Safe Inverse Marginalization in Bayesian Networks

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Abstract

Safe inverse marginalization (SIM) was recently proposed for augmenting a Bayesian network with new discrete variables such that their marginalization exactly recovers the original network, allowing re-certification to focus exclusively on the new variables. Graph-safe marginalization (GSM) was introduced to describe when marginalizing the new variable yields a distribution that factorizes according to the original DAG, with constraint-optimization methods proposed for constructing new conditional probability tables (CPTs). In this paper, we first show that arc-reversal without fill-in (AR-NFI) strictly subsumes GSM as a sufficient graphical condition for SIM. We then propose constructing new CPTs via unity-potential expansion (UPE) rather than optimization. AR-NFI combined with UPE provides a concrete structural route to SIM. More fundamentally, UPE recovers the original Bayesian network exactly by reconstructing its factorization, from which the original DAG is uniquely identified. Hence, UPE alone guarantees SIM, establishing that neither AR-NFI nor GSM is necessary. Taken together, these results show that SIM is fundamentally a parametric property, with structural conditions characterizing only when recovery can be realized via structure-preserving transformations.

Keywords: Bayesian networks, safe inverse marginalization, arc-reversal

1. Introduction

Bayesian networks provide a compact and interpretable representation of joint probability distributions using a directed acyclic graph (DAG) together with conditional probability tables (CPTs) (Darwiche, 2009; Pearl, 1988; Koller and Friedman, 2009). They are widely used in high-stakes applications such as clinical decision support systems (CDSSs), where models are often validated or certified prior to deployment (Kyrimi et al., 2021). In such

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settings, incorporating new information can substantially improve decision-making such as in the ENDORISK model for endometrial cancer risk stratification (Reijnen et al., 2020). However, even minor structural or parametric changes may invalidate prior certification and necessitate revalidation.

Safe inverse marginalization (SIM) (Kwisthout and Renooij, 2025) augments a Bayesian network with a new variable and additional edges such that marginalizing the added variable exactly recovers the original model. This allows new components to be introduced while preserving both the conditional independencies and the CPTs of the original network, limiting validation effort to the augmented portion. Graph-safe marginalization (GSM) captures when marginalizing the added variable preserves the graphical factorization of the original network. Constraints on the new CPTs, together with optimization techniques for obtaining suitable parameters, were proposed in (Kwisthout and Renooij, 2025).

We first relate GSM to arc-reversal (AR) (Olmsted, 1983; Shachter, 1986), a well-known exact inference algorithm that produces a valid Bayesian network factorization of the marginal distribution. Specifically, we show that the sufficient conditions for GSM in Proposition 2 imply arc-reversal without fill-in (AR-NFI). We further demonstrate that AR-NFI can hold when these sufficient conditions do not, establishing that AR-NFI defines a strictly larger class of structure-preserving augmentations than that characterization. Importantly, even when AR-NFI holds, AR guarantees only a valid factorization of the marginal distribution according to the original DAG and does not by itself recover the original CPT parameterization.

We then introduce unity-potential expansion (UPE), a closed-form, optimization-free construction of augmented CPTs. Existing CPTs are extended by multiplying them with unity potentials over newly introduced parents, while the CPT of the added variable is specified independently of the existing CPTs. UPE guarantees that marginalizing the added variable exactly recovers both the original joint distribution and its CPT parameterization. Consequently, AR-NFI together with UPE provides a concrete structural route to SIM. More fundamentally, UPE reconstructs the original Bayesian network exactly from its factorization, from which the original DAG is uniquely identified. Hence, UPE alone guarantees SIM, establishing that neither GSM nor AR-NFI is necessary. Taken together, these results show that SIM is fundamentally a parametric property, with structural conditions characterizing only when recovery can be realized via structure-preserving transformations.

2. Background

We review Bayesian networks, graph-safe marginalization (GSM), safe inverse marginalization (SIM), and arc-reversal (AR), distinguishing between structural properties of the graph and parametric properties of the associated conditional probability tables (CPTs).

Let $\boldsymbol{V}$ be a set of discrete random variables with joint distribution P. Uppercase letters (e.g., V, X, C, Y) denote variables, lowercase letters denote their assignments, and boldface denotes sets of variables and their joint assignments. For a variable V, let $\Omega(V)$ denote its domain, extended to sets in the standard way.

A Bayesian network $\mathcal{B} = (G, P)$ over variables $\boldsymbol{V}$ consists of a directed acyclic graph (DAG) $G = (\boldsymbol{V}, \boldsymbol{A})$ with arcs $\boldsymbol{A}$ together with a conditional probability table (CPT) $P(V_i \mid \pi_G(V_i))$ for each node V_i, where $\pi_G(V_i)$ denotes its parents. The network encodes the

factorization

$$P(\boldsymbol{V}) = \prod_i P(V_i \mid \pi_G(V_i)).$$

In particular, the factorization together with its specified CPT scopes uniquely determines the represented DAG G, since each parent set $\pi_G(V_i)$ is specified in its CPT.

A topological ordering is an ordering $\prec$ of the variables in a Bayesian network $\mathcal{B}$ such that for every arc (V_i, V_j) in $\mathcal{B}$, we have $V_i \prec V_j$. In this paper, we assume a fixed topological ordering $\prec$, which is used to order the children of an eliminated variable during AR and thereby ensure that each arc reversal is admissible.

A unity potential over a set $\boldsymbol{U}$, denoted $1(\boldsymbol{U})$, satisfies $1(\boldsymbol{u}) = 1$ for all assignments $\boldsymbol{u}$. In particular, $1(\emptyset) = 1$.

Graph-safe marginalization (GSM) is a structural property of a DAG that characterizes when marginalization preserves the graphical factorization. We write $G \setminus \{X\}$ for the induced subgraph obtained by removing node X and all edges incident to it.

Definition 1 (Kwisthout and Renooij, 2025) *Marginalization of X from a DAG G' is* graph-safe *if the marginal distribution $\sum_X P'$ factorizes according to the DAG $G = G' \setminus \{X\}$.*

In general, marginal distributions of DAG models need not themselves be representable by DAGs. Evans (2016) characterizes such marginal models using marginal DAGs (mDAGs), a richer class of graphical structures. Here, we focus on conditions under which marginalization preserves a prescribed DAG factorization.

We use the following sufficient structural conditions for graph-safeness.

Proposition 2 (Kwisthout and Renooij, 2025) *Let X be a node in DAG G' such that:*

(1) X and its children appear consecutively in some topological order, and

(2) for each child C_i,

$$\big(\pi_{G'}(X) \cup \boldsymbol{C}_{\prec i} \cup \pi_{G'}(\boldsymbol{C}_{\prec i})\big) \subseteq \pi_{G'}(C_i),$$

where $\boldsymbol{C}_{\prec i}$ are the children preceding C_i, then marginalizing X from G' is graph-safe.

Two additional propositions providing other sufficient structural conditions for GSM are given in (Kwisthout and Renooij, 2025). Throughout this paper, we focus on the conditions in Proposition 2.

Example 1 shows how graph-safeness under these conditions is established in (Kwisthout and Renooij, 2025) via variable elimination, chain-rule factorization, and removal of superfluous edges using conditional independence relations. We later show that these conditions can be more naturally understood in terms of arc-reversal.

Example 1 *Marginalization of variable X from the Bayesian network in Figure 1 (left), where V_i is depicted as i for brevity, is graph-safe, since*

$$\begin{aligned} &P(V_7, V_8 \mid V_2, V_3, V_5, V_6) \\ &= \sum_X P(X \mid V_2, V_3) P(V_7 \mid V_2, V_3, V_5, X) P(V_8 \mid V_2, V_3, V_5, V_6, V_7, X). \end{aligned}$$

Factorizing $P(V_7, V_8 \mid V_2, V_3, V_5, V_6)$ *into singleton CPTs by the chain rule following* $\prec$ *yields*

$$P(V_7, V_8 \mid V_2, V_3, V_5, V_6) = P(V_7 \mid V_2, V_3, V_5, V_6)P(V_8 \mid V_2, V_3, V_5, V_6, V_7),$$

as shown in Figure 1 (middle). Lastly, edge (V_6, V_7) *is deleted giving Figure 1 (right), since* V_7 *is conditionally independent of* V_6 *given* $\{V_2, V_3, V_5\}$ *in Figure 1 (left).*

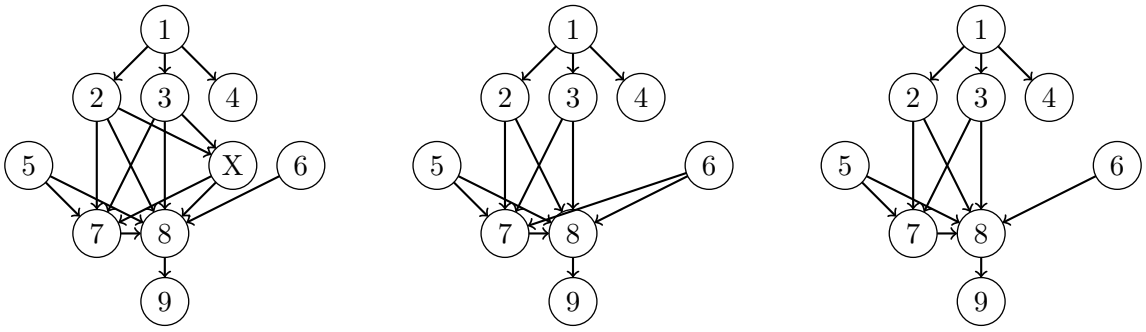


Figure 1: Under the conditions of Proposition 2, graph-safeness is established via variable elimination, refactorization, and removal of superfluous edges.

Concerning the full Bayesian network, we now define safe inverse marginalization (SIM).

Definition 3 *Let* $\mathcal{B} = (G, P)$ *be a Bayesian network over* $\boldsymbol{V}$*, and let* $\mathcal{B}' = (G', P')$ *be an augmentation obtained by adding a variable* X*. We say that inverse marginalization with respect to* X *is* safe *if*

$$\sum_X P'(\boldsymbol{V}, X) = P(\boldsymbol{V}),$$

and the resulting distribution factorizes over G *with identical CPTs as* P*.*

Our formulation differs from (Kwisthout and Renooij, 2025), which separates inverse marginalization and graph-safeness. Here, we combine them into a single definition and make recovery of the original CPT parameterization explicit, emphasizing that SIM is a parametric property.

Arc-reversal (AR) (Olmsted, 1983; Shachter, 1986) eliminates a variable X while maintaining a valid Bayesian network factorization of the marginal distribution. Although termed "arc-reversal," AR may introduce additional edges (fill-in). To avoid cycles during successive eliminations, added edges are oriented according to a fixed topological order $\prec$ of the network. While AR guarantees a valid factorization of the marginal distribution, it does not in general recover the original CPT parameterization.

AR eliminates a variable X with k children by reversing the arcs (X, C_i) for each child C_i, where $i = 1, \ldots, k$, updating CPTs along the way, and finally removing X and its incident edges. Let (X, C_i) be an arc such that there is no other directed path from X to

C_i. Reversing a single arc (X, C_i) proceeds via:

$$P(C_i \mid \pi(X) \cup \pi(C_i) \setminus \{X\}) = \sum_X P(X \mid \pi(X)) P(C_i \mid \pi(C_i)), \tag{1}$$

$$P(X \mid \pi(X) \cup \{C_i\} \cup \pi(C_i) \setminus \{X\}) = \frac{P(X \mid \pi(X)) P(C_i \mid \pi(C_i))}{P(C_i \mid \pi(X) \cup \pi(C_i) \setminus \{X\})}. \tag{2}$$

3. Arc-Reversal and Graph-Safe Marginalization

We relate graph-safe marginalization to arc-reversal from a graphical perspective by comparing GSM with arc-reversal without fill-in (AR-NFI).

Definition 4 *Let X be a node in a DAG G'. Arc-reversal eliminates X with no fill-in (AR-NFI) if eliminating X by arc-reversal yields exactly the induced subgraph $G' \setminus \{X\}$.*

We show that GSM as characterized by Proposition 2 implies AR-NFI.

Lemma 5 *Let X be a node in a DAG G' satisfying the conditions of Proposition 2. Then eliminating X by AR introduces no fill-in edges.*

Proof Let $C_1 \prec \cdots \prec C_k$ be an ordering of the children $\sigma_{G'}(X) = \{C_1, \ldots, C_k\}$ of X in G' with respect to a topological order $\prec_{G'}$ satisfying Proposition 2.

Define

$$F_X = \{X\} \cup \pi_{G'}(X),$$

and

$$F_j = \{C_j\} \cup \pi_{G'}(C_j).$$

By standard arc-reversal parent propagation, after reversing $(X, C_1), \ldots, (X, C_k)$, the resulting parent set of C_i, denoted $\pi_{\mathrm{AR}}(C_i)$, is

$$\pi_{\mathrm{AR}}(C_i) = \big(F_X \cup F_1 \cup \cdots \cup F_{i-1} \cup \pi_{G'}(C_i)\big) \setminus \{X\}, \tag{3}$$

for $i = 1, \ldots, k$. That is, the resulting parent sets are

$$\begin{aligned}
\pi_{\mathrm{AR}}(C_1) &= \big(F_X \cup \pi_{G'}(C_1)\big) \setminus \{X\}, \\
\pi_{\mathrm{AR}}(C_2) &= \big(F_X \cup F_1 \cup \pi_{G'}(C_2)\big) \setminus \{X\}, \\
\pi_{\mathrm{AR}}(C_3) &= \big(F_X \cup F_1 \cup F_2 \cup \pi_{G'}(C_3)\big) \setminus \{X\}, \\
&\vdots \\
\pi_{\mathrm{AR}}(C_k) &= \big(F_X \cup F_1 \cup \cdots \cup F_{k-1} \cup \pi_{G'}(C_k)\big) \setminus \{X\}.
\end{aligned}$$

By Condition (2) of Proposition 2, $\pi_{G'}(X)$, the preceding children $C_1, \ldots, C_{i-1}$, and all of their parents are already contained in $\pi_{G'}(C_i)$. Hence each union in (3) adds no new variables, so

$$\pi_{\mathrm{AR}}(C_i) = \pi_{G'}(C_i) \setminus \{X\}$$

for every i. Therefore, arc-reversal introduces no new parents for any child and hence no fill-in edges. ■

Lemma 5 shows that the sufficient conditions for GSM in Proposition 2 imply AR-NFI. In these cases, elimination of X via AR reduces to the deletion of node X and its incident edges. Importantly, AR-NFI does not imply that the sufficient conditions in Proposition 2 hold, as the next example demonstrates.

Example 2 *Consider a DAG G on variables $\{C_1, Y, C_2\}$ as depicted in Figure 2 (a). Let G' be the augmentation obtained by adding a new variable X as illustrated in Figure 2 (b), where X has children C_1 and C_2. In G', any topological ordering must satisfy $C_1 \prec Y \prec C_2$. Hence, the children of X cannot appear consecutively in any topological order, violating Condition (1) of Proposition 2. Therefore, the sufficient conditions for GSM in Proposition 2 are not satisfied when marginalizing X from G'. Nevertheless, it can be verified that eliminating X using arc-reversal yields $G' \setminus \{X\} = G$, so AR-NFI holds.*

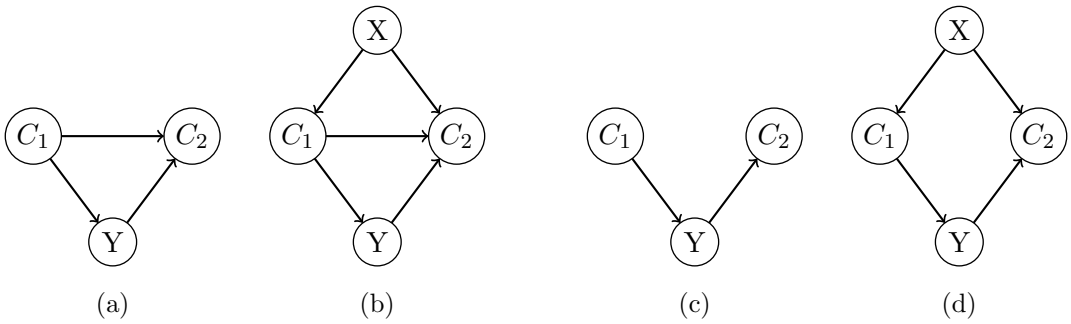


Figure 2: Augmenting the original DAG G (a) with a new variable X, yielding G' (b). AR-NFI of X from G' yields back G, yet the sufficient conditions for GSM in Proposition 2 are not satisfied. Augmenting the original BN G (c) with a new variable X, yielding G' (d), with new CPTs built by Algorithm 1. Marginalization of X from G' is safe and yields back G, yet AR-NFI is not satisfied in G' as arc (C_1, C_2) would be added.

We conclude that AR-NFI defines a strictly larger class of structure-preserving augmentations than the sufficient conditions for GSM in Proposition 2. In the next section, we extend our discussion to recovering both the original DAG and the original CPTs.

4. Unity-Potential Expansion for Safe Inverse Marginalization

When augmentation is restricted to a single variable and its incident edges, we present a direct, closed-form CPT construction method that achieves safe inverse marginalization.

We refer to the following construction as *unity-potential expansion* (UPE). UPE provides a simple closed-form construction that guarantees safe inverse marginalization; it is not intended to characterize all possible constructions. Existing CPTs are extended by multiplying them with unity potentials over newly introduced parents, while the CPT of the added variable is specified independently. Formally, let G be the original BN and G'

its augmentation by a variable X and edges incident only to X. Choose any prior $P'(X)$. Define the new CPT for X in G' as

$$P'(X \mid \pi_{G'}(X)) \;=\; P'(X)\, 1(\pi_{G'}(X))$$

and for each variable W in G, define

$$P'(W \mid \pi_{G'}(W)) \;=\; P\big(W \mid \pi_G(W)\big)\, 1\big(\pi_{G'}(W) \setminus \pi_G(W)\big).$$

We first show that this expansion yields valid CPTs.

Theorem 6 *Let $P(V \mid \boldsymbol{Z})$ be a CPT and let $\boldsymbol{U}$ be disjoint from $\{V\} \cup \boldsymbol{Z}$. Then*

$$\phi(V \mid \boldsymbol{Z}, \boldsymbol{U}) = P(V \mid \boldsymbol{Z})\, 1(\boldsymbol{U})$$

is a valid CPT over V given $\boldsymbol{Z} \cup \boldsymbol{U}$.

Proof For each assignment $(\boldsymbol{z}, \boldsymbol{u})$,

$$\sum_V \phi(V \mid \boldsymbol{z}, \boldsymbol{u}) = \sum_V P(V \mid \boldsymbol{z}) = 1.$$

■

We now illustrate UPE implies SIM in the structural regime where AR-NFI holds.

Example 3 *Let G be a BN on variables $\{C_1, Y, C_2\}$ as illustrated in Figure 2 (a), and let G' be the augmentation obtained by adding a new variable X as in Figure 2 (b). Construct the CPTs in G' using UPE by choosing any prior $P'(X)$ and defining*

$$\begin{aligned} P'(C_1 \mid X) &= P(C_1)\, 1(X), \\ P'(Y \mid C_1) &= P(Y \mid C_1), \\ P'(C_2 \mid C_1, Y, X) &= P(C_2 \mid C_1, Y)\, 1(X). \end{aligned}$$

Since AR-NFI holds, elimination of X proceeds by reversing (X, C_1) and (X, C_2) without introducing fill-in.

Reversing (X, C_1) yields

$$\begin{aligned} P_{\text{new}}(C_1) &= \sum_X P'(X)\, P'(C_1 \mid X) \\ &= \sum_X P'(X)\, P(C_1)\, 1(X) \\ &= P(C_1), \end{aligned}$$

and

$$\begin{aligned} P_{\text{new}}(X \mid C_1) &= \frac{P'(X)\, P'(C_1 \mid X)}{P_{\text{new}}(C_1)} \\ &= \frac{P'(X)\, P(C_1)\, 1(X)}{P(C_1)} \\ &= P'(X). \end{aligned}$$

Reversing (X, C_2) *then yields*

$$\begin{aligned} P_{\text{new}}(C_2 \mid C_1, Y) &= \sum_X P_{\text{new}}(X \mid C_1)\, P'(C_2 \mid C_1, Y, X) \\ &= \sum_X P'(X)\, P(C_2 \mid C_1, Y)\, 1(X) \\ &= P(C_2 \mid C_1, Y). \end{aligned}$$

Thus, the original CPTs $P(C_1)$, $P(Y \mid C_1)$, *and* $P(C_2 \mid C_1, Y)$ *are recovered, and removing* X *and its incident edges yields the original DAG* G.

Example 3 shows that UPE integrates naturally with AR-NFI. Let us first formalize UPE in Algorithm 1.

Algorithm 1: Unity-potential expansion (UPE) for safe inverse marginalization

Input: Original BN $\mathcal{B} = (G, P)$ and augmented graph G' with new variable X
Output: Augmented BN $\mathcal{B}' = (G', P')$

Choose any prior $P'(X)$
$P'(X \mid \pi_{G'}(X)) \leftarrow P'(X)\, \mathbf{1}(\pi_{G'}(X))$
for *each variable* $W \in G$ **do**
  Let $U \leftarrow \pi_{G'}(W) \setminus \pi_G(W)$
  $P'(W \mid \pi_{G'}(W)) \leftarrow P(W \mid \pi_G(W))\, \mathbf{1}(U)$
end

We now show that UPE alone suffices to guarantee SIM.

Theorem 7 *Let* $\mathcal{B} = (G, P)$ *be a Bayesian network over variables* $\boldsymbol{V}$, *and let* G' *be any augmentation obtained by adding a single variable* X *with edges incident only to* X. *Construct* $\mathcal{B}' = (G', P')$ *using Algorithm 1. Then*

$$\sum_X P'(\boldsymbol{V}, X) = P(\boldsymbol{V}),$$

and the resulting distribution factorizes over G *with identical CPTs as* P.

Proof For each original node V, the constructed CPT has the form

$$P'(V \mid \pi_{G'}(V)) = P(V \mid \pi_G(V))\, 1(U),$$

where U contains any newly added parents. Since unity potentials evaluate to 1, they do not affect the product of factors.

For the added variable X, we have

$$P'(X \mid \pi_{G'}(X)) = P'(X)\, 1(\pi_{G'}(X)),$$

so

$$\sum_X P'(X \mid \pi_{G'}(X)) = 1.$$

Thus, when forming the joint and summing over X, all factors involving X cancel, yielding $P(\boldsymbol{V}) = \prod_{V_i \in \boldsymbol{V}} P(V_i \mid \pi_G(V_i))$. ■

Theorem 7 establishes a universal existence result. For any Bayesian network and any augmentation obtained by adding a single variable with edges incident only to it, UPE provides a construction achieving SIM. Unlike arc reversal alone, this construction guarantees recovery of the original CPT parameterization. The proof establishes existence; other constructions satisfying the same marginalization constraints may also be possible. We illustrate UPE by directly marginalizing X from the augmented model, rather than applying arc-reversal equations.

Example 4 *Consider the BN G in Figure 1 (right), and let G' be an augmentation introducing X in Figure 1 (left). Let $P'(X)$ be any prior. Then*

$$P'(X \mid V_2, V_3) = P'(X)\, 1(V_2, V_3),$$

and the child CPTs are

$$P'(V_7 \mid V_2, V_3, V_5, X) = P(V_7 \mid V_2, V_3, V_5)\, 1(X),$$
$$P'(V_8 \mid V_2, V_3, V_5, V_6, V_7, X) = P(V_8 \mid V_2, V_3, V_5, V_6, V_7)\, 1(X).$$

Marginalizing X by variable elimination yields

$$\begin{aligned}
&\sum_X P'(X \mid V_2, V_3)\, P'(V_7 \mid V_2, V_3, V_5, X)\, P'(V_8 \mid V_2, V_3, V_5, V_6, V_7, X) \\
&= \sum_X P'(X)\, 1(V_2, V_3)\, P(V_7 \mid V_2, V_3, V_5)\, 1(X)\, P(V_8 \mid V_2, V_3, V_5, V_6, V_7)\, 1(X) \\
&= P(V_7 \mid V_2, V_3, V_5)\, P(V_8 \mid V_2, V_3, V_5, V_6, V_7) \sum_X P'(X) \\
&= P(V_7 \mid V_2, V_3, V_5)\, P(V_8 \mid V_2, V_3, V_5, V_6, V_7),
\end{aligned}$$

recovering the original CPT factors exactly.

5. Safe Inverse Marginalization Beyond Arc-Reversal with No Fill-in

We now show that safe inverse marginalization extends beyond arc-reversal with no fill-in (AR-NFI). Specifically, some augmentations violate the structural conditions for AR-NFI yet still exactly recover the original Bayesian network under marginalization.

Example 5 *Let G be a BN on variables $\{C_1, Y, C_2\}$ as illustrated in Figure 2 (c). Let G' be the augmentation obtained by adding a new variable X as illustrated in Figure 2 (d), where new CPTs are built using UPE in Algorithm 1. That is, $P'(X)$ is any valid prior and Algorithm 1 constructs augmented CPTs using unity-potential expansion:*

$$P'(C_1 \mid X) = P(C_1)\, 1(X),$$
$$P'(Y \mid C_1) = P(Y \mid C_1),$$
$$P'(C_2 \mid X, Y) = P(C_2 \mid Y)\, 1(X).$$

Now, marginalizing X yields

$$\begin{aligned}
&\sum_X P'(X)\, P'(C_1 \mid X)\, P'(Y \mid C_1)\, P'(C_2 \mid X, Y) \\
&= \sum_X P'(X)\, P(C_1)\, 1(X)\, P(Y \mid C_1)\, P(C_2 \mid Y)\, 1(X) \\
&= P(C_1)\, P(Y \mid C_1)\, P(C_2 \mid Y) \sum_X P'(X) \\
&= P(C_1)\, P(Y \mid C_1)\, P(C_2 \mid Y),
\end{aligned}$$

recovering the original factorization exactly. Since the factorization uniquely determines the parent sets, the original DAG G is recovered.

Two remarks concerning Example 5 are warranted. First, eliminating X by AR from the augmented BN G' in Figure 2 (d) introduces the fill-in edge (C_1, C_2), so AR-NFI does not hold. Nevertheless, the augmented CPTs constructed via UPE ensure that the contribution of X cancels exactly under marginalization, yielding the original factorization and hence the original DAG. This shows that AR-NFI is not necessary for SIM. Moreover, since the recovered marginal distribution factorizes according to G, the example is graph-safe under Definition 1, showing that AR-NFI is not necessary for GSM either.

Second, in the augmented BN G' in Figure 2 (d), C_1 and C_2 are not d-separated given Y. UPE nevertheless defines the expanded CPTs so that, for each value of X, $P'(C_1 \mid X) = P(C_1)$ and $P'(C_2 \mid Y, X) = P(C_2 \mid Y)$. Consequently, C_1 and C_2 remain numerically conditionally independent given Y, allowing the marginal distribution to factorize according to G. This independence need not hold for arbitrary choices of the augmented CPTs.

Since UPE provides an algebraic mechanism that guarantees exact recovery independently of structural constraints, SIM extends strictly beyond the structural regimes captured by the sufficient conditions for GSM in Proposition 2 and by AR-NFI.

6. Algebraic Properties of Unity-Potential Expansion

Given that unity-potential expansion alone suffices to guarantee safe inverse marginalization, it is natural to examine the algebraic properties underlying this construction. In this section, we characterize the key properties that ensure UPE preserves the original CPTs and yields exact recovery under marginalization.

The following propositions isolate the essential algebraic mechanisms of UPE.

Proposition 8 *Let $P(V \mid \boldsymbol{Z})$ be a CPT and let $\boldsymbol{U}$ be disjoint from $\{V\} \cup \boldsymbol{Z}$. Then $P'(V \mid \boldsymbol{Z}, \boldsymbol{U}) = P(V \mid \boldsymbol{Z})\, 1(\boldsymbol{U})$ has scope $\{V\} \cup \boldsymbol{Z} \cup \boldsymbol{U}$, and $P'(V \mid \boldsymbol{z}, \boldsymbol{u}) = P(V \mid \boldsymbol{z})$ for every assignment $(\boldsymbol{z}, \boldsymbol{u})$.*

Proof Since $1(\boldsymbol{U}) = 1$ for all assignments $\boldsymbol{u}$, multiplication by $1(\boldsymbol{U})$ leaves the values of $P(V \mid \boldsymbol{Z})$ unchanged while extending its scope. ■

This strengthens Theorem 6 beyond normalization in that the conditional probabilities are preserved pointwise. Thus, unity-potential expansion acts as a row-replication operator, repeating the same conditional distribution across all assignments of the added variables.

Proposition 9 *Let V be a variable and let $\boldsymbol{Z}$, $\boldsymbol{U}$, and $\boldsymbol{W}$ be pairwise disjoint sets of variables. Let $P'(V \mid \boldsymbol{Z}, \boldsymbol{U}) = P(V \mid \boldsymbol{Z})\,1(\boldsymbol{U})$. Then, for any CPT $P(\boldsymbol{U} \mid \boldsymbol{W})$, $\sum_{\boldsymbol{U}} P'(V \mid \boldsymbol{Z}, \boldsymbol{U})\,P(\boldsymbol{U} \mid \boldsymbol{W}) = P(V \mid \boldsymbol{Z})$.*

This property explains why added variables cancel under marginalization, since unity potentials can be multiplied into CPTs without altering their pointwise values.

Proposition 10 *Let V be a variable and let $\boldsymbol{Z}$ and $\boldsymbol{U} = \{U_1, \ldots, U_k\}$ be disjoint sets of variables. Then $P(V \mid \boldsymbol{Z})\,1(U_1) \cdots 1(U_k) = P(V \mid \boldsymbol{Z})\,1(\boldsymbol{U})$.*

Proof Each unity potential equals one, and the product of unity potentials over disjoint variables equals a unity potential over their union. Since multiplication is associative and commutative, the resulting expanded CPT is independent of the order in which the unity potentials are applied. ■

The above propositions show that unity-potential expansion (i) extends CPT scope without altering values (Proposition 8), (ii) preserves conditional distributions when marginalizing (Proposition 9), and (iii) composes under repeated application, with the expanded CPT independent of the order in which unity potentials are applied (Proposition 10).

7. Relation to Prior Work

Safe inverse marginalization was introduced by Kwisthout and Renooij (2025) as a method for extending a Bayesian network while preserving its distribution. Their work proposes graph-safe marginalization (GSM) as sufficient structural conditions under which marginalizing the added variable yields a distribution that factorizes according to the induced subgraph, together with consistency constraints on the extended CPTs.

Our results extend this perspective by showing that the sufficient conditions for GSM in Proposition 2 imply fill-in–free arc-reversal (AR-NFI). Since this implication is strict, AR-NFI defines a broader class of structure-preserving augmentations than those conditions.

Arc-reversal (AR) (Olmsted, 1983; Shachter, 1986) is a standard method for eliminating variables while preserving the marginal distribution. The CPT constraints in prior SIM formulations coincide with those from AR updates. Graph-safeness under the conditions of Proposition 2 was established via variable elimination, chain-rule factorization, and conditional independence arguments, whereas our results show these conditions also guarantee the absence of fill-in under AR. AR guarantees a valid factorization of the marginal distribution but does not in general recover a prescribed CPT parameterization.

Our approach also complements constraint-based CPT construction. Prior work provides constraints on the extended CPTs together with optimization techniques for obtaining suitable parameters (Kwisthout and Renooij, 2025). In contrast, UPE provides a direct, closed-form construction that yields valid CPTs by design, guarantees exact recovery of the original factorization, and eliminates optimization as a means of establishing existence. It can also serve as a starting point for constraint-based refinement when augmented CPTs encoding additional dependencies or other application-specific properties are desired.

Finally, we place these structural conditions within a broader hierarchy. While AR-NFI defines a strictly larger structural regime than the sufficient conditions for GSM in

Proposition 2, SIM is not limited to AR-NFI. Using UPE, we show that exact recovery is possible even when arc-reversal introduces fill-in. Thus, Proposition 2 and AR-NFI characterize structural regimes in which SIM can be realized, but neither is necessary.

Conceptually, UPE introduces *vacuous parent* variables, additional parents that expand CPT scope while replicating the original conditional probabilities over the extended domain. This provides a simple algebraic mechanism for preserving distributions, guarantees exact recovery of the original factorization, and further sharpens the distinction between structural admissibility and parametric realization.

8. Conclusion

Safe inverse marginalization (SIM) augments a Bayesian network with new variables such that marginalization exactly recovers the original network, allowing re-certification to focus on the added variables. Graph-safe marginalization (GSM) was introduced as a sufficient graphical condition supported by constraint-based CPT constructions. We showed that GSM as characterized by Proposition 2 entails no fill-in under arc-reversal (AR-NFI), while Example 2 shows the converse fails, so AR-NFI strictly subsumes this characterization as a sufficient graphical condition for SIM. We then introduced unity-potential expansion (UPE), a closed-form, optimization-free construction extending CPTs via unity potentials (Algorithm 1), with validity established by Theorem 6. Our central result, Theorem 7, shows that UPE guarantees SIM: marginalizing the added variable exactly recovers both the original DAG and CPTs. Thus, AR-NFI together with UPE provides a concrete structural route to SIM, while UPE alone suffices for any single-variable augmentation. Example 5 shows that SIM extends beyond GSM and AR-NFI, establishing that neither is necessary.

Taken together, these results separate the graphical and probabilistic aspects of SIM. AR-NFI characterizes a broader class of structure-preserving eliminations than GSM as characterized by Proposition 2, whereas UPE guarantees exact recovery independently of structural constraints. Unlike the sufficient structural conditions and augmented-CPT constraints of Kwisthout and Renooij (2025), UPE enforces SIM through a parametric construction that renders marginalization invariant. It reconstructs the exact factorization, whose specified CPT scopes uniquely determine the represented DAG, thereby showing that SIM is a parametric property. Although presented for a single node, UPE extends to multiple nodes by composition. While UPE provides a simple constructive existence result guaranteeing SIM, it is not unique. In practice, augmented CPTs encoding additional dependencies while preserving SIM can be obtained using the GSM constraints in (Kwisthout and Renooij, 2025). Characterizing such parameterizations beyond the cases considered by Kwisthout and Renooij remains an important direction for future work.

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