On the Relationship between Sum-Product Networks and Bayesian Networks

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Outline

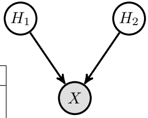
Bayesian Network

Definition

A graphical representation of a set of random variables $\mathbf{X}_{1:N}$ and their conditional dependencies.

- Node corresponds to random variables (observable or latent) and edges represent conditional dependency between pairs of variables.

H_1	$\Pr(H_1)$
0	0.35
1	0.65



H_2	$\Pr(H_2)$
0	0.2
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H_1	H_2	X	$\Pr(X\|H_1, H_2)$
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0	0	1	0.7
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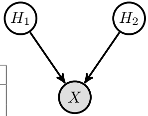

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- A directed acyclic graph (DAG).

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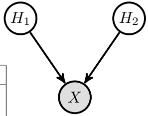

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Bayesian Network

Definition

Local Markov property: each variable is conditionally independent of its non-descendants given its parents.

$$\Pr(\mathbf{X}_{1:N}) = \prod_{i=1}^{N} \Pr(X_i \mid \mathbf{X}_{1:i-1}) = \prod_{i=1}^{N} \Pr(X_i \mid Pa(X_i))$$

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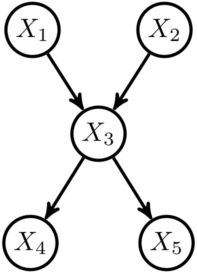
Independence induced by the structure of BN

Bayesian Network

Example

A Bayesian Network over 5 random variables:



$$\Pr(\mathbf{X}_{1:5}) = \Pr(X_5|\mathbf{X}_{1:4}) \Pr(X_4|\mathbf{X}_{1:3}) \Pr(X_3|\mathbf{X}_{1:2}) \Pr(X_2|X_1) \Pr(X_1)$$
$$=$$

Bayesian Network

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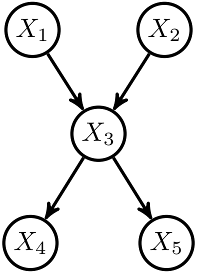

$$\begin{aligned}\Pr(\mathbf{X}_{1:5}) &= \Pr(X_5|\mathbf{X}_{1:4})\Pr(X_4|\mathbf{X}_{1:3})\Pr(X_3|\mathbf{X}_{1:2})\Pr(X_2|X_1)\Pr(X_1)\\ &= \Pr(X_5|X_3)\Pr(X_4|X_3)\Pr(X_3|X_1,X_2)\Pr(X_2)\Pr(X_1)\end{aligned}$$

Bayesian Network

Inference

Joint, marginal and conditional probabilistic query in Bayesian Network. Consider the marginal query $\Pr(X_N = \texttt{True})$

$$\Pr(X_N = \texttt{True}) = \sum_{X_1} \cdots \sum_{X_{N-1}} \Pr(\mathbf{X}_{1:N-1}, X_N = \texttt{True})$$

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$$= \sum_{\mathbf{X}_{1:4}} \Pr(X_5 = \texttt{True} | X_3) \Pr(X_4 | X_3) \Pr(X_3 | X_1, X_2) \Pr(X_2) \Pr(X_1)$$

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$$= \sum_{X_3} \Pr(X_5 = \texttt{True}|X_3) \sum_{X_2} \Pr(X_2) \sum_{X_1} \Pr(X_1) \Pr(X_3|X_1, X_2)$$

$$\sum_{X_4} \Pr(X_4|X_3)$$

Exact inference algorithms for Bayesian Networks:

- **Variable Elimination/Sum-Product algorithm**
- Belief Propagation/Message Passing algorithm

General question:

$$\sum_{\mathbf{X}_H \subseteq \mathbf{X}} \prod_{n=1}^{N} \Pr(X_n \mid Pa(X_n))$$

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1: $\pi \leftarrow$ an ordering of the hidden variables to be eliminated
2: $\Phi \leftarrow \{\mathcal{T}_H \mid H \text{ is a hidden variable}\}$
3: **for** each hidden variable H in π **do**
4: $\quad P \leftarrow \{\mathcal{T}_X \mid \mathcal{T}_X \text{ includes H}\}$
5: $\quad \Phi \leftarrow \Phi \backslash P \cup \{\sum_H \prod_{\mathcal{T} \in P} \mathcal{T}\}$
6: **end for**

Algebraic Decision Diagram

Motivation

How to represent the conditional probability distribution (CPD) associated with each variable in Bayesian Network?

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Tabular representation

A real function over 4 boolean variables

X_1	X_2	X_3	X_4	$f(\cdot)$	X_1	X_2	X_3	X_4	$f(\cdot)$
0	0	0	0	0.4	1	0	0	0	0.4
0	0	0	1	0.6	1	0	0	1	0.6
0	0	1	0	0.3	1	0	1	0	0.3
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Observation: Once $X_1 = 0$, the value of the function is independent of the value taken by X_2.

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Let X, Y and Z be three random variables.

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$$X \perp\!\!\!\perp Y \Rightarrow \forall x, y \quad \Pr(x, y) = \Pr(x)\Pr(y)$$

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$$X \perp\!\!\!\perp Y \mid Z \Rightarrow \forall x, y, z \quad \Pr(x, y|z) = \Pr(x|z) \Pr(y|z)$$

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Context Specific conditional Independence (CSI)

$$X \perp\!\!\!\perp Y \mid Z = z \Rightarrow \exists z \forall x, y \quad \Pr(x, y|z) = \Pr(x|z) \Pr(y|z)$$

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Both independence and conditional independence can be encoded in the structure of Bayesian Network, but CSI cannot.

Algebraic Decision Diagram

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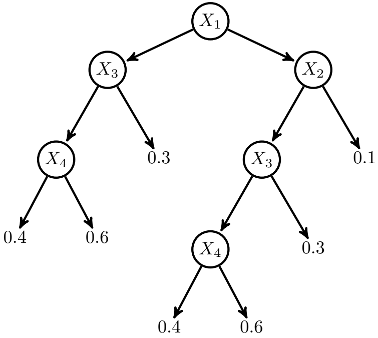
Decision Tree representation

Use decision tree to capture the context specific dependencies



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X_2 does not appear in the left branch of X_1 and X_4 does not appear in the branch when X_3 takes value 1.

Algebraic Decision Diagram

Decision Tree cannot reuse isomorphic sub-graphs

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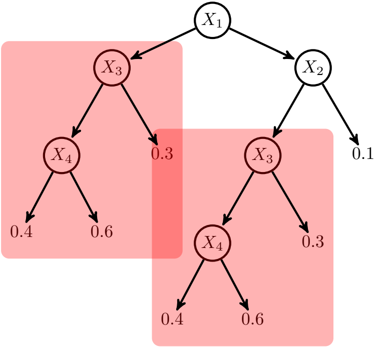
Decision Tree cannot reuse isomorphic sub-graphs



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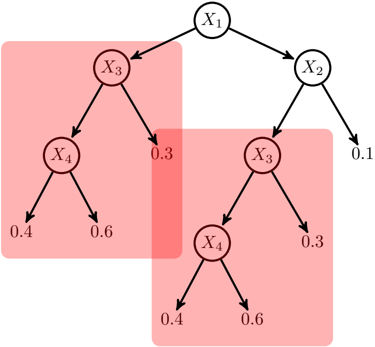

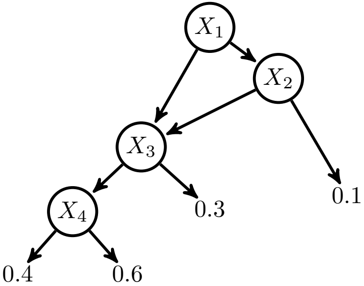

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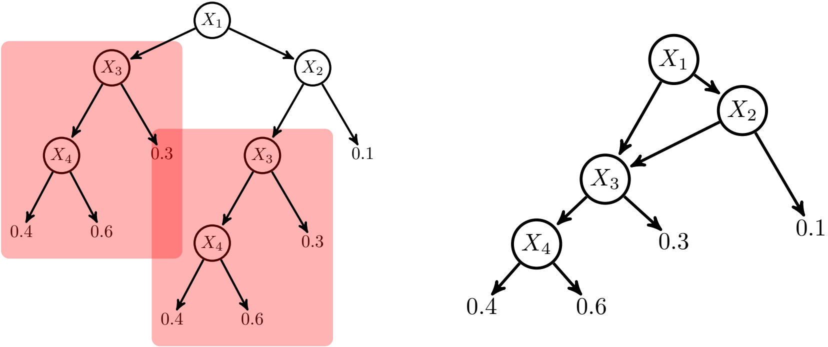


Using directed acyclic graphs instead of trees!

Algebraic Decision Diagram

Discussion

- Algebraic Decision Diagram is a data structure to compactly encode any discrete function with finite support.
- Context Specific Independence (CSI) can be encoded using Algebraic Decision Diagram (better than tabular representation).
- Efficiently avoid the replication problem by reusing isomorphic subgraph (better than decision tree representation).
- We use Algebraic Decision Diagram to encode local CPDs in Bayesian Network.

Sum-Product Network

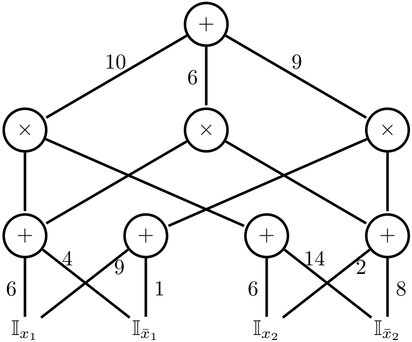
Definition

A Sum-Product Network is a

- Directed acyclic graph of indicator variables, sum nodes and product nodes.
- Each edge emanated from a sum node is associated with a non-negative weight.
- Value of a product node is the product of its children.
- Value of a sum node is the weighted sum of its children.

Sum-Product Network

Example



$f(\mathbb{I}_{x_1}, \mathbb{I}_{\bar{x}_1}, \mathbb{I}_{x_2}, \mathbb{I}_{\bar{x}_2}) = 10(6\mathbb{I}_{x_1} + 4\mathbb{I}_{\bar{x}_1})(6\mathbb{I}_{x_2} + 14\mathbb{I}_{\bar{x}_2}) + 6(6\mathbb{I}_{x_1} + 4\mathbb{I}_{\bar{x}_1})(2\mathbb{I}_{x_2} + 8\mathbb{I}_{\bar{x}_2}) + 9(9\mathbb{I}_{x_1} + \mathbb{I}_{\bar{x}_1})(2\mathbb{I}_{x_2} + 8\mathbb{I}_{\bar{x}_2}) = 594\mathbb{I}_{x_1}\mathbb{I}_{x_2} + 1776\mathbb{I}_{x_1}\mathbb{I}_{\bar{x}_2} + 306\mathbb{I}_{\bar{x}_1}\mathbb{I}_{x_2} + 824\mathbb{I}_{\bar{x}_1}\mathbb{I}_{\bar{x}_2}$

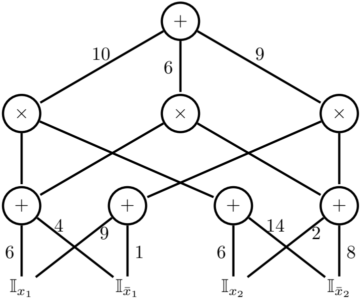
Sum-Product Network

Inference

Joint/Marginal/Conditional queries can be answered in linear time in Sum-Product Network.

Joint Inference

$\Pr(X_1 = 1, X_2 = 0)$?



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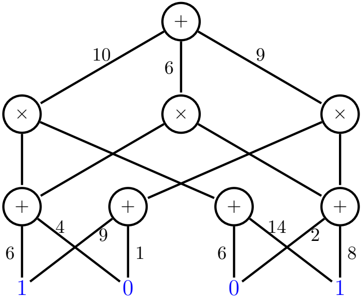

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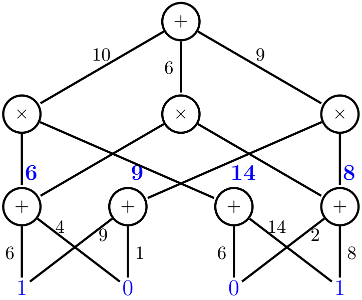

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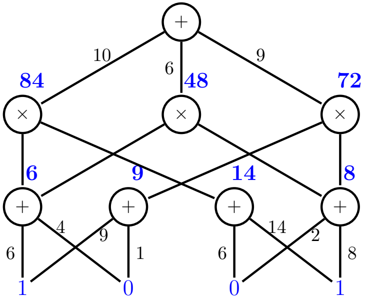

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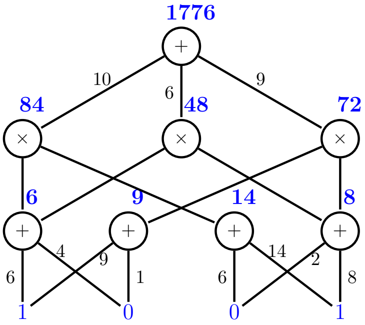

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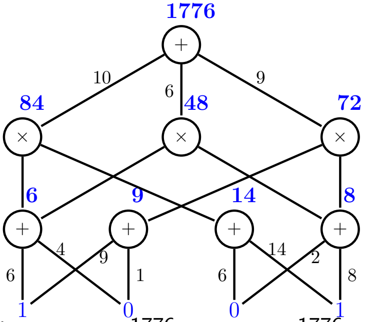

$\Pr(X_1 = 1, X_2 = 0) = \frac{1776}{594+1776+306+824} = \frac{1776}{3500}$

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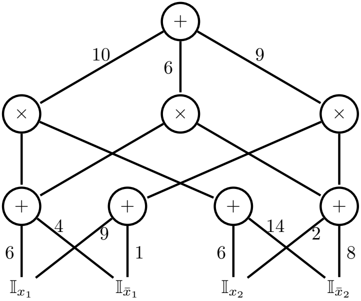
Marginal Inference

$\Pr(X_1 = 1)$?



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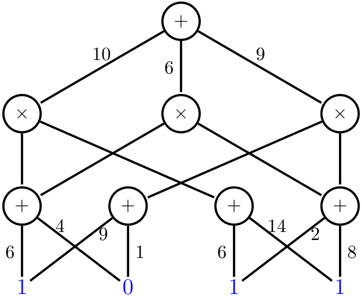

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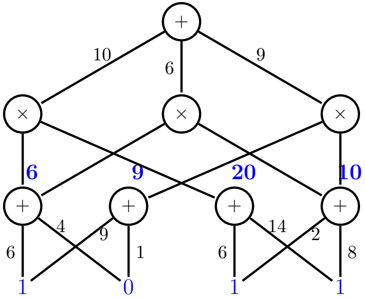

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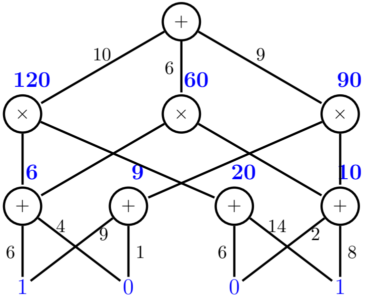

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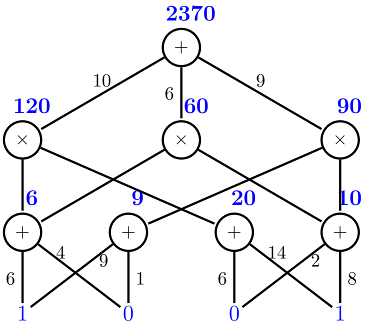

Sum-Product Network

Inference

Joint/Marginal/Conditional queries can be answered in linear time in Sum-Product Network.

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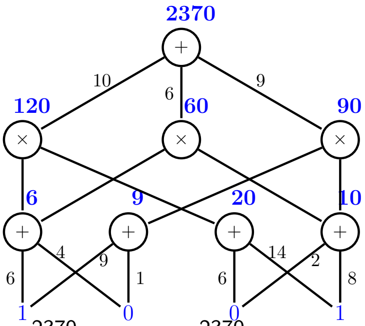

$$\Pr(X_1 = 1) = \frac{2370}{594+1776+306+824} = \frac{2370}{3500}$$

Joint/Marginal/Conditional queries can be answered in linear time in Sum-Product Network.

Conditional Inference

$\Pr(X_2 = 0 | X_1 = 1)$?

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Two passes through the Sum-Product Network, one to compute $\Pr(X_1 = 1, X_2 = 0)$, the other to compute $\Pr(X_1 = 1)$.

Sum-Product Network

Deep Learning Perspective

Deep structure

- Sum node $\Leftrightarrow$ Weighted linear activation function
- Product node $\Leftrightarrow$ Component-wise nonlinear activation function

Sum-Product Network

Definition

Definition (scope)

The *scope* of a node in an SPN is defined as the set of variables that have indicators among the node's descendants: For any node v in an SPN, if v is a terminal node, say, an indicator variable over X, then $\text{scope}(v) = \{X\}$, else $\text{scope}(v) = \bigcup_{\tilde{v} \in Ch(v)} \text{scope}(\tilde{v})$.

Definition (Complete)

An SPN is *complete* iff each sum node has children with the same scope.

Definition (Consistent)

An SPN is consistent iff no variable appears negated in one child of a product node and non-negated in another.

Sum-Product Network

Definition

Definition (Decomposable)

An SPN is decomposable iff for every product node v, $\text{scope}(v_i) \bigcap \text{scope}(v_j) = \varnothing$ where $v_i, v_j \in Ch(v), i \neq j$.

Definition (Valid)

An SPN is said to be *valid* iff it defines a (unnormalized) probability distribution.

Theorem (Poon and Domingos)

If an SPN $\mathcal{S}$ is complete and consistent, then it is valid.

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Valid SPN induces a (unnormalized) probability distribution by the network polynomial defined by the root of the SPN.

Main Theorems

SPN-BN

Let $|\mathcal{S}|$ be the size of the SPN, i.e., the number of nodes plus the number of edges in the graph. For a BN $\mathcal{B}$, the size of $\mathcal{B}$, $|\mathcal{B}|$, is defined by the size of the graph *plus* the size of all the CPDs in $\mathcal{B}$.

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Theorem (SPN-BN)

There exists an algorithm that converts any complete and decomposable SPN $\mathcal{S}$ over Boolean variables $\mathbf{X}_{1:N}$ into a BN $\mathcal{B}$ with CPDs represented by ADDs in time $O(N|\mathcal{S}|)$. Furthermore, $\mathcal{S}$ and $\mathcal{B}$ represent the same distribution and $|\mathcal{B}| = O(N|\mathcal{S}|)$.

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Corollary (SPN-BN)

There exists an algorithm that converts any complete and consistent SPN $\mathcal{S}$ over Boolean variables $\mathbf{X}_{1:N}$ into a BN $\mathcal{B}$ with CPDs represented by ADDs in time $O(N|\mathcal{S}|^2)$. Furthermore, $\mathcal{S}$ and $\mathcal{B}$ represent the same distribution and $|\mathcal{B}| = O(N|\mathcal{S}|^2)$.

Main Theorems

SPN-BN

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Remark

The BN $\mathcal{B}$ generated from $\mathcal{S}$ has a simple bipartite DAG structure, where all the source nodes are hidden variables and the terminal nodes are the Boolean variables $\mathbf{X}_{1:N}$.

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Remark

Assuming sum nodes alternate with product nodes in SPN $\mathcal{S}$, the depth of $\mathcal{S}$ is proportional to the maximum in-degree of the nodes in $\mathcal{B}$, which, as a result, is proportional to a lower bound of the tree-width of $\mathcal{B}$.

Main Theorems

BN-SPN

Theorem (BN-SPN)

Given the BN $\mathcal{B}$ with ADD representation of CPDs generated from a complete and decomposable SPN $\mathcal{S}$ over Boolean variables $\mathbf{X}_{1:N}$, the original SPN $\mathcal{S}$ can be recovered by applying the Variable Elimination algorithm to $\mathcal{B}$ in $O(N|\mathcal{S}|)$.

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Remark

The combination of the above two theorems shows that distributions for which SPNs allow a compact representation and efficient inference, BNs with ADDs also allow a compact representation and efficient inference (i.e., no exponential blow up).

Road Map

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Normal Sum-Product Network

Definition

Definition (Normal Sum-Product Network)

An SPN is said to be normal if

1. It is complete and decomposable.
2. For each sum node in the SPN, the weights of the edges emanating from the sum node are nonnegative and sum to 1.
3. Every terminal node in an SPN is a univariate distribution over a Boolean variable and the size of the scope of a sum node is at least 2 (sum nodes whose scope is of size 1 are reduced into terminal nodes).

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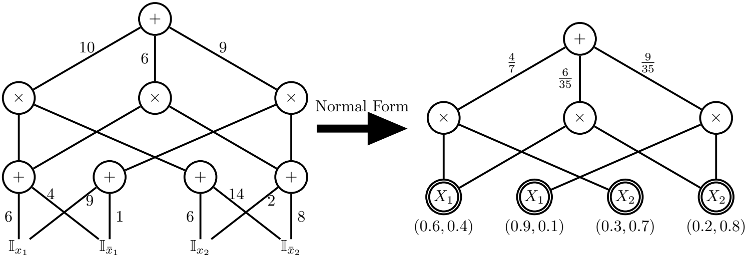
Theorem (Normal Transformation)

For any complete and consistent SPN $\mathcal{S}$, there exists a normal SPN $\mathcal{S}'$ such that $\Pr_{\mathcal{S}}(\cdot) = \Pr_{\mathcal{S}'}(\cdot)$ and $|\mathcal{S}'| = O(|\mathcal{S}|^2)$.

Normal Sum-Product Network

Example



- Each terminal node is a univariate distribution.

Normal Sum-Product Network

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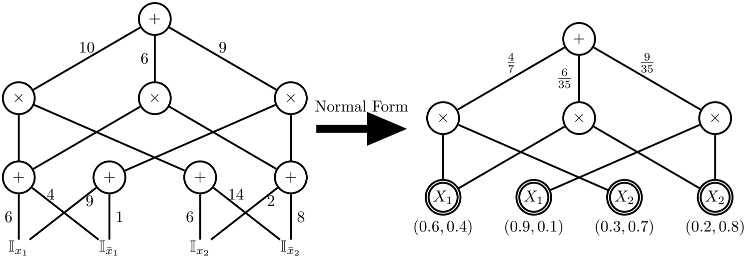

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Normal Sum-Product Network

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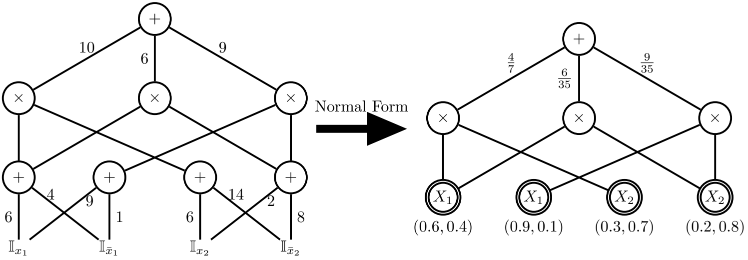

- Each terminal node is a univariate distribution.
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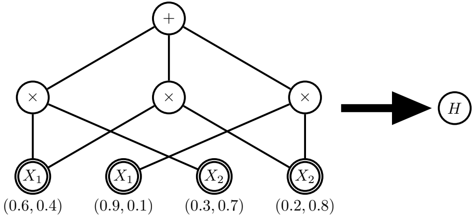
- Each internal product node encodes a rule of context specific independence over its children.

SPN-BN

Structure Construction

Given a normal SPN $\mathcal{S}$ over $\mathbf{X}_{1:N}$, construct:

- A hidden node H_v for each sum node v in $\mathcal{S}$.



SPN-BN

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Given a normal SPN $\mathcal{S}$ over $\mathbf{X}_{1:N}$, construct:

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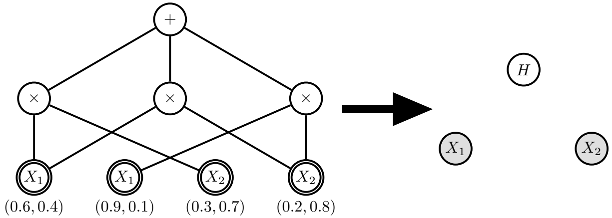

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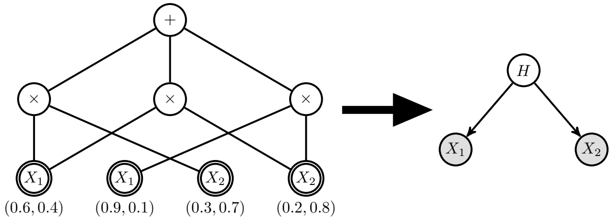

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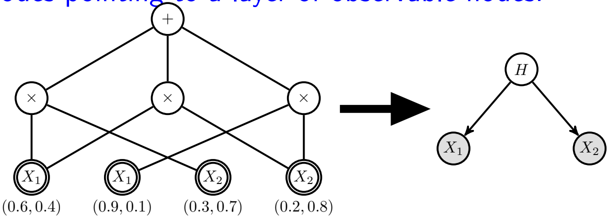
The structure of $\mathcal{B}$ is a directed bipartite graph, with a layer of hidden nodes pointing to a layer of observable nodes.



SPN-BN

CPD Construction

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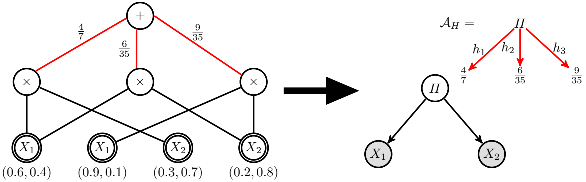

SPN-BN

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Given a normal SPN $\mathcal{S}$ over $\mathbf{X}_{1:N}$, construct:

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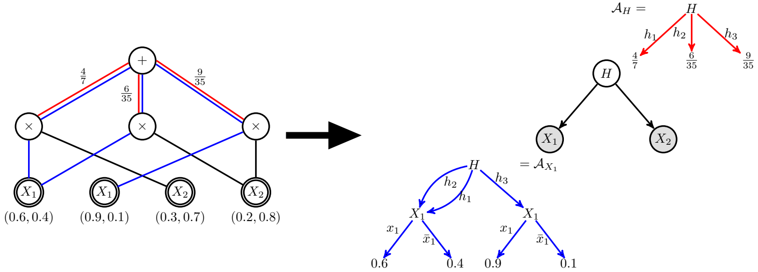

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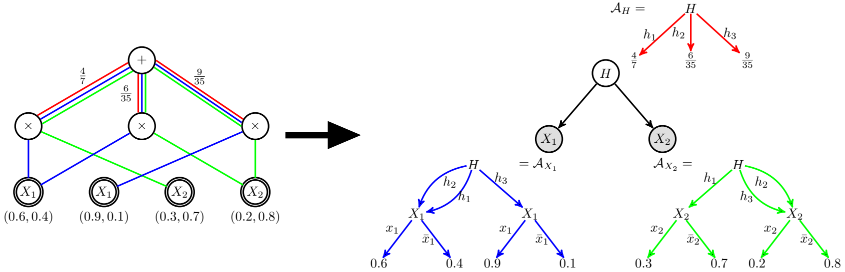

SPN-BN

Theorems

Theorem

For any normal SPN $\mathcal{S}$ *over* $\mathbf{X}_{1:N}$*, the constructed BN* $\mathcal{B}$ *encodes the same probability distribution, i.e.,* $\Pr_{\mathcal{S}}(\mathbf{x}) = \Pr_{\mathcal{B}}(\mathbf{x}), \forall \mathbf{x}$.

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Theorem

$|\mathcal{B}| = O(N|\mathcal{S}|)$*, where BN* $\mathcal{B}$ *is constructed from the normal SPN* $\mathcal{S}$ *over* $\mathbf{X}_{1:N}$.

Extend Algebraic Decision Diagram to *Symbolic* Algebraic Decision Diagram where $+, -, \times, /$ are allowed to be internal nodes.

BN-SPN

Algorithm

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Example

Given symbolic ADDs $\mathcal{A}_{X_1}$ over X_1 and $\mathcal{A}_{X_2}$ over X_2. A symbolic ADD $\mathcal{A}_{X_1,X_2}$ over X_1, X_2 encodes a function over X_1 and X_2 such that $\mathcal{A}_{X_1,X_2}(x_1, x_2) \triangleq (\mathcal{A}_{X_1} \otimes \mathcal{A}_{X_2})(x_1, x_2) = \mathcal{A}_{X_1}(x_1) \times \mathcal{A}_{X_2}(x_2)$.

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Define two operations in symbolic ADD:

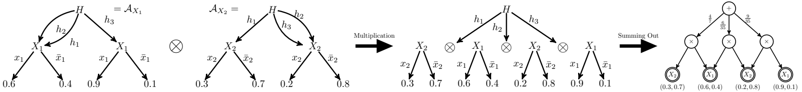
- *Multiplication* between pairs of symbolic ADDs
- *Summing Out* one internal variable in symbolic ADD

BN-SPN

Algorithm

Theorem (SPN-BN)

There exists a variable ordering such that applying Variable Elimination with the ordering to BN with ADDs builds the original SPN $\mathcal{S}$ in $O(N|\mathcal{S}|)$.



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- The depth of SPN is linearly proportional to a lower bound of the tree-width of the BN.
- SPNs can be viewed as hierarchical mixture models with reusability.
- CSI are key to allow linear exact inference on BN with high tree-width.

Thanks

Thanks

Question and Answering

short version: ICML 2015

full version: arXiv:1501.01239