Advances in Learning Sum-Product Networks

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Outline

- · Introduction to Sum-Product Networks
- Parameter Learning
- Structure Learning
- Applications of Sum-Product Networks

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- Introduction to Sum-Product Networks
- Parameter Learning
 - semi-supervised learning
 - effects of overparameterization
- Structure Learning
 - principled structure learning
- Applications of Sum-Product Networks
 - · out-of-domain detection
 - non-linear probabilistic regression

Introduction

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- · Answer probabilistic queries q on a probabilistic model m.

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- $X = \{Day, Time, JamA1, JamA2, ..., JamA_n\}.$
- $q(m) = p_m(Day = Monday, JamA2 = 1).$
- Therefore, we need to be able marginalise out variables, such as Date and JamA2.

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- A class of queries Q on a class of models M is tractable, iff for any query q ∈ Q and model m ∈ M the computational complexity is at most polynomial O(|q| · |m|).
- SPNs admit many probabilistic inference tasks, such as marginalisation, in linear time.
- To model a probability distribution over X, SPNs use an explicit representation.

Note: Most recent generative models, such as GANs, are implicitly defined, intractable and require approximate inference.

Sum-Product Networks

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Note: This definition is conceptually different to the classic definition of SPNs.

Computational Graph G

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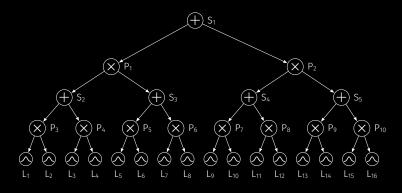


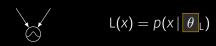
Figure 1: Example of a tree-shaped computational graph.

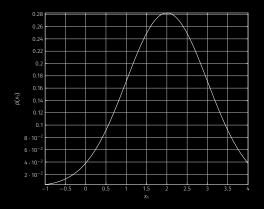
Leaves L in G



$$L(x) = p(x \mid \theta_L)$$

Leaves L in G



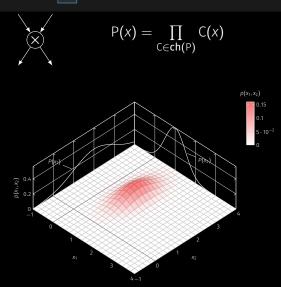


Product Nodes P in G



$$P(x) = \prod_{C \in \mathsf{ch}(P)} C(x)$$

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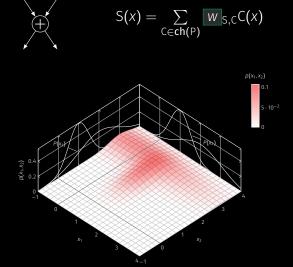


Sum Nodes S in G



$$S(x) = \sum_{C \in ch(P)} w_{S,C}C(x)$$

Sum Nodes S in G



Note: We assume that $w_{S,C} \ge 0$ and $\sum_{C \in ch(P)} w_{S,C} = 1$.

Scope Function ψ

 ψ is a function assigning each node N in the graph a sub-set of X.¹

¹This sub-set is often referred to as the scope of a node.

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A scope function has to fulfil the following properties:

- 1. If N is the root node, then ψ (N) = X.
- 2. If N is a sum or product, then

$$\psi$$
 (N) = $\bigcup_{N' \in \mathsf{ch}(N)} \psi$ (N').

- 3. For each $S \in S$ we have $\forall N, N' \in ch(S)$: $\psi(N) = \psi(N')$ (completeness).
- 4. For each $P \in P$ we have $\forall N, N' \in ch(P)$: $\psi(N) \cap \psi(N') = \emptyset$ (decomposability).

This sub-set is often referred to as the scope of a node.

Completeness $|\psi|$

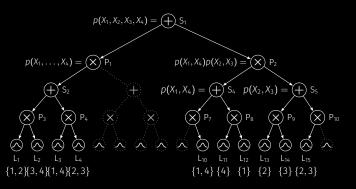
Completeness can be understood as requiring each sum node to be a well-defined mixture distribution.

Decomposability ψ

Decomposability ensures that each product node is a proper factorisation of its scope. Also, decomposability ensures we can "pull" down expensive operations, such as marginalisation or computation of expectations, down to the leaves enabelling tractable inference.

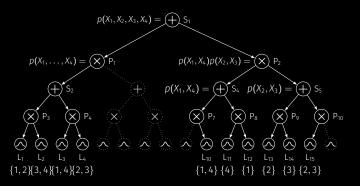
Example SPN
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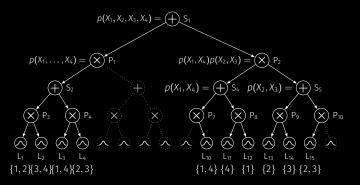
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Example SPN
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After applying a scope function $|\psi|$ on $|\mathcal{G}|$ we obtain the SPN.



Note: We define that L(x) := 1 for every x if and only if ψ (L) = \emptyset . Also note: Most structure learners learn \mathcal{G} and ψ in an entangled way.

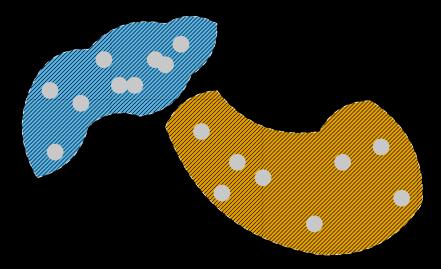
Parameter Learning of

Sum-Product Networks

Parameter Learning

- State-of-the-art SPN parameter learning covers a wide range of well-developed techniques.
- The following selection is a small and biased sub-selection of the existing literature.

Goal: Model the data distribution to be able to generate new data.



Let $\mathcal{X} = \{x_n\}_n^N$ with $xn \in \mathbb{R}^D$ denote training samples and $\phi = (W, \theta)$.

²Note: $S(*|\phi)$ denotes the partition function which is a normalisation constant. If the SPN is normalised this evaluates to one.

Let $\mathcal{X} = \{x_n\}_n^N$ with $xn \in \mathbb{R}^D$ denote training samples and $\phi = (W, \theta)$.

To learn the parameters, we maximise the log-likelihood:²

$$\mathcal{L}(\phi \mid \mathcal{X}) = \sum_{n=1}^{N} \log \mathcal{S}(\mathbf{x}_n \mid \phi) - \log \mathcal{S}(* \mid \phi)$$
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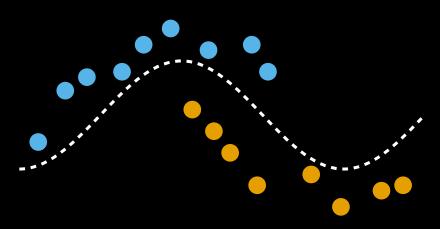
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This is usually done using expectation-maximisation or gradient-based optimisation.

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Goal: Find a separation of pre-defined classes given labelled training examples.



Let $\mathcal{X} = \{x_n\}_n^N$ with $xn \in \mathbb{R}^D$ denote training samples and $\boldsymbol{\lambda} = \{\lambda_n\}_n^N$ with $\lambda_n \in \mathbb{R}$ their respective class labels and $\phi = (\underline{W}, \underline{\theta})$.

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To learn the parameters, we maximise the conditional log-likelihood (or the cross-entropy):

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Note: [Peharz2019] proposed a hybrid generative-discriminative loss.

Goal: Find a separation of pre-defined classes given few labelled and many unlabelled training examples.

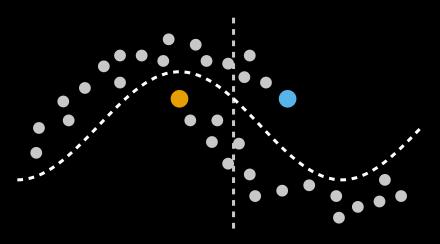


Figure 2: Example of a semi-supervised learning problem.

Let $\mathcal{X} = \{x_n\}_n^N$ with $xn \in \mathbb{R}^D$ denote labelled training samples and $\boldsymbol{\lambda} = \{\lambda_n\}_n^N$ with $\lambda_n \in \mathbb{R}$ their respective class labels.

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Further, let $\mathcal{U}=\{u_n\}_m$ with $u_n\in\mathbb{R}^D$ denote unlabelled training samples and let $q\in\Delta_{K-1}$ denote soft-labels with $q_m\in\Delta_{K-1}\in$ that we aim to infer. ϕ^+ denotes the parameters of an SPN trained solely on labelled data.

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$$\underset{\phi \in \Phi}{\operatorname{arg}} \underset{q \in \Delta_{K-1}}{\min} \mathcal{L}(\phi, \lambda, q \mid \mathcal{X}, \mathcal{U}) - \mathcal{L}(\phi^+, \lambda, q \mid \mathcal{X}, \mathcal{U}) \quad (3)$$

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$$\operatorname*{arg\,max}_{\phi \in \Phi}\operatorname*{arg\,min}_{\boldsymbol{q} \in \Delta_{K-1}} \mathcal{L}(\phi, \boldsymbol{\lambda}, \boldsymbol{q} \,|\, \mathcal{X}, \mathcal{U}) - \mathcal{L}(\phi^+, \boldsymbol{\lambda}, \boldsymbol{q} \,|\, \mathcal{X}, \mathcal{U}) \tag{3}$$

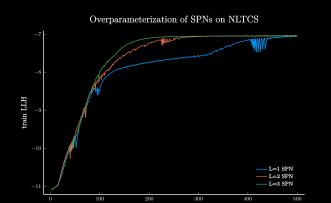
Intuitively, this objective (contrastive pessimistic likelihood estimation) tries to find the best semi-supervised learner (ϕ) under the worst soft-labels q.

Overparameterization in SPNs [Trapp2019b]

Gradient-based optimisation of the weights of any deep treestructured sum-product network with small (fixed) learning rate η and near zero initialisation of the weights w is equivalent to gradient-based optimisation with adaptive and timevarying learning rate and momentum term.

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Sum-Product Networks

Learners tailored to images

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- Later, [Gens2012] proposed a structure that decomposes images into parts.
- Recently, [Peharz2019] presented a randomly constructed structure that divides images into randomly defined sub-regions. ³

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General-purpose learners

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- Later, a wide range of variants of LearnSPN have been proposed to allow structure learning on continuous data or heterogeneous data and to prune the structures in order to improve the generalisation of the structures.⁴

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- However, all of the existing approaches refrain from asking What is a good structure?
- Recently, we presented the first principled approach that aims to change this practice! [Trapp2019]

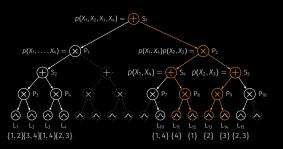
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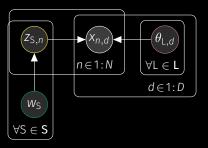


Figure 3: Generative model for Bayesian parameter learning.

Bayesian Structure & Parameter Learning [Trapp2019]

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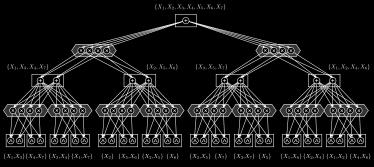


Figure 4: Example region-graph. Based on the illustration by [Peharz2019].

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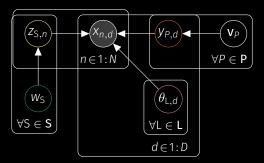


Figure 5: Generative model for Bayesian structure and parameter learning.

Posterior Inference

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- We perform Gibbs sampling alternating between i) updating parameters w, θ (fixed y), and ii) updating y (fixed w, θ) to learn Bayesian SPNs.
- This emperically approach has shown to be sufficient for real-world dataset with up to 1556 dimensions.
- More sophisticated approaches, e.g. particle Gibbs sampling or variational inference, might be interesting future avenues.

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Note: Existing approach cannot handle missing data during structure learning, so we either removed the samples with missing data or used k-NN imputation.

Experiments (discrete)

Dataset	LearnSPN	RAT-SPN	СССР	ID-SPN	ours	ours∞	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	<u>-12.68</u>	<u>-12.94</u>	-11.84
Audio	-40.50	-39.96	-40.02	-39.79	-39.77	<u>-39.79</u>	-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	<u>-34.10</u>	-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	<u>-31.34</u>	<u>-31.96</u>	-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	<u>-10.74</u>	<u>-10.77</u>	-10.52
MSWeb	-10.25	-10.12	-9.97	-9.73	-9.88	<u>-9.89</u>	-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	<u>-156.02</u>	-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 (missing data)

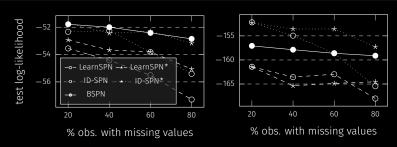
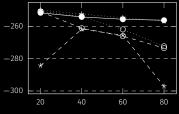


Figure 6: EachMovie (D: 500, N: 5526) Figure 7: WebKB (D: 839, N: 3361)



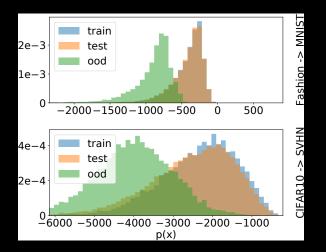
% obs. with missing values

Figure 8: BBC (D: 1058, N: 1895)

Recent Applications

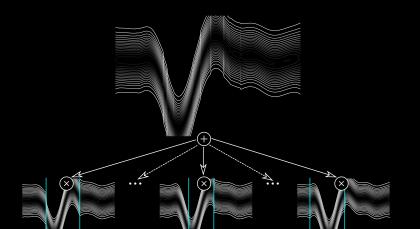
Out-Of-Domain Detection [Peharz2019]

Histograms of the log-likelihoods of RAT-SPNs on the native data set (blue: train, orange: test) and out-of-domain (ood) data set (green).



Non-linear Probabilistic Regression [Trapp2019c]

Deep structured mixtures of Gaussian processes combine exact inference in Gaussian processes with exact and efficient inference in SPNs to obtain an efficient probabilistic non-linear regression model for large-scale data.



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- However, most structure learning approaches are based on intuition and refrain from declaring the goal of structure learning.
- We recently proposed an approach that aims to *change* this practice using a Bayesian formulation.

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