Bayesian Learning of Sum-Product Networks

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- We introduce a well-principled Bayesian framework for SPN structure learning by decomposing the problem into:
    1. laying out a computational graph, and
    2. learning the so-called scope function over the graph.
- We propose a natural parametrisation for an important and widely used special case of SPNs, incorporate the parameters into a Bayesian model, and perform posterior inference over structure and parameters jointly.

Sum-Product Networks

What is a Sum-Product Network?

- Let $\mathbf{X} = \{X_1, \ldots, X_D\}$ be set of D random variables, for which N i.i.d. samples are available.
- An SPN is a distribution over $\mathbf{X}$ defined as a 4-tuple $\mathcal{S} = (\mathcal{G}, \psi, w, \theta)$.

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  - w denotes the set of sum-weights and θ the set of leaf node parameters.
- Note: This definition is conceptually different to the classic definition of SPNs as it disentangles the definition of the SPNs structure into a computational graph, which has only few requirements, and a scope function, which ensures completeness and decomposability.

Computational Graph $\mathcal{G}$

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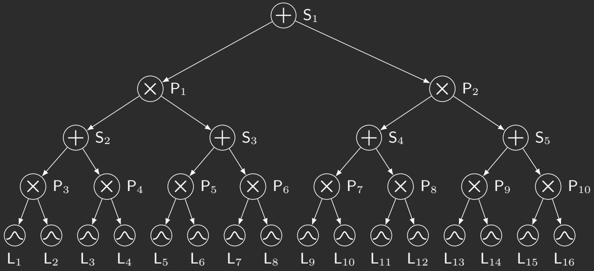

Figure: Example of a tree-shaped computational graph with two layers.

Scope Function ψ

- Let **N** denote the set of all nodes.
- ψ a function ψ: $\mathbf{N} \mapsto 2^{\mathbf{X}}$ assigning each node in the graph a sub-set of X ($2^{\mathbf{X}}$ denotes the power set of $\mathbf{X}$).

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It has the following properties:

1. If N is the root node, then $\psi(\mathsf{N}) = \mathbf{X}$.
2. If N is a sum or product, then $\psi(\mathsf{N}) = \bigcup_{\mathsf{N}' \in \mathbf{ch}(\mathsf{N})} \psi(\mathsf{N}')$.
3. For each $\mathsf{S} \in \mathbf{S}$ we have
   $\forall \mathsf{N}, \mathsf{N}' \in \mathbf{ch}(\mathsf{S}) \colon \psi(\mathsf{N}) = \psi(\mathsf{N}')$ (*completeness*).
4. For each $\mathsf{P} \in \mathbf{P}$ we have
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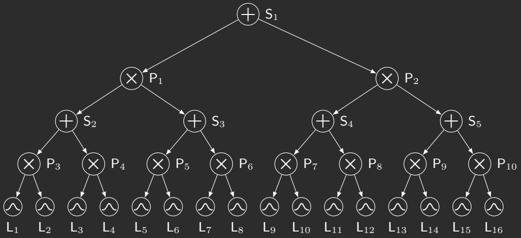
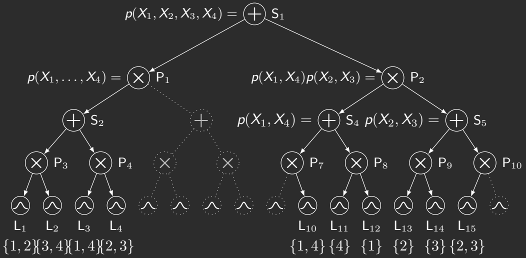
Note: Completeness and decomposability are necessary for any SPN to be a well-defined probability distribution and to allow exact inference in linear time (in the model size).

Example SPN $\mathcal{S} = (\mathcal{G}, \psi, w, \theta)$



$\downarrow$ Apply scope function ψ on $\mathcal{G}$



Bayesian Learning of Sum-Product Networks

Bayesian Parameter Learning

- The key insight for Bayesian parameter learning [Zhao2016, Rashwan2016, Vergari2019] is that sum nodes can be interpreted as latent variables Z_S, clustering data instances.

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$$\begin{aligned}\mathcal{S}(\mathbf{x}) &= \sum_{\mathbf{z}} \prod_{\mathsf{S}\in\mathbf{S}} w_{\mathsf{S},z_\mathsf{S}} \prod_{\mathsf{L}\in T(\mathbf{z})} L(\mathbf{x}_\mathsf{L}) \\ &= \sum_{\mathcal{T}} \prod_{(\mathsf{S},\mathsf{N})\in\mathcal{T}} w_{\mathsf{S},\mathsf{N}} \prod_{\mathsf{L}\in\mathcal{T}} \mathsf{L}(\mathbf{x}_\mathsf{L}) \underbrace{\left(\sum_{\bar{\mathbf{z}}} \prod_{\mathsf{S}\in\bar{\mathbf{S}}_\mathcal{T}} w_{\mathsf{S},\bar{z}_\mathsf{S}} \right)}_{=1}\end{aligned} \tag{1}$$

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- $\mathcal{T}$ is a so-called induced tree [Zhao2016] which is a sub-tree in $\mathcal{S}$ such that the root of $\mathcal{S}$ is the root of $\mathcal{T}$, each $\mathsf{S} \in \mathcal{T}$ has only one child and each $\mathsf{P} \in \mathcal{T}$ has the same children as in $\mathcal{S}$.
- $T(\mathbf{z})$ is a surjective (not injective) function that assigns to each value $\mathbf{z}$ the induced tree $\mathcal{T}$ determined by $\mathbf{z}$.

Bayesian Parameter Learning (cont.)

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Generative model for Bayesian parameter learning:

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\begin{aligned}
w_{\mathsf{S}} \mid \alpha &\sim \mathcal{D}ir(w_{\mathsf{S}} \mid \alpha) \;\; \forall \mathsf{S}\,, & z_{\mathsf{S},n} \,\Big|\, w_{\mathsf{S}} &\sim \mathcal{C}at(z_{\mathsf{S},n} \mid w_{\mathsf{S}}) \;\; \forall \mathsf{S}\, \forall n, \\
\theta_{\mathsf{L}} \mid \gamma &\sim p(\theta_{\mathsf{L}} \mid \gamma) \;\; \forall \mathsf{L}\,, & \mathbf{x}_n \mid \mathbf{z}_n, \theta &\sim \prod_{\mathsf{L} \in T(\mathbf{z}_n)} \mathsf{L}(\mathbf{x}_{\mathsf{L},n} \mid \theta_{\mathsf{L}}) \;\; \forall n.
\end{aligned} \tag{2}
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- We introduce Bayesian learning of SPNs by considering the case in which $\mathcal{G}$ is a tree-shaped region graph.
- A region graph $\mathcal{R}$ can be understood as a vectorised representation of SPNs and is a connected DAG containing two types of nodes: regions ($R \in \mathbf{R}$) and partitions ($P \in \mathbf{P}$).

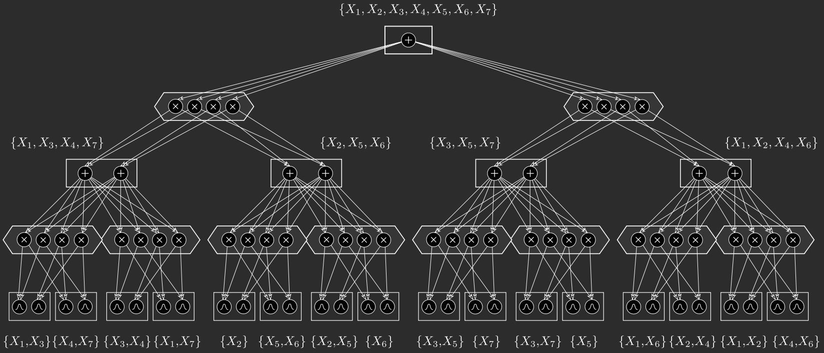

Figure: Example region-graph. Based on the illustration by [Peharz2019].

Bayesian Structure & Parameter Learning (cont.)

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Generative model for joint Bayesian learning:

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\begin{aligned}
w_{\mathsf{S}} \mid \alpha &\sim \mathcal{D}ir(w_{\mathsf{S}} \mid \alpha) \;\; \forall \mathsf{S}, & z_{\mathsf{S},n} \mid w_{\mathsf{S}} &\sim \mathcal{C}at(z_{\mathsf{S},n} \mid w_{\mathsf{S}}) \;\; \forall \mathsf{S} \forall n, \\
\mathbf{v}_P \mid \beta &\sim \mathcal{D}ir(\mathbf{v}_P \mid \beta) \;\; \forall P, & y_{P,d} \mid \mathbf{v}_P &\sim \mathcal{C}at(v_{P,d} \mid \mathbf{v}_P) \;\; \forall P \forall d, \\
\theta_{\mathsf{L}} \mid \gamma &\sim p(\theta_{\mathsf{L}} \mid \gamma) \;\; \forall \mathsf{L}, & \mathbf{x}_n \mid \mathbf{z}_n, \mathbf{y}, \theta &\sim \prod_{\mathsf{L} \in T(\mathbf{z}_n)} \mathsf{L}(\mathbf{x}_{\mathbf{y},n} \mid \theta_{\mathsf{L}}) \;\; \forall n.
\end{aligned} \tag{3}
$$

$\mathbf{x}_{\mathbf{y},n}$ denotes the evaluation of L on the scope induced by $\mathbf{y}$.

Posterior Inference

- We perform Gibbs sampling alternating between i) updating parameters w, θ (fixed $\mathbf{y}$), and ii) updating $\mathbf{y}$ (fixed w, θ) to learn Bayesian SPNs.

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- We perform Gibbs sampling alternating between i) updating parameters w, θ (fixed $\mathbf{y}$), and ii) updating $\mathbf{y}$ (fixed w, θ) to learn Bayesian SPNs.
- This approach has shown to be sufficient for most real-world dataset, but more sophisticated approaches, e.g. particle Gibbs combined with Hamiltonian Monte Carlo sampling; variational inference or posterior bootstrap, might be a interesting future avenues for large-scale problems.

Experiments (discrete data)

Dataset	LearnSPN	RAT-SPN	CCCP	ID-SPN	ours	ours$^\infty$	BTD
NLTCS	−6.11	−6.01	−6.03	−6.02	−6.00	−6.02	−5.97
MSNBC	−6.11	−6.04	−6.05	−6.04	−6.06	−6.03	−6.03
KDD	−2.18	−2.13	−2.13	−2.13	−2.12	−2.13	−2.11
Plants	−12.98	−13.44	−12.87	−12.54	−12.68	−12.94	−11.84
Audio	−40.50	−39.96	−40.02	−39.79	−39.77	−39.79	−39.39
Jester	−53.48	−52.97	−52.88	−52.86	−52.42	−52.86	−51.29
Netflix	−57.33	−56.85	−56.78	−56.36	−56.31	−56.80	−55.71
Accidents	−30.04	−35.49	−27.70	−26.98	−34.10	−33.89	−26.98
Retail	−11.04	−10.91	−10.92	−10.85	−10.83	−10.83	−10.72
Pumsb-star	−24.78	−32.53	−24.23	−22.41	−31.34	−31.96	−22.41
DNA	−82.52	−97.23	−84.92	−81.21	−92.95	−92.84	−81.07
Kosarak	−10.99	−10.89	−10.88	−10.60	−10.74	−10.77	−10.52
MSWeb	−10.25	−10.12	−9.97	−9.73	−9.88	−9.89	−9.62
Book	−35.89	−34.68	−35.01	−34.14	−34.13	−34.34	−34.14
EachMovie	−52.49	−53.63	−52.56	−51.51	−51.66	−50.94	−50.34
WebKB	−158.20	−157.53	−157.49	−151.84	−156.02	−157.33	−149.20
Reuters-52	−85.07	−87.37	−84.63	−83.35	−84.31	−84.44	−81.87
20 Newsgrp	−155.93	−152.06	−153.21	−151.47	−151.99	−151.95	−151.02
BBC	−250.69	−252.14	−248.60	−248.93	−249.70	−254.69	−229.21
AD	−19.73	−48.47	−27.20	−19.05	−63.80	−63.80	−14.00

Experiments (heterogeneous data)

Dataset	MSPN	ABDA	ours	ours^{∞}
Abalone	9.73	2.22	3.92	3.99
Adult	-44.07	-5.91	-4.62	-4.68
Australian	-36.14	-16.44	-21.51	-21.99
Autism	-39.20	-27.93	-0.47	-1.16
Breast	-28.01	-25.48	-25.02	-25.76
Chess	-13.01	-12.30	-11.54	-11.76
Crx	-36.26	-12.82	-19.38	-19.62
Dermatology	-27.71	-24.98	-23.95	-24.33
Diabetes	-31.22	-17.48	-21.21	-21.06
German	-26.05	-25.83	-26.76	-26.63
Student	-30.18	-28.73	-29.51	-29.9
Wine	-0.13	-10.12	-8.62	-8.65

Experiments (missing data)

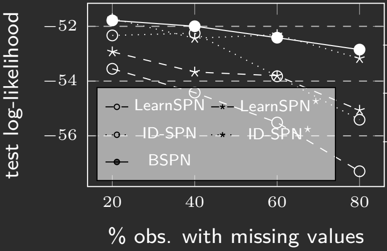

Figure: EachMovie (D: 500, N: 5526)

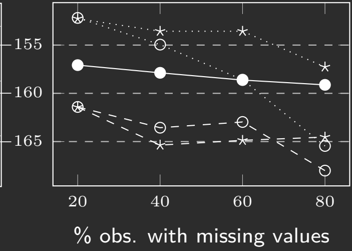

Figure: WebKB (D: 839, N: 3361)

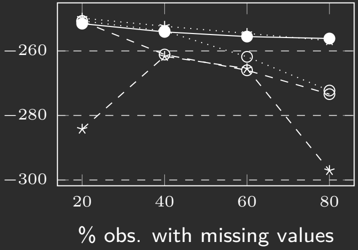

Figure: BBC (D: 1058, N: 1895)

Conclusion

- Structure learning is an important topic in SPNs, and many promising directions have been proposed in recent years.
- However, most of these approaches are based on intuition and refrain from declaring an explicit and global principle to structure learning.
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- We phrase structure (and joint parameter) learning as Bayesian inference in a latent variable model.
- In various experiments we show that this principled approach competes well with prior art and that we gain several benefits, such as *automatic protection against overfitting*, *robustness under missing data* and a natural extension to nonparametric formulations.

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- A critical insight for our approach is to decompose structure learning into: constructing a computational graph and separately learning the SPN's scope function.

References

[Poon2011] H. Poon and P. Domingos. Sum-product networks: A new deep architecture. In Proceedings of UAI, pages 337–346, 2011.

[Zhao2016] H. Zhao, T. Adel, G. J. Gordon, and B. Amos. Collapsed variational inference for sum-product networks. In Proceedings of ICML, pages 1310–1318, 2016.

[Rashwan2016] A. Rashwan, H. Zhao, and P. Poupart. Online and distributed Bayesian moment matching for parameter learning in sum-product networks. In Proceedings of AISTATS, pages 1469–1477, 2016.

[Vergari2019] A. Vergari, A. Molina, R. Peharz, Z. Ghahramani, K. Kersting, and I. Valera. Automatic Bayesian density analysis. In Proceedings of AAAI, 2019.

[Peharz2019] R. Peharz, A. Vergari, K. Stelzner, A. Molina, X. Shao, M. Trapp, K. Kersting, and Z. Ghahramani. Random sum-product networks: A simple but effective approach to probabilistic deep learning. In Proceedings of UAI, 2019.

[Trapp2019] M. Trapp, R. Peharz, H. Ge, F. Pernkopf, and Z. Ghahramani. Bayesian Learning of Sum-Product Networks. To appear at NeurIPS, 2019.