equivalence class that have the fewest number of edges in the recovery output.

To conclude, the identifiability of Algorithm 2 can be summarized by the following proposition.

Algorithm 1: AOG Recovery algorithm for linear LV-SEM-ME.

- **Input:** Recovered mixing matrix  $\mathbf{W}^*$ , observability indicators of the variables (whether each variable is observed or measured).
- 1 Define n as the vector with the *i*-th entry as the number of non-zero entries in row *i* of  $\mathbf{W}^*$ .
- 2 Define m as the vector with the *j*-th entry as the number of non-zero entries in column *j* of  $\mathbf{W}^*$ .
- 3 Initialize  $\tilde{\mathbf{W}} \leftarrow \mathbf{W}^*, \mathcal{C}_{cogent} \leftarrow [], \mathcal{C}_{mleaf} \leftarrow [], \mathcal{C}_{unobserved} \leftarrow [].$
- 4 while W is not empty do
- 5 Find the rows in  $\hat{\mathbf{W}}$  that contain the fewest number of non-zero entries. Among them, choose one with the lowest corresponding value in  $\mathbf{n}$  (break ties at random). Denote the selected row by  $\mathbf{w}$ , the variable corresponding to this row by  $Z_w$ , and its corresponding value in  $\mathbf{n}$  by  $n_0$ .
- 6 Consider the rows in W with the same support (non-zero entries) as w, including w itself. Denote the set of variables that correspond to these rows as  $Z_I$ , and the the noise terms corresponding to the support of w as  $N_I$ .
- 7 Denote the set of variables in  $\mathcal{Z}_I$  with corresponding value  $n_0$  in **n** as  $\mathcal{Z}_J$ , and the set of noise terms in  $\mathcal{N}_I$  with the smallest corresponding value in **m** as  $\mathcal{N}_J$ .
- 8 Assign each variable in  $Z_I \setminus Z_J$  to a separate group in  $C_{mleaf}$ . Assign each exogenous noise term in  $\mathcal{N}_I \setminus \mathcal{N}_J$  to a separate group in  $C_{unobserved}$ .
- 8 Randomly select one noise term  $N_m$  in  $\mathcal{N}_J$ . Consider the submatrix  $\mathbf{W}_0$  of  $\mathbf{W}^*$  where the rows correspond to the (column) support of  $N_m$ , and the columns correspond to the (row) support of  $Z_w$ .
- 10 **if**  $\mathbf{W}_0$  includes any zero entry then
- 11 Assign each variable in  $Z_J$  to a separate group in  $C_{mleaf}$ . Assign each exogenous noise term in  $\mathcal{N}_J$  to a separate group in  $C_{unobserved}$ .
- 12 else if  $Z_J$  includes any observed variable then
- Assign the observed variable in  $\mathcal{Z}_J$  and all exogenous noise terms in  $\mathcal{N}_J$  to a single group in  $\mathcal{C}_{cogent}$ . Assign each remaining variable in  $\mathcal{Z}_J$  to a separate group in  $\mathcal{C}_{mleaf}$ .
- 14 else

15

- Assign all variables in  $\mathcal{Z}_J$  and all exogenous noise terms in  $\mathcal{N}_J$  to a single group in  $\mathcal{C}_{cogent}$ .
- Remove from W the rows corresponding to the variables in  $Z_I$ , and the columns corresponding to the noise terms in  $N_I$ . Remove the corresponding entries in m and n.

**Output:**  $C_{unobserved}$ ,  $C_{cogent}$ ,  $C_{mleaf}$ .

- **Proposition 8** (a) Under Assumptions 2 and 4, Algorithm 2 outputs  $\mathcal{M}_{AOG}$  which is the AOG equivalence class of the LV-SEM-ME corresponding to the input  $\mathbf{W}^*$ .
  - (b) Under Assumptions 3 and 4, Algorithm 2 outputs both  $\mathcal{M}_{AOG}$  and  $\mathcal{M}_{DOG}$ , where  $\mathcal{M}_{DOG}$  is the DOG equivalence class of the LV-SEM-ME corresponding to the input  $\mathbf{W}^*$ .

**Computational complexity** Recovering AOG of the model requires  $O(p_cmn)$  time complexity and O(mn) space complexity as discussed above. Recovering the underlying model given each choice of row and col requires  $O(p_cmn)$  calculation and O(mn) space. Calculating the number of edges in each single model requires O(mn) calculation and O(1) space. Denote the total number of choices of the centers and noises (i.e., size of Row and Col) by  $M_{Row}$  and  $M_{Col}$ . Note that  $M_{Row}$  and  $M_{Col}$  are bounded by  $|D|^{p_c}$ , where |D| is the maximum group size. Therefore, total time complexity for recovering  $\mathcal{M}_{AOG}$  and  $\mathcal{M}_{DOG}$  is  $O(M_{Row}M_{Col}p_cmn)$ , and the space complexity is O(mn).

#### **F Proofs**

#### F.1 Proof of Proposition 4

The proof includes two parts. We first show the sufficiency: For an unobserved variable  $H_i$  in the ground truth model M, if it has an mleaf child that satisfies the condition described in Proposition

Algorithm 2: Recovering all models in the AOG / DOG Equivalence Class

Input: Recovered mixing matrix W<sup>\*</sup>, observability indicators of the variables.

- 1 Obtain the AOG of the true model using Algorithm 1.
- 2 Denote row as a selection of centers in the groups in  $C_{cogent}$ . Define Row as the set of all rows.
- 3 Denote *col* as a selection of noises in the groups in  $C_{cogent}$ . Define *Col* as the set of all *cols*.
- 4 Initialize  $\mathcal{M}_{AOG} = \emptyset$ .
- **5** for all  $row \in Row$  and  $col \in Col$  do
- 6  $\mathbf{C} = \mathbf{I} (\mathbf{W}^*[row, col])^{-1}$
- 7  $\mathbf{B}^C = (\mathbf{I} \mathbf{C})\mathbf{W}^*[row, col^C].$
- 8  $\mathbf{D} = \mathbf{W}^*[row^C, col](\mathbf{I} \mathbf{C}).$
- 9  $| \mathbf{B}^L = \mathbf{W}^*[row^C, col^C] \mathbf{D}(\mathbf{I} \mathbf{C})^{-1}\mathbf{B}^C.$
- 10  $M = \{ \mathbf{B} = [\mathbf{B}^L; \mathbf{B}^C], \mathbf{C}, \mathbf{D} \}.$  Add M to  $\mathcal{M}_{AOG}$ .

11 Define  $\mathcal{M}_{DOG}$  as the set of models in  $\mathcal{M}_{AOG}$  that have the fewest total number of non-zero entries in **B**, **C**, **D**.

**Output:**  $\mathcal{M}_{AOG}$ ,  $\mathcal{M}_{DOG}$ .

4, then M is not minimal, i.e., there exists an alternative model M' without  $H_i$  that has the same mixing matrix and satisfies Assumption 1. Next, we show the necessity: If M is not minimal, then there must exist an unobserved variable  $H_i$  and one of its mleaf child  $Z_j$  such that the described condition is satisfied.

#### F.1.1 Proof of sufficiency

Suppose there exists latent variable  $H_i$  and a mleaf child  $Z_j$  of  $H_i$  in M such that the condition described in Proposition 4 holds. In the following we construct the alternative model M' that includes all variables in M except for  $H_i$ . The idea is to consider  $N_{H_i}$  as the exogenous noise term of  $Z_j$ . Further, for any other child  $V_k$  of  $H_i$ , replace the edge  $H_i \to V_k$  in M by edges from  $Z_j$  (and parents of  $Z_j$ ) to  $V_k$  in M'.

The structural equation of  $Z_j$  in M can be written as

$$Z_j = \sum_{l: V_l \in Pa_M(Z_j) \cap \mathcal{V}^C} a_{jl} V_l + \sum_{l_j: H_{l_j} \in Pa_M(Z_j) \cap \mathcal{H}} b_{jl_j} H_{l_j}.$$
(4)

Consider  $N_{H_i}$  as the exogenous noise term of  $Z_j$  in M'. The structural equation of  $Z_j$  in M' is

$$Z_{j} = \sum_{l:Z_{l} \in Pa_{M}(Z_{j}) \cap \mathcal{V}^{C}} a_{jl}Z_{l} + \sum_{l_{j}:H_{l_{j}} \in Pa_{M}(Z_{j}) \cap \mathcal{H} \setminus \{H_{i}\}} b_{jl_{j}}H_{l_{j}} + b_{ji}N_{H_{i}}.$$
(5)

For any other children  $V_k$  of  $H_i$  in M, the structural equation of  $V_k$  in M can be written as

$$V_{k} = \sum_{l:Z_{l} \in Pa_{M}(V_{k}) \cap \mathcal{V}^{C}} a_{kl}Z_{l} + \sum_{l_{k}:H_{l_{k}} \in Pa_{M}(V_{k}) \cap \mathcal{H}} b_{kl_{k}}H_{l_{k}} + N_{V_{k}}.$$
 (6)

By considering  $N_{H_i}$  in Equation (6) to be the exogenous noise of  $Z_j$ , the structural equation of  $Z_m$  in M' can be written as

$$V_{k} = \sum_{l:Z_{l} \in Pa_{M}(V_{k}) \cap \mathcal{V}^{C}} a_{kl}Z_{l} + \sum_{l_{k}:H_{l_{k}} \in Pa_{M}(V_{k}) \cap \mathcal{H} \setminus \{H_{i}\}} b_{kl_{k}}H_{l_{k}} + N_{Z_{m}} + b_{ki}b_{ji}^{-1} \left( Z_{j} - \sum_{l:Z_{l} \in Pa_{M}(Z_{j}) \cap \mathcal{V}^{C}} a_{jl}Z_{l} - \sum_{l_{j}:H_{l_{j}} \in Pa_{M}(Z_{j}) \cap \mathcal{H} \setminus \{H_{i}\}} b_{jl_{j}}H_{l_{j}} \right).$$
(7)

Since  $H_i$  and  $Z_j$  satisfy the condition in Proposition 4,  $V_k$  cannot be an ancestor of  $Z_j$  or variables in  $Pa_M(Z_j)$  in M, otherwise we have  $V_k \in \bigcup_{Z \in Pa(Z_j)} An_M(Z = An_M(Z_j) \subseteq An_M(V_k)$ . This implies that M' is still acyclic. Further, since  $An_M(Z_j) \subseteq An_M(V_k)$ , there are no additional ancestors introduced to  $V_k$  in M' compared with M. Lastly, we note that there might be edge cancellations in (4). In particular, the coefficient of the direct edge from a variable in  $Z \in Pa_M(V_k) \cap V^C$  to  $V_k$  may change in M' if  $Z \in Pa_M(Z_j)$  and hence may be cancelled out. However, Z is still an ancestor of  $V_k$  in M', as there is the path  $Z \to Z_j \to V_k$ . As M and M' has the same mixing matrix, the conventional faithfulness is still satisfied.

In conclusion, if such  $H_i$  and  $Z_j$  exists in  $\mathcal{M}$ , then there exists an alternative model  $\mathcal{M}'$  such that we cannot distinguish  $\mathcal{M}'$  from  $\mathcal{M}$  under Assumption 1 while having one less latent variable. Hence the sufficiency is proved.

#### F.1.2 Proof of necessity

Suppose M is not minimal. Then there exists an alternative model M' that has the same mixing matrix as M and also satisfies conventional faithfulness assumption, while having fewer unobserved variables. Without loss of generality, suppose M' is minimal. Note that since both models correspond to the same mixing matrix, this implies that the number of measured cogent variables in M is strictly less than M', which equals to the number of columns of in the mixing matrix subtract the number of unobserved variables.

Now, we partition the cogent and mleaf variables in M and M' as follows, where we put measured variables with the same row support in the mixing matrix in the same group. We note that in M', this is the same partition as the ancestral ordered grouping among these variables.

Consider the set of measured cogent variables in M. According to the definition, they must have different row support hence each of them must belong to a separate group. Therefore, since M has fewer measured cogent variables than M', there exists at least one group  $\mathcal{G}$ , where variables  $\mathcal{G}$  are all mleaf variables in M and one of the variables in  $\mathcal{G}$  is a measured cogent variable in M'. Denote this measured cogent variable in M' as  $Z_j$ . Consider the column corresponding to the exogenous noise term of  $\mathcal{G}$  in the mixing matrix.

We first show that this column corresponds to a latent confounder in M by contradiction. Suppose this column corresponds to the exogenous noise of a measured cogent variable  $Z_i$  in M. Therefore  $Z_i$  must be an ancestor of  $Z_j$  in M, and the entry with row corresponding to  $Z_i$  and column corresponding to this noise is not zero. Denote  $Supp(Z_i)$ ,  $Supp(Z_j)$  as the support of the row corresponding to  $Z_i$  and  $Z_j$ , respectively. Since M satisfies conventional faithfulness, the total causal effects from all ancestors of  $Z_i$  on  $Z_j$  in M is not zero. Hence  $Supp(Z_i) \subseteq Supp(Z_j)$ . Similarly, consider  $Z_i$  in M'. Since  $Z_j$  is the a measured cogent variable,  $Z_j$  is an ancestor of  $Z_i$ , and  $Supp(Z_j) \subseteq Supp(Z_i)$ . Therefore we have  $Supp(Z_j) = Supp(Z_i)$ , and hence both belong to the same group  $\mathcal{G}$ . However, no variables in  $\mathcal{G}$  are cogent variables in M, which leads to a contradiction. Therefore, this column must correspond to a latent confounder in M denote this latent confounder as  $H_i$  in M.

Next, we consider any other child  $V_k$  of  $H_i$  in M.  $V_k$  must be an descendant of  $Z_j$ , hence  $Supp(Z_j) \subseteq Supp(V_k)$ . As M satisfies conventional faithfulness, this implies that  $An(Z_j) \subseteq An(V_k)$ . Therefore the condition in the proposition is satisfied on M.

# F.2 Enumerating all models in the AOG and DOG equivalence classes by different choice of centers

We first show that an LV-SEM-ME can be uniquely deduced given the mixing matrix  $W^*$  of the LV-SEM-ME, and a choice of the centers (and their corresponding exogenous noises) in each group. This has been described in Algorithm 2, where the matrices B, C, D can be found through matrix calculation.

In this following, given the ground-truth model M, we will show how to deduce the structural equations of the variables in the alternative model M', where M and M' has the same mixing matrix and the same (ancestral ordered or directed ordered) grouping of the variables. Specifically, we consider the case when the centers of the groups are the same between M and M' except for one group. We denote the center of this only group in M as  $V_i$  with exogenous noise  $N_{V_i}$ , while the center and the corresponding exogenous noise in M' are  $Z_j$  and  $N_{H_l}$ , where  $Z_j$  and  $H_k$  belong to the same group as  $V_i$  in M. We will show the structural equations of all variables that are affected by this difference. This will be used in the proof of AOG and DOG results in F.3 and F.4, respectively.

The structural equation of  $V_i$  in M can be written as:

$$V_{i} = \sum_{m_{i}:H_{m_{i}} \in Pa_{\mathcal{H}}(V_{i})} b_{im_{i}}H_{m_{i}} + \sum_{n_{i}:V_{n_{i}} \in Pa_{\mathcal{V}^{C}}(V_{i})} a_{in_{i}}V_{n_{i}} + N_{V_{i}}$$
(8)

Note that  $H_l \in Pa_{\mathcal{H}}(V_i)$ . For  $Z_j$ , since it is an mleaf child of  $V_i$ , we have:

$$Z_{j} = a_{ji}V_{i} + \sum_{m_{j}:H_{m_{j}}\in Pa_{\mathcal{H}}(Z_{j})} b_{jm_{j}}H_{m_{j}} + \sum_{n_{j}:V_{n_{j}}\in Pa_{\mathcal{V}^{C}}(Z_{j})\setminus\{V_{i}\}} a_{jn_{j}}V_{n_{j}}.$$
(9)

We can also write down the equations of any other children  $V_{k_i}$  of  $V_i$ , and any other children  $V_{k_l}$  of  $H_l$ :

$$V_{k_{i}} = a_{k_{i}i}V_{i} + \sum_{m_{k_{i}}:H_{m_{k_{i}}}\in Pa_{\mathcal{H}}(V_{k_{i}})} b_{k_{i}m_{k_{i}}}H_{m_{k_{i}}} + \sum_{n_{k_{i}}:V_{n_{k_{i}}}\in Pa_{\mathcal{V}C}(V_{k_{i}})\setminus\{V_{i}\}} a_{k_{i}n_{k_{i}}}V_{n_{k_{i}}} + N_{V_{k_{i}}},$$

$$V_{k_{l}} = b_{k_{l}l}H_{l} + \sum_{m_{k_{l}}:H_{m_{k_{l}}}\in Pa_{\mathcal{H}}(V_{k_{l}})\setminus\{H_{l}\}} b_{k_{l}m_{k_{l}}}H_{m_{k_{l}}} + \sum_{n_{k_{l}}:V_{n_{k_{l}}}\in Pa_{\mathcal{V}C}(V_{k_{l}})} a_{k_{l}n_{k_{l}}}V_{n_{k_{l}}} + N_{V_{k_{l}}}.$$

$$(10)$$

(11)

Now, consider M'. We can first write down the equation for  $V_i$ , which is now a mleaf:

$$V_{i} = a_{ji}^{-1} \left( Z_{j} - \sum_{m_{j}: H_{m_{j}} \in Pa_{\mathcal{H}}(Z_{j})} b_{jm_{j}} H_{m_{j}} - \sum_{n_{j}: V_{n_{j}} \in Pa_{\mathcal{V}^{C}}(Z_{j}) \setminus \{V_{i}\}} a_{jn_{j}} V_{n_{j}} \right).$$
(12)

For  $Z_j$ , by plugging in  $V_i$  from (8) to (9), we have:

$$Z_{j} = a_{ji} \left( b_{il}H_{l} + \sum_{m_{i}:H_{m_{i}} \in Pa_{\mathcal{H}}(V_{i}) \setminus \{H_{l}\}} b_{im_{i}}H_{m_{i}} + \sum_{n_{i}:V_{n_{i}} \in Pa_{\mathcal{V}^{C}}(V_{i})} a_{in_{i}}V_{n_{i}} + N_{V_{i}} \right)$$
$$+ \sum_{m_{j}:H_{m_{j}} \in Pa_{\mathcal{H}}(Z_{j})} b_{jm_{j}}H_{m_{j}} + \sum_{n_{j}:V_{n_{j}} \in Pa_{\mathcal{V}^{C}}(Z_{j}) \setminus \{V_{i}\}} a_{jn_{j}}V_{n_{j}}.$$

Next, since  $N_{H_l}$  is the exogenous noise term of  $Z_j$ , and  $N_{V_i}$  is the exogenous noise of  $H_l$ , we can rewrite it as

$$Z_{j} = a_{ji} \left( H_{l} + \sum_{m_{i}:H_{m_{i}} \in Pa_{\mathcal{H}}(V_{i}) \setminus \{H_{l}\}} b_{im_{i}}H_{m_{i}} + \sum_{n_{i}:V_{n_{i}} \in Pa_{\mathcal{V}C}(V_{i})} a_{in_{i}}V_{n_{i}} \right) + \sum_{m_{j}:H_{m_{j}} \in Pa_{\mathcal{H}}(Z_{j})} b_{jm_{j}}H_{m_{j}} + \sum_{n_{j}:V_{n_{j}} \in Pa_{\mathcal{V}C}(Z_{j}) \setminus \{V_{i}\}} a_{jn_{j}}V_{n_{j}} + a_{ji}b_{il}N_{H_{l}}.$$
(13)

For  $V_{k_i}$ , by plugging in  $V_i$  from (12) to (10), we have

$$V_{k_{i}} = \frac{a_{k_{i}i}}{a_{ji}} \left( Z_{j} - \sum_{m_{j}:H_{m_{j}} \in Pa_{\mathcal{H}}(Z_{j})} b_{jm_{j}}H_{m_{j}} - \sum_{n_{j}:V_{n_{j}} \in Pa_{\mathcal{V}C}(Z_{j}) \setminus \{V_{i}\}} a_{jn_{j}}V_{n_{j}} \right) + \sum_{m_{k_{i}}:H_{m_{k_{i}}} \in Pa_{\mathcal{H}}(V_{k_{i}})} b_{k_{i}m_{k_{i}}}H_{m_{k_{i}}} + \sum_{n_{k_{i}}:V_{n_{k_{i}}} \in Pa_{\mathcal{V}C}(V_{k_{i}}) \setminus \{V_{i}\}} a_{k_{i}n_{k_{i}}}V_{n_{k_{i}}} + N_{V_{k_{i}}}.$$
(14)

Lastly, for  $V_{k_l}$ , we substitute  $H_l$  in (11) by  $N_{H_l}$  in (13) and have

$$V_{k_{l}} = \frac{b_{k_{l}l}}{a_{ji}b_{il}}Z_{j} - \frac{b_{k_{l}l}}{b_{il}}\left(H_{l} + \sum_{m_{i}:H_{m_{i}}\in Pa_{\mathcal{H}}(V_{i})\setminus\{H_{l}\}}b_{im_{i}}H_{m_{i}} + \sum_{n_{i}:V_{n_{i}}\in Pa_{\mathcal{V}C}(V_{i})}a_{in_{i}}V_{n_{i}}\right) - \frac{b_{k_{l}l}}{a_{ji}b_{il}}\left(\sum_{m_{j}:H_{m_{j}}\in Pa_{\mathcal{H}}(Z_{j})}b_{jm_{j}}H_{m_{j}} + \sum_{n_{j}:V_{n_{j}}\in Pa_{\mathcal{V}C}(Z_{j})\setminus\{V_{i}\}}a_{jn_{j}}V_{n_{j}}\right) + \sum_{m_{k_{l}}:H_{m_{k_{l}}}\in Pa_{\mathcal{H}}(V_{k_{l}})\setminus\{H_{l}\}}b_{k_{l}m_{k_{l}}}H_{m_{k_{l}}} + \sum_{n_{k_{l}}:V_{n_{k_{l}}}\in Pa_{\mathcal{V}C}(V_{k_{l}})}a_{k_{l}n_{k_{l}}}V_{n_{k_{l}}} + N_{V_{k_{l}}}.$$
(15)

We note that if  $V_i \in Pa(V_{k_l})$ , then we have to replace  $a_{k_l i}V_i$  by the right hand side of Equation (12). To summarize, compared with M, the changes in the parent-child relationships among variables in M' can be summarized as follows:

- (i) For  $V_i$ , since it is an mleaf node in M', its parents in M' are the parents of  $Z_j$  in M (excluding  $V_i$  itself), plus  $Z_j$ .
- (ii) For  $Z_j$ , since it is the new center, its parents in M' are the parents of  $Z_j$  itself in M (excluding  $V_i$ ), plus the parents of  $V_i$  in M.
- (iii) For any child  $V_{k_i}$  of  $V_i$  in M (other than  $Z_j$ ), compared with its parent set in M, the new parent set in M replaces  $V_i$  by  $Z_j$ , and includes additional variables that are the parents of  $Z_j$  in M.
- (iv) For any child  $V_{k_l}$  of  $H_l$  in M (other than  $V_i$ ), compared with its parent set in M, the new parent set in M' additionally includes the new center  $Z_j$  and all parents of  $Z_j$  in M' (i.e., parents of  $V_i$  and  $Z_j$  in M).

Note that there may be changes of model coefficients if the "additional variables" are already in the parent set of  $V_{k_i}$  and  $V_{k_l}$ . In particular, this change may lead to removal of variables from the parent set if the coefficients cancel out each other.

#### F.3 Proof of the identification result under conventional faithfulness

In this subsection, we provide the proof of the result regarding the AOG equivalence class in LV-SEM-ME, i.e., Theorem 2(a). Note that the proof of the result for SEM-ME and LV-SEM, i.e., Theorem 1(a), can be deduced from it.

To show that the extent of identifiability of an LV-SEM-ME under conventional faithfulness is the AOG equivalence class, we need to show that, for the ground-truth model M, any other model M' in the AOG equivalence class of M, and any model M'' that has the same mixing matrix but does not belong to the AOG equivalence class of M:

- (1.a) M' satisfies conventional faithfulness.
- (1.b) M' is consistent with any causal order among the ancestral ordered groups that is consistent with M.
- (1.c) M'' violates conventional faithfulness.

Recall that for each cogent variable  $V_i$ , the ancestral ordered group of  $V_i$  includes its mleaf child  $Z_j$  if  $V_i$  is measured and all other parents of  $Z_j$  are also ancestors of  $V_i$ , and unobserved parent  $H_l$  if all other children of  $H_l$  are also descendants of  $V_i$ .

**Proof of (1.a).** We note that it suffices to show (a) when the choices of centers (and/or the corresponding exogenous noise) of M' only differs from the choices of M in one group. This is because if there are p differences in the choices of centers, then we can always find a finite sequence of models  $M_0 \rightarrow M_1 \rightarrow \cdots \rightarrow M_p$ , where  $M_0 = M$ ,  $M_p = M'$ , and for each  $M_{k_p}$ ,  $k_p \in [p]$ , the choices of centers only differs from the choices of centers of  $M_{k_p-1}$  in one group. If (a) hold for models with one difference of the choices, then following the sequence of the models, (a) must also hold for  $M_p$ .

We prove by contradiction. Suppose V is an ancestor of V' in M' and the total causal effect from V to V' is zero. Note that the total causal effect from V to V' is equal to the sum of path products from the exogenous noise of V to V'. Suppose the exogenous noise of V in M' is the exogenous noise of  $V_0$  in M. Since M satisfies Assumption 2,  $V_0$  is not an ancestor of V' in M. This means that the added edges in M' introduces additional ancestors to V'.

Note that if  $V' = Z_j$ , then we compare the addition of ancestors to  $Z_j$  in M' with the ancestors of  $V_j$  in M as both are the center variable in the corresponding model. Similarly, we compare the addition of ancestors to  $V_j$  in M' with the ancestors of  $V_i$  in M.

However, as we described in Appendix F.2, all added edges in M' can be categorized as follows:

- If  $V' = Z_j$ . According to (ii), all added edges in M' are from parents of  $Z_j$  in M to  $Z_j$ . However, parents of  $Z_j$  are all ancestors of  $V_i$  in M. Therefore no additional ancestors are introduced.
- If  $V' = V_{k_i}$ . According to (iii), all added edges in M' are also from parents of  $Z_j$  in M to  $Z_j$ . Since there is  $V_i$  is a parent of  $V_{k_i}$  in M, parents of  $Z_j$  are all ancestors of  $V_{k_i}$  in M.
- If  $V' = V_{k_l}$ . According to (iv), all added edges in M' are also from parents of  $V_i$  or  $Z_j$  in M to  $Z_j$ . Since  $V_i$  is an ancestor of  $V_{k_l}$  in M, parents of  $V_i$  or  $Z_j$  are all ancestors of  $V_{k_l}$ .

In conclusion, the added edges in M' does not introduce any additional ancestors to V', which leads to a contradiction. Therefore M' satisfies Assumption 2.

**Proof of (1.b).** Since M and M' both satisfies conventional faithfulness, then Proposition 5 holds. Further, for any group g, define Supp(g) as the row support of variables in g in  $\mathbf{W}^*$  if g includes any observed or measured variables, and if  $g = \{H_i\} \subseteq \mathcal{H}$ , define Supp(g) as  $\{N_{H_i}\}$ . Similarly, define  $Supp(N_g)$  as the column support of the exogenous noises of the variables in g in  $\mathbf{W}^*$  if g includes any cogent or unobserved variables, and if  $g = \{Z_L\} \subseteq \mathcal{Z}^L$ , define Supp(g) as  $\{Z_L\}$ . We have the following property.

**Proposition 9** For two different ancestral ordered groups  $g_i$  and  $g_j$ , the following three conditions are equivalent:

- (i) There exists a causal path from one variable in the group of  $g_i$  to one variable in the group of  $g_j$ .
- (ii)  $Supp(g_i) \subset Supp(g_j)$ .
- (iii)  $Supp(N_{q_i}) \subset Supp(N_{q_i}).$

Therefore, given M, a causal order among the groups is consistent with the causal order among the variables if and only if the set relations in the mixing matrix hold. Since M and M' have the same mixing matrix and satisfy Assumption 2, they are consistent with the same set of causal order among the groups.

**Proof of (1.c).** Suppose M'' does not belong to the AOG equivalence class of M. First, consider the number of cogent variables in M'', which is equal to the number of columns of  $\mathbf{W}^*$  minus the number of unobserved variables. Given that M is minimal, M'' cannot have more cogent variables than M. Similarly, if M'' has fewer cogent variables than M, then M'' is not minimal. Therefore, M and M'' must have equal number of cogent variables.

Next, consider the cogent variables in M'', and their position in the AOG of M. Denote these cogent variables as  $\mathcal{P}$ . Firstly, note that no two variables in  $\mathcal{P}$  belongs to the same ancestral ordered group of M. This is because the mixing matrix corresponding to  $\mathcal{P}$  must be lower-triangular following the causal order, which is impossible when two variables in  $\mathcal{P}$  have the same row support. Therefore,  $\mathcal{P}$  includes at most one variable in each group. Similarly, the exogenous noises of variables in  $\mathcal{P}$  in M'', denoted by  $N_{\mathcal{P}}$ , includes the exogenous noise of at most one variable in each group. Suppose g is the a group with cogent variables where either (I) g does not include any variable in  $\mathcal{P}$ , or (II) g does not include any variable whose corresponding exogenous noise is in  $N_{\mathcal{P}}$ . Note that such a group must exist, otherwise M'' belongs to the same AOG equivalence class. Denote this cogent variable in M as  $V_i$ , and its exogenous noise  $N_{V_i}$ .

(I): Suppose g does not include any variable in  $\mathcal{P}$ . Then  $V_i$  is an mleaf in M''. Consider  $N_{V_i}$  in M''. If there exists one parent of  $V_i$  in M'' that also includes  $N_{V_i}$  (i.e., is affected by  $N_{V_i}$  directly or indirectly), denote this variable as  $V_j$ , which must be in  $\mathcal{P}$  and not in g. Since  $V_j$  includes  $N_{V_i}$ , it must be a descendant of  $V_i$  in M. However, since M satisfies conventional faithfulness and  $V_j \notin g$ , the row support of  $V_j$  must be a superset of  $V_i$ . This implies that conventional faithfulness is violated on M''.

Therefore, none of the parents of  $V_i$  in M'' is affected by  $N_{V_i}$ , and there must be a directed edge from  $N_{V_i}$  to  $V_i$ . Since  $V_i$  is an mleaf,  $N_{V_i}$  corresponds to a latent confounder in M''. Further, for any other children V of  $N_{V_i}$  in M'', it must be a descendant of  $V_i$  in M, and hence  $Supp(V_i) \subseteq Supp(V)$ . According to Proposition 4, this implies that M'' is not minimal.

(II): Suppose g does not include any variable whose exogenous noise is in  $N_{\mathcal{P}}$ . Then  $N_{V_i}$  corresponds to an unobserved confounder in M''. Similarly, consider  $V_i$  in M''. If there is one cogent variable in M'' that is a child of  $N_{V_i}$  and affects  $V_i$  (or  $V_i$  is this cogent variable), denote the exogenous noise of this cogent variable as  $N_V$ , which is in  $N_{\mathcal{P}}$ . Since  $N_V$  is an ancestor of  $V_i$  in M,  $Supp(N_{V_i}) \subseteq Supp(N_V)$ . Further, as  $N_V$  is not the exogenous noise of any (observed or latent) variable in g,  $Supp(N_{V_i})$  must be a strict subset of  $Supp(N_V)$ . As any descendants of  $N_V$  must also be a descendant of  $N_{V_i}$  in M'', this implies that conventional faithfulness is violated on M''.

Therefore, none of the parents of  $V_i$  in M'' is affected by  $N_{V_i}$ , and  $V_i$  cannot be a cogent variable. Hence  $V_i$  is an mleaf variable in M'' and is directly affected by  $N_{V_i}$ . Similarly, for any other children V of  $N_{V_i}$  in M'', it must be a descendant of  $V_i$  in M, and hence  $Supp(V_i) \subseteq Supp(V)$ . According to Proposition 4, this implies that M'' is not minimal.

#### F.4 Proof of the identification result under LV-SEM-ME faithfulness

In this subsection, we provide the proofs of all results regarding the DOG equivalence class in LV-SEM-ME, i.e., Proposition 3, and 7, and Theorem 2(b). These proof of the results for for SEM-ME and LV-SEM, i.e., Proposition 2 and Theorem 1(b) can be deduced from it.

To show that the extent of identifiability of an LV-SEM-ME under LV-SEM-ME faithfulness is the DOG equivalence class, the proof includes two parts.

First, we show that, for the ground-truth model M, any other model M' in the DOG equivalence class:

- (2.a) M' does not add extra edge compared with M.
- (2.b) M' does not remove any edge compared with M.
- (2.c) M' satisfies LV-SEM-ME faithfulness.

Therefore we cannot distinguish M' from M. Next, any other model M'' that is in the AOG equivalence class of M but not the DOG equivalence class:

- (2.d) M'' adds at least one extra edge compared with M.
- (2.e) M'' does not remove any edge compared with M, and there is at least one added edge that is not removed.
- (2.f) M'' violates LV-SEM-ME faithfulness.

Therefore we can distinghuish M' from M.

#### F.4.1 Model within the same DOG equivalence class

Similar to (1.a) in the AOG proof, we only need to show the result if M' only differs from M in the choices of centers (and/or the corresponding exogenous noise) in one group. If there are p differences in the choices of centers between M and M', then we can always find a finite sequence of models  $M_0 \to M_1 \to \cdots \to M_p$ , where  $M_0 = M$ ,  $M_p = M'$ , and for each  $M_{k_p}$ ,  $k_p \in [p]$ , the choices of centers only differs from the choices of centers of  $M_{k_p-1}$  in one group.

In the following, we show (2.a) - (2.c) together for the one difference in the choices of centers. Specifically, for (2.b), we show that if one edge is cancelled out, then M violates LV-SEM-ME faithfulness. Further, for (2.c), we show that a single change still preserves LV-SEM-ME faithfulness. Following the sequence of the models, all three properties hold for M'.

**Proof of (2.a).** Following the description in Appendix F.2, after replacing the center  $V_i$  in M with  $Z_j$ , and replacing the exogenous noise  $N_{V_i}$  in M with  $N_{H_l}$ , where  $Z_j$  and  $H_l$  belong to the same direct ordered group as  $V_i$  in M, all added edges in M' can be categorized as follows:

- For  $V_i$ : No edges are added.
- For Z<sub>j</sub>: According to (ii), all added edges in M' are from parents of Z<sub>j</sub> (excluding V<sub>i</sub>) in M to Z<sub>j</sub>. However, according to Condition 1(a), since Z<sub>j</sub> belongs to the same direct ordered group as V<sub>i</sub>, Pa(Z<sub>j</sub>) \ {V<sub>i</sub>} is a subset of Pa(V<sub>i</sub>). Therefore no edges are added.
- For V<sub>ki</sub>: According to (iii), all added edges in M' are from parents of Z<sub>j</sub> in M (excluding V<sub>i</sub>) to V<sub>ki</sub>. Still, according to Condition 1(b), since Z<sub>j</sub> belongs to the same direct ordered group as V<sub>i</sub>, Pa(Z<sub>j</sub>) is a subset of Pa(V<sub>ki</sub>). Therefore no edges are added.
- For V<sub>kl</sub>: According to (iv), the added edges are from Z<sub>j</sub> and parents of V<sub>i</sub> and V<sub>j</sub> in M to V<sub>kl</sub>. Since H<sub>l</sub> belongs to the same direct ordered group as V<sub>i</sub> in M, {V<sub>i</sub>} ∩ Pa(V<sub>i</sub>) ⊆ Pa(V<sub>kl</sub>) in M. Since the center is replaced by Z<sub>j</sub> and Pa(Z<sub>j</sub>) \ {V<sub>i</sub>} is a subset of Pa(V<sub>i</sub>), no edges are added.

Therefore no edges are added to M' compared with M.

**Proof of (2.b).** We show that if any edge is cancelled out in M' described in Appendix F.2, then M violates LV-SEM-ME faithfulness. Similarly, all removed edges in M' can be categorized as follows:

- For  $V_i$ : No edges are removed.
- For  $Z_j$ : According to (ii), the edge from V to  $V_i$  in M may be cancelled out in M' if V is also a parent of  $Z_j$ . Suppose the edge from V to  $V_i$  is cancelled out in M' because of this. We show that if this happens, then M violates LV-SEM-ME faithfulness. Note that V can be either cogent or unobserved.

If V is cogent: Consider variable  $Z_j$ , the set of cogent ancestors  $J = An_{M'}(Z_j) \cap \mathcal{V}^C$  in M', and the set of cogent parents  $K = Pa_{M'}(Z_j) \cap \mathcal{V}^C$  in M'. We have  $An_{M'}(Z_j) \cap \mathcal{V}^C = An_V(V_j) \setminus \{V_i\}$  and  $K \subset Pa_V(V_i)$ , because  $V \notin K$ . Next, following the structural equation of  $Z_j$  in M', we have:  $Rank(\mathbf{W}_{K\cup\{Z_j\}}^J) = |K|$ . However, the minimal bottleneck from J to  $K \cup \{Z_j\}$  in M is at least |K| + 1, because  $K \subset J$ , and there is one extra path in M ( $V \to V_i \to Z_j$ ) that is not blocked by K. Therefore,  $Z_j$  violates Assumption 3(b). If V is unobserved: Consider the set of cogent ancestors  $J = An_{M'}(Z_j) \cap \mathcal{V}^C$  plus  $\{V\}$  in M', and the set of cogent parents  $K = Pa_{M'}(Z_j) \cap \mathcal{V}^C$  in M'. In this case, K may equal to  $Pa_V(V_i)$ . However, we can still show that  $Rank(\mathbf{W}_{K\cup\{Z_j\}}^J) = |K|$  (since there is no direct connection from V to  $Z_j$  in M'), but the minimal bottleneck from J to  $K \cup \{Z_j\}$  in M is at least |K| + 1, because the path  $V \to V_i \to Z_j$  is not blocked. Therefore  $Z_j$  still violates Assumption 3(b).

• For  $V_{k_i}$ : According to (iii), the edge from V to  $V_{k_i}$  in M may be cancelled out in M' if V is also a parent of  $Z_j$ . Suppose the edge from V to  $V_{k_i}$  is cancelled out in M' because of this. Similarly, V can be either cogent or observed.

If V is cogent: Consider variable  $V_{k_i}$ ,  $J = An_V(V_{k_i}) \setminus \{V_i\} \cup \{H_l\}$ , and the set of cogent parents  $K = Pa_{M'}(V_{k_i}) \cap \mathcal{V}^C$  in M'. We have  $K \subset PP(V_{k_i})$  (note that  $Z_j$  is an mleaf in M), and  $|K| < Pa_V(V_{k_i})$ . Further, J includes all variables with the exogenous noise corresponding to the cogent ancestors of  $Z_j$  in M'. Therefore, we have  $Rank(\mathbf{W}_{K\cup\{V_{k_i}\}}^J) = |K|$ . However, the minimal bottleneck from J to  $K \cup \{V_{k_i}\}$  in M is at least |K| + 1. Firstly,  $K \setminus \{Z_j\}$  is a subset of J so they are included in any bottleneck. Additionally, there are two distinct paths from J to  $K \cup \{V_{k_i}\}$  that cannot be blocked by  $K \setminus \{Z_j\}$ :  $V \to V_{k_i}$  and  $H_l \to V_i \to Z_j$ . Therefore  $V_{k_i}$  violates Assumption 3(a).

If V is unobserved: Similarly, consider  $J = An_V(V_{k_i}) \setminus \{V_i\} \cup \{V, H_l\}$  and  $K = Pa_{M'}(V_{k_i}) \cap \mathcal{V}^C$ . Note that  $V \neq H_l$  as V is a parent of  $V_{k_i}$  in M. The results above still hold, as  $Rank(\mathbf{W}_{K\cup\{V_{k_i}\}}^J) = |K|$ , and the same two paths,  $V \to V_{k_i}$  and  $H_l \to V_i \to Z_j$ , cannot be blocked by  $K \setminus \{Z_j\}$ . Therefore  $V_{k_i}$  violates Assumption 3(a).

• For  $V_{k_l}$ : According to (iv), the edge from V to  $V_{k_l}$  in M may be cancelled out in M' if  $V = Z_j$ , or  $V \in Pa_{M'}(Z_j) \cap V^C$ . Suppose the edge from V to  $V_{k_l}$  is cancelled out in M' because of this.

If *V* is cogent and  $V \in Pa_V(V_i)$ : Consider variable  $V_{k_l}$ , the set of cogent ancestors  $J = An_V(V_{k_l}) \setminus \{V_i\} \cup \{H_l\}$  in *M*, and the set of cogent parents  $K = Pa_{M'}(V_{k_l}) \cap \mathcal{V}^C$  in *M'*. Similarly, we have  $K \subset PP(V_{k_l})$ , and  $|K| < Pa_V(V_{k_l})$ . We have  $Rank(\mathbf{W}_{K \cup \{V_{k_l}\}}) = |K|$ . Further, the minimal bottleneck from *J* to  $K \cup \{V_{k_l}\}$  in *M* is at least |K| + 1. Firstly,  $K \setminus \{Z_j\}$  is a subset of *J* so they are included in any bottleneck. Additionally, there are two distinct paths from *J* to  $K \cup \{V_{k_l}\}$  that cannot be blocked by  $K \setminus \{Z_j\}$ :  $V \to V_{k_l}$  and  $H_l \to V_i \to Z_j$ . Therefore  $V_{k_l}$  violates Assumption 3(a).

If  $V = Z_j$ : Consider the same J and K as above. The main difference here is that  $Z_j \notin K$ and hence  $K \subset J$ . Therefore,  $Rank(\mathbf{W}_{K\cup\{V_{k_l}\}}^J) = |K|$ , and the minimal bottleneck at least includes all variables in K, and one extra variable on the edge  $H_l \to V_{k_l}$ . Therefore  $V_{k_l}$  violates Assumption 3(a).

If V is unobserved: Consider  $J = An_V(V_{k_l}) \setminus \{V_i\} \cup \{H_l, V\}$  in M, and  $K = Pa_{M'}(V_{k_l}) \cap \mathcal{V}^C$  in M'. We have  $Rank(\mathbf{W}_{K\cup\{V_{k_l}\}}^J) = |K|$ , and the minimal bottleneck includes all variables in  $K \setminus \{Z_j\}$ , as well as two variables on the paths  $V \to V_{k_l}$  and  $H_l \to V_i \to Z_j$ . Therefore  $V_{k_l}$  violates Assumption 3(a).

In conclusion, if an edge is cancelled in M', then M violates Assumption 3.

**Proof of (2.c).** From (2.a) and (2.b), we show that M' has the same unlabeled graph structure as M. We can construct a mapping  $\sigma_M$  on variables in  $\mathcal{Z} \cup \mathcal{Y}$ , where

$$\sigma(V_i) = Z_j; \quad \sigma(Z_j) = V_i; \quad \sigma(V) = V, \quad V \neq V_i, Z_j.$$

Similarly, define a mapping  $\sigma_N$  on variables in  $\mathcal{V}^C \cup \mathcal{H}$ , where

$$\sigma_N(V_i) = H_l; \quad \sigma(H_l) = V_i; \quad \sigma(V) = V, \quad V \neq V_i, H_l.$$

We note that for all variable V except  $V_i$  and  $Z_j$ ,  $PP_M(V) = PP_{M'}(V)$ ,  $An_{M'}(V) = An_M(V)$ . This is because PP(V) either includes both  $V_i$  and  $Z_j$ , or include neither of them, as all parents of  $Z_j$  in M are ancestors of  $V_i$ . Similarly,  $An_M(V)$  either includes both  $H_l$  and  $V_i$ , or neither of them, because  $H_l$  is a parent of  $V_i$ , and all other children of  $H_l$  are descendants of  $V_i$ .

In the following, we show that if M satisfies Assumption 3, then M' also satisfies Assumption 3 with probability one. In particular, following the rewriting procedure described in Appendix F.2, we can construct an invertible mapping between the model parameters in M and in M'. Since Assumption 3 is violated with probability zero on the model parameters in M, the same results hold on the model parameters in M'.

We note that the differences in the model parameters that are different between M and M' can be summarized as follows:

- (i) The edge weight from  $Z_j$  to  $V_i$  is the inverse of the edge weight from  $V_i$  to  $Z_j$ ,  $a_{ji}$ ;
- (ii) The edge weight from other parents of  $V_i$  to  $V_i$  in M' can be written as the edge weight from other parents of  $Z_j$  to  $Z_j$  in M multiplied by  $-a_{ji}^{-1}$ ;
- (iii) The edge weight from  $Pa(Z_j)$  to  $Z_j$  in M' can be written as a function of  $a_{ji}$ , the edge weight from  $Pa(V_i)$  to  $V_i$  in M and the edge weight from  $Pa(Z_j)$  to  $Z_j$ ;
- (iv) The edge weight from  $Z_j$  to  $V_{k_i}$  is edge weight from  $V_i$  to  $V_{k_i}$ ,  $a_{k_i i}$  divided by  $a_{ji}$ ;
- (v) The edge weight from other parents of  $V_{k_i}$  to  $V_{k_i}$  in M' can be written as a function of  $a_{k_i i}$ ,  $a_{ji}$  the edge weight from  $Pa(V_{k_i})$  to  $V_{k_i}$  and the edge weight from  $Pa(Z_j)$  to  $Z_j$  in M;
- (vi) The edge weight from  $H_l$  to  $V_{k_l}$  is edge weight from  $H_l$  to  $V_{k_l}$ ,  $b_{k_l l}$ , divided by  $b_{il}$  (note that  $b_{il}$  is included in (iii));
- (vii) The edge weight from  $Z_j$  to  $V_{k_l}$  is a function of the edge weight from  $V_i$  to  $V_{k_l}$   $(a_{k_l i}), a_{ji}, b_{il}, b_{k_l l}$ ;
- (viii) The edge weight from  $Pa(V_{k_l})$  to  $V_{k_l}$  in M' can be written as a function of the edge weight from  $Pa(V_{k_l})$  to  $V_{k_l}$ , and the edge weight from  $Pa(Z_j)$  to  $Z_j$ , and  $Pa(V_i)$  to  $V_i$  in M.

Therefore, if we arrange the model parameters in M and in M' following (i)-(viii) above, we can clearly see that the mapping that translates model parameters in M to model parameters in M' is

invertible. This is consistent with the fact that since M and M' belong to the same DOG, we can equivalently write the model parameters in M using model parameters in M'. Therefore, since the model parameters in M satisfy Assumption 3 with probability one, the model parameters in M' also satisfy Assumption 3 with probability one.

Lastly, we note that, since the number of models in the DOG equivalence class is finite, if the ground-truth model satisfies Assumption 3, then the probability that models in the DOG equivalence class all satisfy Assumption 3 is also one.

#### F.4.2 Model outside the DOG equivalence class

Without loss of generality, we only need to show the result if all the differences in the choices of centers in M'' are outside the corresponding direct ordered group of the cogent variable in M, but in the same ancestral ordered group. That is, we consider M to be the model that is closest to M'' in terms of the differences of the centers. We have shown above that this closest model also satisfies LV-SEM-ME faithfulness and share the same unlabeled graph structure.

**Proof of (2.d).** We first show that if M'' differs from M only in one choice of the centers, then there will be at least one edge added to M''. The proof also follows the procedure described in Appendix F.2. That is, if  $Z_j$  belong to the same ancestral ordered group but not the same direct ordered group as  $V_i$ , then Condition 1 is satisfied. In this case, there will be one additional edge either from parents of  $Z_j$  in M to  $Z_j$ , or to  $V_{k_i}$ . Similarly, if  $H_l$  belong to the same ancestral ordered group but not the same direct ordered group but not the same direct ordered group as  $V_i$ , then Condition 2 is satisfied. In this case, there will be one additional edge from  $Z_j$ , or the parents of  $Z_j$  or  $V_i$  to  $V_{k_l}$ . In conclusion, there will be at least one added edge in M'' compared with M.

We note that if there are multiple differences in the centers between M'' and M, then we may not able to use the above analysis. In particular, since one added edge may change the parent-child relation among variable, it might be the case that no edges are added to  $M_2$  compared with  $M_1$ . Nevertheless, we can still show that  $M_2$  has at least one more edge compared with  $M_0$ . Repeating this procedure following the chain  $M_0 \to M_1 \to \cdots \to M_p$  completes the proof.

**Proof of (2.e).** We note that we can use the same method as in (2.b) to show that if any edge is removed in M, then M violates Assumption 3. Specifically, in (2.b), we only used the fact that  $Z_j$  is a child of  $V_i$ , and  $H_l$  is a parent of  $V_i$ . Both still hold true for AOG. In the following, we will only show the latter part, that is, there is at least one added edge that is not removed.

We prove by contradiction. Suppose all added edges are removed in M'', and suppose the edge from  $V_0$  to V is added but finally removed. We further assume that among all the added edges  $V_1 \rightarrow V_2$ ,  $V_0$  has the smallest index (following the causal order in M), and for any  $V' \in De(V_0) \cap An(V)$ , no edges from  $V_0$  to V' is added. That is, for any causal path from  $V_0$  to V, no edges are added from  $V_0$  to any other variable V' on this path. Note that  $V_0$  and V refers to their position (center or non-center) in M, i.e., they may represent different variables in M'' and  $M_q$ .

Suppose  $M_s$  is the first model following the sequence where this edge is added, and  $M_{q-1}$  is the last model following the sequence where this edge is present. Denote the center of the ancestral ordered group that changes between  $M_{s-1}$  and  $M_s$  as  $V_{i_s}$ , and between  $M_{q-1}$  and  $M_q$  as  $V_{i_q}$ . Since the edge from  $V_0$  to V is added in  $M_s$ , it must belong to one of the following three cases: There is a causal path  $V_0 \rightarrow V_{i_s} \rightarrow V$ , or there exists a latent confounder with  $V_0 \rightarrow V_{i_s} \leftarrow H_{l_s} \rightarrow V$  (note that  $V_0$  may be  $V_{i_s}$ ) or  $V_0 \rightarrow Z_{j_s} \leftarrow V_{i_s} \leftarrow H_{l_s} \rightarrow V$  in  $M_{q-1}$ . Note that in the latter two cases, since  $Z_{j_s}, V_{i_s}, H_{l_s}$  all belong to the same ancestral ordered group,  $V_0$  is an ancestor of  $V_{i_s}$ , and  $V_{i_s}$  is an ancestor of V.

We consider the following cases:

- $V = Z_{j_a}$ . This step does not include edge removals.
- $V = V_{i_q}$ . Since the edge is removed in  $M_q$ ,  $V_0 \in Pa_{M_{q-1}}(Z_{j_q})$  in  $M_{q-1}$ , where  $V_0$  is not a parent of  $V_{i_q}$  in M, and is not a parent of  $Z_{j_q}$  in M''. We note that the edge from  $V_0$  to  $Z_{j_q}$  cannot be an added edge. Because this edge is not removed in  $M_q$ , and will never be removed for all  $M_{q+1}, \dots, M_p = M''$ . Therefore this edge is in M.

Consider  $Z_{j_q}$ , and consider J as the set of (unobserved or cogent) variable V' in M where  $N_{V'}$  corresponds to the exogenous noise of a variable in  $\{V_0\} \cup (An_{M''}(Z_{j_q}) \cap \mathcal{V}^C)$ . In other

words,  $J = An_{M''}(Z_{j_q}) \cap \mathcal{V}^C$  if  $V_0$  is a cogent variable, and J additionally includes  $V_0$  if it is unobserved. Further, consider  $K = Pa_{M''}(Z_{j_q}) \cap \mathcal{V}^C$ . It follows that  $K \subseteq PP_M(V_{i_q})$ , and  $J \subseteq An_M(Z_{j_q}) \setminus \{V_{i_q}\}$ .

We have  $Rank(\mathbf{W}_{K\cup\{Z_{j_q}\}}^J) = |K|$ . However, note that we can find K distinct paths from variables in J to variables in K. Specifically, for each variable V' in K, define f(V') as the variable in J whose exogenous noise in M is the exogenous noise of V' in M''. Note that f(V') = V' if there is no change on V' and  $N_{V'}$  on both models. Further, f(V') and V' must belong to the same ancestral ordered group and hence there is a causal path  $f(V') \rightsquigarrow V'$  in M. Therefore, a minimal bottleneck from J to  $K \cup \{Z_{j_q}\}$  must at least include K variables. However, there is still one path  $V_0 \rightarrow Z_{j_q}$  that is not blocked, as  $V_0$  is not a parent of  $Z_{j_q}$  in M'' (meaning  $V_0 \notin K$ ). Hence M violates Assumption 3.

•  $V = V_{k_i}$  for some  $V_{k_i}$ . Note that this variable  $V_{k_i}$  may have different positions (center or non-center) in  $M_q$  and M''. For simplicity of notation, denote this variable as  $V_{k_q}$ . Then there exist paths  $V_0 \to V_{i_q} \to V_{k_q}$ ,  $V_0 \to V_{k_q}$ , and  $V_0 \to Z_{j_q}$  in  $M_{q-1}$ . Note that the edge  $V_{i_q} \to V_{k_q}$  and  $V_0 \to Z_{j_q}$  are in M.

If  $V_{k_q}$  does not change the position. Consider J as the set of (unobserved or cogent) variable V' in M where  $N_{V'}$  corresponds to the exogenous noise of a variable in  $\{V_0\} \cup (An_{M''}(V_{k_q}) \cap \mathcal{V}^C)$ , and  $K = Pa_{M''}(V_{k_q}) \cap \mathcal{V}^C$ . It follows that  $K \subseteq PP_M(V_{k_q})$ , and  $J \subseteq An_M(V_{k_q})$ . Further,  $Rank(\mathbf{W}_{K\cup\{V_{k_q}\}}^J) = |K|$ . However, a minimal bottleneck from J to  $K \cup \{V_{k_q}\}$  must at least include: One variable between V' and f(V') for each  $V' \in K$ , except for  $Z_{j_q}$ ; One variable on the edge  $V_{i_q} \to V_{k_q}$ ; One variable on the edge  $V_0 \to Z_{j_q}$ . Therefore the size of the minimal bottleneck is at least |K| + 1. Hence M violates Assumption 3.

If  $V_{k_q}$  changes the position from non-center to center. That is, it can be denoted by  $Z_{j_r}$  for some  $q < r \le p$ . Note that the reason we consider M'' in the above analysis is because there may still be edge additions or removals on  $V_{k_q}$  after  $M_q$ . However, if  $V = Z_{j_r}$ , then we know that there will be no edge additions/removals on V after  $M_r$ . Therefore, consider J as the set of variable V' in  $M_r$  where  $N_{V'}$  corresponds to the exogenous noise of a variable in  $\{V_0\} \cup (An_{M_r}(Z_{j_r}) \cap \mathcal{V}^C)$ , and  $K = Pa_{M_r}(Z_{j_r}) \cap \mathcal{V}^C$ . This implies that  $J \subseteq An(Z_{j_r}) \setminus \{V_{i_r}\}$ , and  $K \subseteq PP(V_{i_r})$ . We have  $Rank(\mathbf{W}_{K\cup\{Z_{j_r}\}}^J) = |K|$ . However, a minimal bottleneck from J to  $K \cup \{V_{k_q}\}$  must at least include: One variable between V' and f(V') for each  $V' \in K$ , except for  $Z_{j_q}$ ; One variable on the edge  $V_{i_q} \to V_{k_q}$ ; One variable on the edge  $V_0 \to Z_{j_q}$ . Therefore the size of the minimal bottleneck is at least |K| + 1. Hence M violates Assumption 3.

If  $V_{k_q}$  changes the position from center to non-center. That is, it can be denoted by  $V_{i_r}$  for some  $q < r \le p$ . Similarly, there are no edge additions or removals involving  $V_{i_r}$  after  $M_r$ . In this case, we consider the variable  $V_{i_r}$  in  $M_{r-1}$ , i.e., J as the set of variable V' in  $M_r$ where  $N_{V'}$  corresponds to the exogenous noise of a variable in  $\{V_0\} \cup (An_{M_{r-1}}(V_{i_r}) \cap \mathcal{V}^C)$ , and  $K = Pa_{M_{r-1}}(V_{i_r}) \cap \mathcal{V}^C$ . The following is the same as when  $V_{k_q}$  does not change the position, and we can conclude that M violates Assumption 3.

•  $V = V_{k_l}$  for some  $V_{k_l}$ . Similarly, for notation simplicity, denote this variable as  $V_{l_q}$ . Note that this is different from  $H_{l_q}$ , which refers to the unobserved variable that is in the same group as  $V_{i_q}$ . Then there exist paths  $V_0 \rightarrow V_{i_q} \leftarrow H_{l_q} \rightarrow V_{l_q}$  or  $V_0 \rightarrow Z_{j_q} \leftarrow V_{i_q} \leftarrow H_{l_q} \rightarrow V_{l_q}$  in  $M_{q-1}$ .

If  $V_{l_q}$  does not change the position. Consider J as the set of variable V' in M where  $N_{V'}$  corresponds to the exogenous noise of a variable in  $\{V_0\} \cup (An_{M''}(V_{l_q}) \cap \mathcal{V}^C)$ , and  $K = Pa_{M''}(V_{l_q}) \cap \mathcal{V}^C$ . It follows that  $K \subseteq PP_M(V_{l_q})$ , and  $J \subseteq An_M(V_{l_q})$ , and  $Rank(\mathbf{W}_{K\cup\{V_{l_q}\}}^J) = |K|$ .

- If  $V_{i_q}$  ( $Z_{j_q}$  if the center is replaced) is not a parent of  $V_{l_q}$  in M''. Note that this includes the case when  $V_0 = V_{i_q}$ . Similar to the above analysis for  $V_{k_i}$ , for each variable V' in K, define f(V') as the variable in J whose exogenous noise in M is the exogenous noise of V' in M''. Then any bottleneck from J to K must include at least one variable between V' and f(V') for each  $V' \in K$ . Further, it must also include one variable on the edge  $H_{l_q} \rightarrow V_{l_q}$ . Therefore the size of the minimal bottleneck must be at least |K| + 1.

- If  $V_{i_q}$  ( $Z_{j_q}$  if the center is replaced) is a parent of  $V_{l_q}$  in M. Then any bottleneck from J to K must include at least one variable between V' and f(V') for each  $V' \in K$  except for  $V_{i_q}$ . Further, it must also include one variable on the edge  $H_{l_q} \rightarrow V_{l_q}$ , and one variable on the edge  $V_0 \rightarrow V_{i_q}$  (or  $V_0 \rightarrow Z_{j_q}$  if  $Z_j$  is the center node in M''). Therefore the size of the minimal bottleneck must also be at least |K| + 1.

Therefore, in both cases, M violates Assumption 3.

If  $V_{l_q}$  changes its position. Similar to the analysis described in  $V_{k_i}$ ,  $V_{l_q}$  can be denoted by  $Z_{j_r}$  or  $V_{i_r}$  for some  $q < r \le p$ . Since there are no edge additions or removals involving  $V_{i_r}$  after  $M_r$ , we can consider the sets J and K defined on  $M_{r-1}$  if  $V = V_{i_r}$ , and the sets J and K defined on  $M_r$  if  $V = Z_{j_r}$ . Following the same analysis as above, we can conclude that M violates Assumption 3.

In conclusion, we show that if all added edges in  $M_1, \dots, M_p$  are removed, then M violates Assumption 3. Therefore at least one of the added edge to M'' is not removed.

**Proof of (2.f).** Lastly, we show that because of this added edge, M'' violates Assumption 3. Suppose the edge from  $V_0$  to V is added in M''. Note that this edge does not introduce any additional ancestral relations as M'' and M belong to the same AOG equivalence class. Therefore for each center or non-center variable V, the ancestor set and possible parent set of V remain the same. The proof of this claim is actually the same as (2.b), but in a reversed manner.

•  $V = Z_j$ . Then V is a center node in M'', and  $V_0 \in Pa_M(Z_j) \setminus Pa_M(V_i)$ . Consider  $V_i$  in M'', which is an mleaf. Consider J as the set of (unobserved or cogent) variable V' in M'' where  $N_{V'}$  corresponds to the exogenous noise of a variable in  $\{V_0\} \cup (An_M(V_i) \cap \mathcal{V}^C)$ , and consider  $K = Pa_M(X_i) \cap \mathcal{V}^C$ . We have  $J \subseteq An_{M''}(V_i \setminus \{Z_j\})$ , and  $K \subseteq PP_{M''}(V_j)$ . Further, according to the structural equation of  $V_i$  in M,  $Rank(\mathbf{W}_{J \cup \{V_i\}}) = |K|$ .

For each variable V' in K, define f(V') as the variable in J whose exogenous noise in M'' is the exogenous noise of V' in M. Then the minimal bottleneck must include at least one variable between V' and f(V') for each  $V' \in K$ , and one variable on the path  $V_0 \rightarrow Z_j \rightarrow V_i$  on M''. Therefore the size of the minimal bottleneck must be at least |K| + 1.

•  $V = V_{k_i}$ . Then  $V_0 \in Pa_M(Z_j) \setminus Pa_M(V_{k_i})$ . Without loss of generality, suppose  $V_{k_i}$  does not change its position between M and M''. If it changes then we can use the same procedure as described in (2.e).

Consider J as the set of variable V' in M" where  $N_{V'}$  corresponds to the exogenous noise of a variable in  $\{V_0\} \cup (An_M(V_{k_i}) \cap \mathcal{V}^C)$ , and consider  $K = Pa_M(V_{k_i}) \cap \mathcal{V}^C$ . We have  $Rank(\mathbf{W}_{K\cup\{V_{k_i}\}}^J) = |K|$ . However, any bottleneck from J to K includes one variable between V' and f(V'), for all  $V' \in K$ . Additionally, it needs to cover the edge  $V_0 \to V$ . Therefore the size of the minimal bottleneck must be at least |K| + 1.

•  $V = V_{k_l}$ . Similarly, we assume that  $V_{k_i}$  does not change its position between M and M''. Consider J as the set of variable V' in M'' where  $N_{V'}$  corresponds to the exogenous noise of a variable in  $\{V_0\} \cup (An_M(V_{k_l}) \cap \mathcal{V}^C)$ , and consider  $K = Pa_M(V_{k_l}) \cap \mathcal{V}^C$ . We have  $Rank(\mathbf{W}_{K\cup\{V_{k_l}\}}^J) = |K|$ . However, any bottleneck from J to K includes one variable between V' and f(V'), for all  $V' \in K$ . Additionally, it needs to cover the edge  $V_0 \to V$ . Therefore the size of the minimal bottleneck must be at least |K| + 1.