Learning Sum-Product Networks

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Introduction

Definition

Definition 1 (Generalized sum-product network).

A sum-product network (SPN) is a DAG where each node n is either:

1. A tractable univariate probability distribution;
2. A product of SPNs: $v_n = \prod_{j \in \mathrm{Ch}(n)} v_j$; or
3. A weighted sum of SPNs: $v_n = \sum_{j \in \mathrm{Ch}(n)} w_{n,j} v_j$.

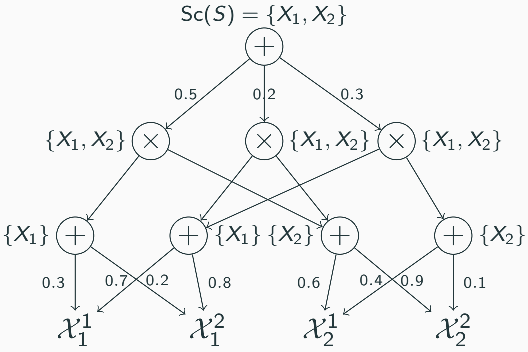
Where v_n is the value of node n, $\mathrm{Ch}(n)$ its set of children and $w_{n,j}$ the weight of edge $n \to j$.

Scope

The scope $\mathrm{Sc}(n)$ of node n is the union of the scope of its children.

The scope of a leaf is the set of all variables in the distribution.

Let S be the root of the SPN below:



Validity

Definition 2 (Validity).

Let S be an SPN. If S correctly computes and marginalizes an unnormalized probability $\phi(\mathbf{X})$, then it is said to be *valid*.

If for every sum node n

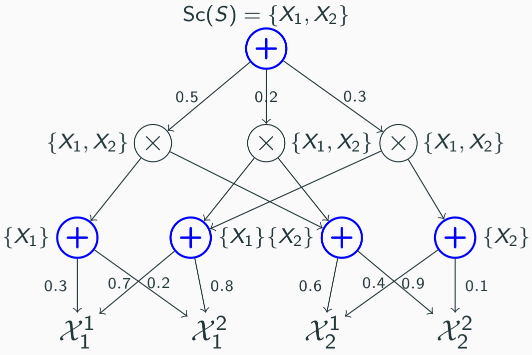
$$\forall j \in \mathrm{Ch}(n), w_{n,j} \geq 0 \text{ and } \sum_{j \in \mathrm{Ch}(n)} w_{n,j} = 1$$

then S represents the probability distribution itself.

A **sufficient**, yet not necessary, condition for validity is *completeness* and *consistency* (Poon and Domingos 2011).

Definition 3 (Completeness).

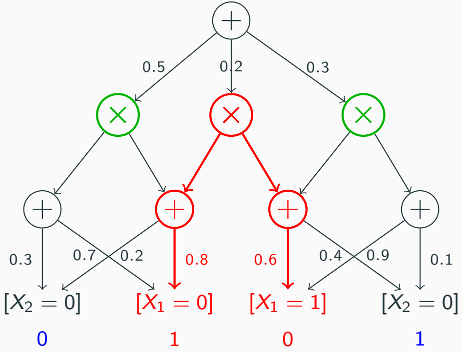
An SPN S is said to be complete, iff for each sum node $s \in S$, all children of s have same scope.



Consistency

Definition 4 (Consistency).

An SPN S is said to be consistent, iff no variable appears with a value v in one child of a product node, and valued u, with $u \neq v$, in another.

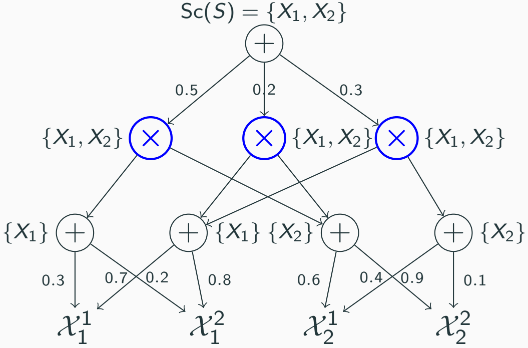


$$X = \{X_1 = 0, X_2 = 1\}$$

Decomposability

Definition 5 (Decomposability).

An SPN is decomposable iff no variable appears in more than one child of a product node (i.e. scopes are disjoint).



Decomposability vs Consistency

Decomposability implies **consistency**.

But **decomposability** is much easier for learning, and allows for an interpretation of product nodes as *independencies* between variables.

Robert Peharz et al. 2015 shows **decomposable** SPNs are as representable as solely **consistent** ones.

Learning

Learning types

Two main types of learning:

Structure learning:

Learn graph structure from data.

Parameter learning:

Learn weights from data given a fixed graph structure.

Both usually attempt to optimize log-likelihood.

Structure learning

- Structure learning:
  1. **Poon-Domingos dense architecture** (Poon and Domingos 2011);
  2. **Gens-Domingos LearnSPN** (Gens and Domingos 2013);
  3. **Dennis-Ventura clustering architecture** (Dennis and Ventura 2012);
  4. **Random Tensorized SPNs (RAT-SPNs)** (R. Peharz et al. 2018);
  5. Indirect-Direct SPNs (ID-SPNs) (Rooshenas and Lowd 2014);
  6. LearnSPN+Chow-Liu Trees (LearnSPN-BTB) (Vergari, Mauro, and Esposito 2015).

Parameter learning

- Parameter learning:
    1. **Generative Gradient Descent** (Poon and Domingos 2011; Darwiche 2003);
    2. **Discriminative Gradient Descent** (Gens and Domingos 2012);
    3. Expectation-Maximization (Poon and Domingos 2011);
    4. Extended Baum-Welch (Rashwan, Poupart, and Zhitang 2018);
    5. Collapsed Variational Inference (Zhao et al. 2016);
    6. Bayesian Moment Matching (Rashwan, Zhao, and Poupart 2016).

Parameter learning

Generative vs Discriminative Gradient Descent

Generative:

- Optimize log-likelihood of $P(X, Y)$
- Gradient: $\frac{\partial}{\partial W} \log P(X, Y)$
- E.g. completion

Discriminative:

- Optimize log-likelihood of $P(Y|X)$
- Gradient: $\frac{\partial}{\partial W} \log P(Y|X)$
- E.g. classification

Generative representation is able to extract its **discriminative**.

$$P(Y|X) = \frac{P(X, Y)}{P(Y)}$$

Derivatives I

Let S be an SPN, and W the set of weights of S. Denote by S_n the sub-SPN rooted at node n.

Objective: find gradient $\frac{\partial}{\partial W} \log S$.

That is, compute each component $\partial S / \partial w_{n,j}$, for each edge $n \to j$.

$$
\begin{aligned}
\frac{\partial S}{\partial w_{n,j}}(X) &= \frac{\partial S}{\partial S_n} \frac{\partial S_n}{\partial w_{n,j}}(X) \\
&= \frac{\partial S}{\partial S_n} \frac{\partial}{\partial w_{n,j}} \left(\sum_{i \in \mathrm{Ch}(n)} w_{n,i} S_i(X) \right) \\
&= \frac{\partial S}{\partial S_n} S_j(X).
\end{aligned}
$$

We now need to find a form for derivative $\frac{\partial S}{\partial S_n}$.

Derivatives II

Let's find the sub-SPN derivative $\frac{\partial S}{\partial S_j}$. From chain rule:

$$\begin{aligned}
\frac{\partial S}{\partial S_j}(X) &= \sum_{n \in \mathrm{Pa}(j)} \frac{\partial S}{\partial S_n}\frac{\partial S_n}{\partial S_j}(X) \\
&= \underbrace{\sum_{\substack{n \in \mathrm{Pa}(j) \\ n\text{: sum}}} \frac{\partial S}{\partial S_n}\frac{\partial S_n}{\partial S_j}(X)}_{(*)} + \underbrace{\sum_{\substack{n \in \mathrm{Pa}(j) \\ n\text{: product}}} \frac{\partial S}{\partial S_n}\frac{\partial S_n}{\partial S_j}(X)}_{(**)}
\end{aligned}$$

Let's analyze two cases: when n is a sum node $(*)$, and when it's a product node $(**)$.

Derivatives III

Case 1: when n is a sum node.

$$
\begin{aligned}
(*) &= \sum_{\substack{n \in \mathrm{Pa}(j) \\ n\text{: sum}}} \frac{\partial S}{\partial S_n} \frac{\partial S_n}{\partial S_j}(X) \\
&= \sum_{\substack{n \in \mathrm{Pa}(j) \\ n\text{: sum}}} \frac{\partial S}{\partial S_n} \frac{\partial}{\partial S_j} \left(\sum_{i \in \mathrm{Ch}(n)} w_{n,i} S_i(X) \right) \\
&= \sum_{\substack{n \in \mathrm{Pa}(j) \\ n\text{: sum}}} \frac{\partial S}{\partial S_n} w_{n,j}
\end{aligned}
$$

Derivatives IV

Case 2: when n is a product node.

$$
\begin{aligned}
(**) &= \sum_{\substack{n \in \mathrm{Pa}(j) \\ n:\ \mathrm{product}}} \frac{\partial S}{\partial S_n} \frac{\partial S_n}{\partial S_j}(X) \\
&= \sum_{\substack{n \in \mathrm{Pa}(j) \\ n:\ \mathrm{product}}} \frac{\partial S}{\partial S_n} \frac{\partial}{\partial S_j} \left(\prod_{i \in \mathrm{Ch}(n)} S_i(X) \right) \\
&= \sum_{\substack{n \in \mathrm{Pa}(j) \\ n:\ \mathrm{product}}} \frac{\partial S}{\partial S_n} \prod_{k \in \mathrm{Ch}(n) \setminus \{j\}} S_k
\end{aligned}
$$

Derivatives V

Going back to our original formula and using the derived forms of $(*)$ and $(**)$:

$$\begin{aligned}\frac{\partial S}{\partial S_j}(X) &= \sum_{\substack{n \in \mathrm{Pa}(j) \\ n:\ \text{sum}}} \frac{\partial S}{\partial S_n} \frac{\partial S_n}{\partial S_j}(X) \quad + \sum_{\substack{n \in \mathrm{Pa}(j) \\ n:\ \text{product}}} \frac{\partial S}{\partial S_n} \frac{\partial S_n}{\partial S_j}(X) \\ &= \sum_{\substack{n \in \mathrm{Pa}(j) \\ n:\ \text{sum}}} \frac{\partial S}{\partial S_n} w_{n,j} \qquad\quad + \sum_{\substack{n \in \mathrm{Pa}(j) \\ n:\ \text{product}}} \frac{\partial S}{\partial S_n} \prod_{k \in \mathrm{Ch}(n) \setminus \{j\}} S_k\end{aligned}$$

Remark: when j is the root node: $\frac{\partial S}{\partial S_j} = \frac{\partial S}{\partial S} = 1$.

The above form lends itself nicely to an algorithmic format.

Algorithm 1 `Backprop`: Backpropagation derivation on SPNs

Input A valid SPN S with pre-computed probabilities $S_n(X)$

Output Partial derivatives of S with respect to every node and weight

1: Initialize $\frac{\partial S}{\partial S_n} = 0$ except $\frac{\partial S}{\partial S} = 1$
2: **for** each node $n \in S$ in top-down order **do**
3:     **if** n is sum node **then**
4:         **for** all $j \in \mathrm{Ch}(n)$ **do**
5:             $\frac{\partial S}{\partial S_j} \leftarrow \frac{\partial S}{\partial S_j} + w_{n,j} \frac{\partial S}{\partial S_n}$
6:             $\frac{\partial S}{\partial w_{n,j}} \leftarrow \frac{\partial S}{\partial S_n} S_j$
7:     **else**
8:         **for** all $j \in \mathrm{Ch}(n)$ **do**
9:             $\frac{\partial S}{\partial S_j} \leftarrow \frac{\partial S}{\partial S_j} + \frac{\partial S}{\partial S_n} \prod_{k \in \mathrm{Ch}(n) \setminus \{j\}} S_k$

Generative gradient descent

Let's go back to our original objective of finding the gradient. For the **generative** (joint distribution) case:

$$\begin{aligned}\frac{\partial}{\partial W}\log P(X,Y) &= \frac{\partial}{\partial W}\log S(X,Y)\\ &= \frac{1}{S(X,Y)}\frac{\partial S}{\partial W}(X,Y) \propto \frac{\partial S}{\partial W}(X,Y)\end{aligned}$$

So it is sufficient to find $\frac{\partial S}{\partial W}$, which we already have. Our weight update is then:

$$\Delta w_{n,j} = \eta\frac{\partial S}{\partial w_{n,j}}(X,Y)$$

Discriminative gradient descent

For the **discriminative** (conditional distribution) case:

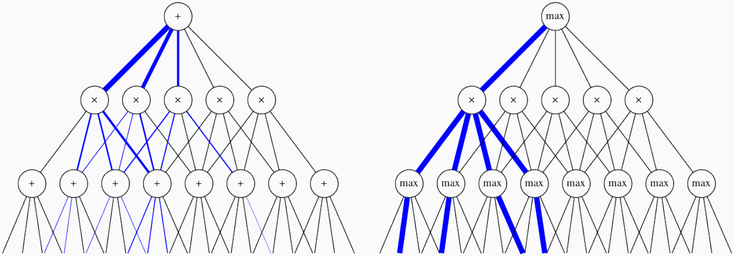
$$\begin{aligned}\frac{\partial}{\partial W}\log P(Y|X) &= \frac{\partial}{\partial W}\log\left(\frac{P(Y,X)}{P(X)}\right)\\ &= \frac{\partial}{\partial W}\log P(Y,X) \quad - \quad \frac{\partial}{\partial W}\log P(X)\\ &= \frac{1}{S(Y,X)}\frac{\partial}{\partial W}S(Y,X) \quad - \quad \frac{1}{S(X)}\frac{\partial}{\partial W}S(X)\end{aligned}$$

Weight updates will take the following form:

$$\Delta w_{n,j} = \eta\left(\frac{1}{S(Y,X)}\frac{\partial S(Y,X)}{\partial w_{n,j}} - \frac{1}{S(X)}\frac{\partial S(X)}{\partial w_{n,j}}\right)$$

Soft vs hard derivation

Results derived in the previous slides are called **soft**. Soft gradient means weight updates are derivatives of network evaluations. The **deeper** the network, the **fainter** the signal.



(a) Soft gradient **(b)** Hard gradient

This is called **gradient diffusion**. A solution to this is **hard** gradient descent.

Hard derivatives I

Let S be an SPN. Instead of $\frac{\partial S}{\partial W}$, we'll derive $\frac{\partial M}{\partial W}$, where M is the Max-Product Network (MPN) of S. M can be extracted from S by replacing sums with max nodes.

Soft:

- $\partial S / \partial W$
- W is the set of weights of S
- Messages are derivatives

Hard:

- $\partial M / \partial W$
- W is the multiset of weights that a forward pass through M visits
- Messages are counts

Hard derivatives II

Objective: find gradient $\frac{\partial M}{\partial W}$

We know that $M(X) = \prod_{w_i \in W} w_i^{c_i}$, where c_i is the number of times w_i appears in W. Let's take the logarithm of M on each component:

$$\frac{\partial \log M}{\partial w_{n,j}}(X) = \frac{\partial}{\partial w_{n,j}} \log \left(\prod_{w_i \in W} w_i^{c_i} \right)$$

$$= \frac{1}{\prod_{w_i \in W} w_i^{c_i}} \cdot c_{n,j} w_{n,j}^{c_{n,j}-1} \cdot \prod_{w_i \in W \setminus \{w_{n,j}\}} w_i^{c_i}$$

$$= c_{n,j} \frac{w_{n,j}^{c_{n,j}-1}}{w_{n,j}^{c_{n,j}}} = \frac{c_{n,j}}{w_{n,j}}$$

Hard generative gradient descent

From our previous result, we know that:

$$\frac{\partial \log M}{\partial w_{n,j}}(X) = \frac{c_{n,j}}{w_{n,j}}$$

But that's exactly the log-likelihood for the generative case! This gives us the following weight update:

$$\Delta w_{n,j} = \eta \frac{c_{n,j}}{w_{n,j}}$$

Note how $c_{n,j}$ is an integer, and $w_{n,j} \in [0, 1]$, meaning the signal passed at learning does not depend on network size or depth, avoiding the problem of gradient diffusion.

Hard discriminative gradient descent I

For the discriminative case we want:

$$\frac{\partial}{\partial W} \log \tilde{P}(Y|X) = \frac{\partial}{\partial W} \log \left(\frac{\tilde{P}(Y,X)}{\tilde{P}(X)} \right) = \frac{\partial}{\partial W} \log \left(\frac{M(Y,X)}{M(X)} \right)$$

Where $\tilde{P}$ is the MAP. Apply chain rule:

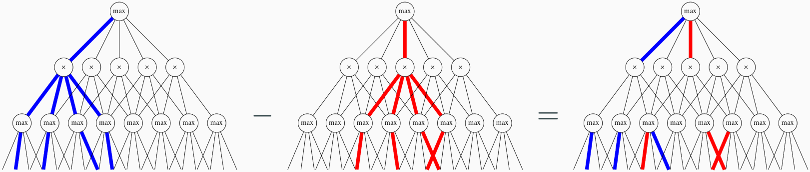
$$\frac{\partial}{\partial W} \log \left(\frac{M(Y,X)}{M(X)} \right) = \frac{\partial}{\partial W} \log M(Y,X) - \frac{\partial}{\partial W} \log M(X)$$

For each component:

$$\begin{aligned}
\frac{\partial}{\partial w_{n,j}} \log \tilde{P}(Y|X) &= \frac{\partial}{\partial w_{n,j}} \log M(Y,X) - \frac{\partial}{\partial w_{n,j}} \log M(X) \\
&= \frac{\partial}{\partial w_{n,j}} c_{n,j} - \frac{\partial}{\partial w_{n,j}} \hat{c}_{n,j} \\
&= \frac{\Delta c_{n,j}}{w_{n,j}}
\end{aligned}$$

Hard discriminative gradient descent II

Visually, $\Delta c_{n,j}$ is the difference between the path of evaluation $M(Y,X)$ and $M(X)$.



$$\frac{\partial}{\partial W}\log M(Y,X) \qquad - \qquad \frac{\partial}{\partial W}\log M(X) \qquad = \qquad \nabla \log \tilde{P}(Y|X)$$

Edges in blue represent positive values, red are negative values and uncolored edges have zero value.

Summary

Generative Gradient Descent

Inference	Weight updates
Soft	$\Delta w_{n,j} = \eta \frac{\partial S}{\partial w_{n,j}}(X, Y)$
Hard	$\Delta w_{n,j} = \eta \frac{c_{n,j}}{w_{n,j}}$

Discriminative Gradient Descent

Inference	Weight updates
Soft	$\Delta w_{n,j} = \eta \left(\frac{1}{S(Y,X)} \frac{\partial S(Y,X)}{\partial w_{n,j}} - \frac{1}{S(X)} \frac{\partial S(X)}{\partial w_{n,j}} \right)$
Hard	$\Delta w_{n,j} = \eta \frac{\Delta c_{n,j}}{w_{n,j}}$

Structure learning

Definition 6 (Dataset).

A dataset is a matrix $D \in M_{m\times n}(\mathbb{Z})$, where **rows** are **instances** and **columns** represent **variables**.

Example 7.

Let D be a 3×2 black and white image dataset, where each pixel can take a value 0 (black) or 1 (white).

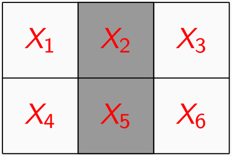
D	X_1	X_2	X_3	X_4	X_5	X_6
I_1	1	0	1	1	0	1
I_2	0	1	0	0	1	0

$\mathbf{X} = \{X_1, \ldots, X_n\}$ is the set of random variables (e.g. pixels) of D.

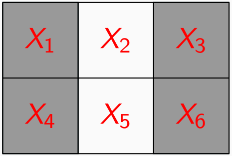
$\mathbf{I} = \{I_1, \ldots, I_m\}$ is the set of instances of D.

Preliminaries II

D	X_1	X_2	X_3	X_4	X_5	X_6
I_1	1	0	1	1	0	1
I_2	0	1	0	0	1	0



I_1



I_2

LearnSPN I

LearnSPN (Gens and Domingos 2013)

The Gens-Domingos LearnSPN schema exploits two SPN properties: **completeness** and **decomposability**.

Completeness:

Interpret sum children as clusters (similar instances).

Decomposability:

Interpret product children as independent sets (disjoint scopes).

Idea:

1. Partition by row through clustering.
2. Partition by column through variable independence tests.
3. Base case: univariate distribution.

LearnSPN II

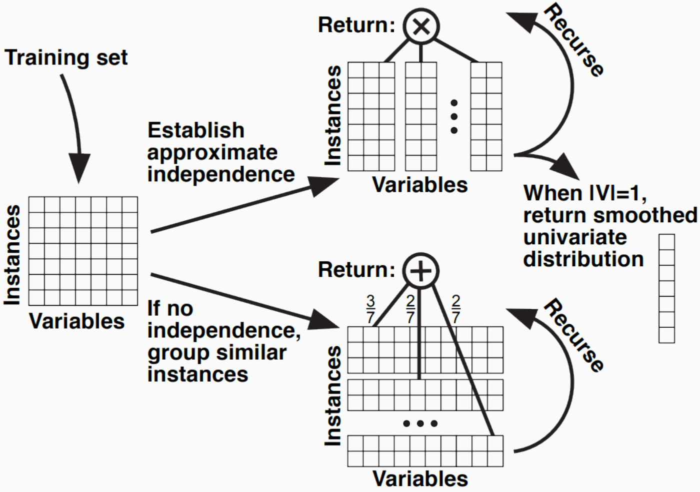
Algorithm 2 `LearnSPN`: Gens-Domingos structure learning schema

Input Set of instances I and scope X

Output SPN structure learned from I and X

if $|X| = 1$ **then**
    return univariate distribution over $I[X]$
Partition X into $P_1, P_2, \ldots, P_m$ st $\forall i, j,\ i \neq j,\ P_i \perp P_j$
if $m > 1$ **then**
    return $\prod_i \texttt{LearnSPN}(D, P_i)$
Cluster I such that $Q_1, Q_2, \ldots, Q_n$ are I's clusters
return $\sum_i \frac{|Q_i|}{|I|} \texttt{LearnSPN}(Q_i, X)$

LearnSPN III



Source: Gens and Domingos 2013

LearnSPN IV

LearnSPN is very flexible and modular.

Clustering:

k-means, k-mode, DBSCAN, ...

Variable independence:

G-test, χ^2 Pearson test, Mutual Information, ...

Univariate distribution:

Multivariate, gaussian, mixture of gaussians, ...

LearnSPN V

Pros:

- Flexible implementation;
- Very deep architecture even with small training size;
- Guarantees completeness and decomposability.

Cons:

- Generates only trees;
- Not as expressive as dense and deep networks;
- Tree-like structure and deepness impact inference speed.

Poon dense architecture I

Poon-Domingos architecture (Poon and Domingos 2011)

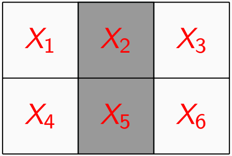
Decompose data into local spatial *neighborhoods*. Call neighborhoods **Regions**, and represent them as sets of sums. **Decomposition** is done with products.

Idea:

1. Define regions as set of sums.
2. Define decompositions of regions as products.
3. Create gaussian mixtures for leaves.
4. Generate dense architecture through decomposition of regions.
5. Learn weights with EM or Gradient Descent (GD).
6. Prune zero weights and redundant sub-SPNs.

Example 8.

In the image domain, regions could be a rectangular set of pixels. Take our previous example.

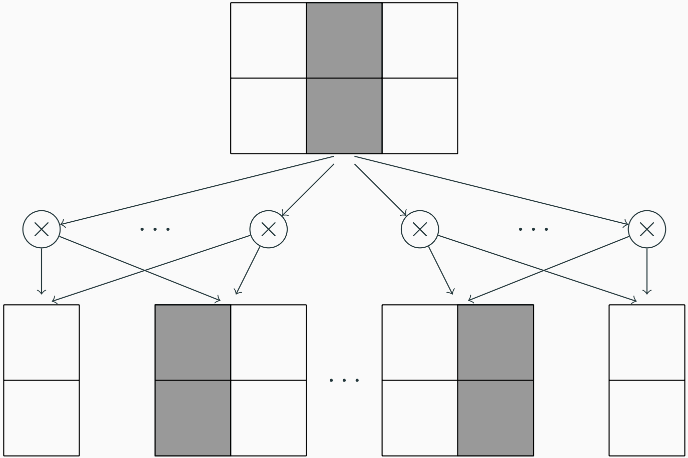


Any rectangular subset of the image is a region. The smallest (e.g. one pixel) regions are called *fine* regions. All others are *coarse* regions. □

Special case: the whole data is a region, represented by a single sum node.

Poon dense architecture III

For each region, find all possible rectangular 2-decompositions (horizontal and vertical) and connect them with m products.



Poon dense architecture IV

Pros:

- Very dense architecture;
- Depth of $2(d-1)$ for $d \times d$ images, though not as deep as LearnSPN;
- Fast to generate dense structure.

Cons:

- Restricted to only local spatial neighborhoods;
- Very short and very long paths from root to a same variable;
- Biased for Viterbi-style inference (e.g. Max-Product for MAP), prefering shorter paths;

Region graphs

Both Dennis-Ventura (DV) and RAT-SPNs use **Region Graphs** to construct an SPN.

Derived from Poon-Domingos' (PD) concept of Region and Decomposition. Introduced by DV.

- **Regions:**
  rectangular spatial neighborhoods vs any neighborhood of variables;
- **Subregions:**
  fixed rectangular decomposition vs any partitioning of the scope;
- **Structure:**
  depth is domain dependent vs depth depends only on data/instances.

Region graph definition

Definition 9 (Region graph).

A region graph G is a rooted DAG with two possible node types: region and partition nodes. The root of G is a region node. Children of region nodes are partition nodes and vice-versa. Scope of G works similarly to complete decomposable SPNs, with region nodes resembling sums and partitions products.

Main ideas:

- Regions act like set of sums;
- Partitions act like set of products;
- Partition nodes partition the parent's scope;
- Regions are the result of this decomposition;
- Region graph is always a tree because of partitioning.

Constructing a region graph

General idea for constructing a region graph:

1. Create a root region from whole data.
2. Partition data k times.
3. Construct partition node for each k split.
4. For each of these k, create two subregions representing split scope as children of corresponding partition node.
5. Recursively repeat until early stop or reach scope of size 1.

Converting a region graph to an SPN

$$
\begin{aligned}
\text{Region node } R \quad &\longrightarrow \quad \begin{cases} m \text{ sum nodes,} & \text{if coarse region;} \\ d \text{ distributions,} & \text{if fine region;} \end{cases} \\
\text{Partition node } P \quad &\longrightarrow \quad m^2 \text{ product nodes}
\end{aligned}
$$

Connect every parent region sum node to every child partition product node. $(R \rightarrow P)$

Connect each partition product node with a distinct pair of children region nodes. $(P \rightarrow R)$

Semantics of a region graph

Thank you.

Questions?

References i

- Darwiche, Adnan (May 2003). “A Differential Approach to Inference in Bayesian Networks”. In: *J. ACM* 50.3, pp. 280–305. ISSN: 0004-5411. DOI: 10.1145/765568.765570. URL: http://doi.acm.org/10.1145/765568.765570.
- Dennis, Aaron and Dan Ventura (2012). “Learning the Architecture of Sum-Product Networks Using Clustering on Variables”. In: *Advances in Neural Information Processing Systems* 25.
- Gens, Robert and Pedro Domingos (2012). “Discriminative Learning of Sum-Product Networks”. In: *Advances in Neural Information Processing Systems 25 (NIPS 2012)*.
- – (2013). “Learning the Structure of Sum-Product Networks”. In: *International Conference on Machine Learning* 30.

- Peharz, R. et al. (2018). "Probabilistic Deep Learning using Random Sum-Product Networks". In: *ArXiv e-prints*.
- Peharz, Robert et al. (2015). "On Theoretical Properties of Sum-Product Networks". In: *International Conference on Artificial Intelligence and Statistics 18 (AISTATS 2015)*.
- Poon, Hoifung and Pedro Domingos (2011). "Sum-Product Networks: A New Deep Architecture". In: *Uncertainty in Artificial Intelligence* 27.

References iii

Rashwan, Abdullah, Pascal Poupart, and Chen Zhitang (2018). "Discriminative Training of Sum-Product Networks by Extended Baum-Welch". In: *Proceedings of the Ninth International Conference on Probabilistic Graphical Models*. Vol. 72. Proceedings of Machine Learning Research, pp. 356–367.

Rashwan, Abdullah, Han Zhao, and Pascal Poupart (Sept. 2016). "Online and Distributed Bayesian Moment Matching for Parameter Learning in Sum-Product Networks". In: *Proceedings of the 19th International Conference on Artificial Intelligence and Statistics*. Ed. by Arthur Gretton and Christian C. Robert. Vol. 51. Proceedings of Machine Learning Research. Cadiz, Spain: PMLR, pp. 1469–1477. URL: http://proceedings.mlr.press/v51/rashwan16.html.

Rooshenas, Amirmohammad and Daniel Lowd (2014). "Learning Sum-Product Networks with Direct and Indirect Variable Interactions". In: *International Conference on Machine Learning 31 (ICML 2014)*.

References v

Vergari, Antonio, Nicola di Mauro, and Floriana Esposito (2015). "Simplifying, Regularizing and Strengthening Sum-Product Network Structure Learning". In: *European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECMLPKDD 2015)*.

Zhao, Han et al. (20–22 Jun 2016). "Collapsed Variational Inference for Sum-Product Networks". In: *Proceedings of The 33rd International Conference on Machine Learning*. Ed. by Maria Florina Balcan and Kilian Q. Weinberger. Vol. 48. Proceedings of Machine Learning Research. New York, New York, USA: PMLR, pp. 1310–1318. URL: http://proceedings.mlr.press/v48/zhaoa16.html.