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LACAM Laboratory
Machine Learning

Simplifying, Regularizing and Strengthening Sum-Product Network Structure Learning

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Introduction

The main task on **Probabilistic Graphical Models** (PGMs), *inference*, is untractable.

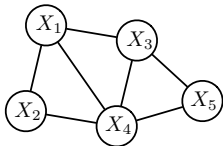
Tractable PGMs are recently gaining interest: tree based models [Meilă and Jordan 2000], Arithmetic Circuits (ACs) [Rooshenas and Lowd 2014], **Sum-Product Networks** (SPNs) [Poon and Domingos 2011].

Sum-Product Networks structure learning: **LearnSPN**.

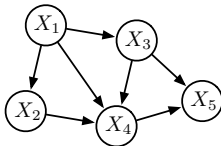
Improving LearnSPN on **structure quality** and **accuracy**, in three ways:

- I **simplifying** by limiting node splits
- II **regularizing** by effective early stopping
- III **strengthening** by model averaging

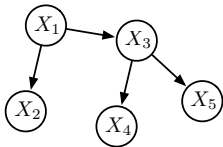
PGMs and Tractability



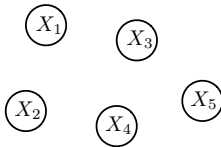
$$P(\mathbf{X}) = \frac{1}{Z} \prod_c \phi_c(\mathbf{X}_c)$$



$$P(\mathbf{X}) = \prod_{i=1}^n P(X_i | \mathbf{Pa}_i)$$

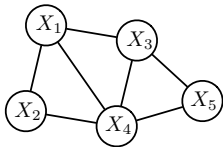


$$P(\mathbf{X}) = \prod_{i=1}^n P(X_i | Pa_i)$$

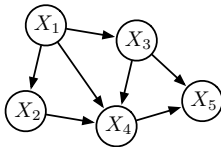


$$P(\mathbf{X}) = \prod_{i=1}^n P(X_i)$$

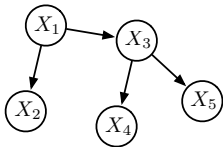
PGMs and Tractability



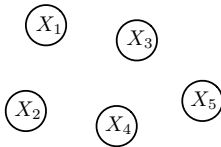
untractable



untractable



tractable

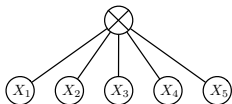


tractable

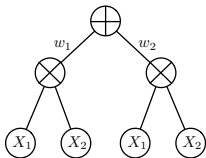
Sum-Product Networks (I)

SPNs are DAGs *compiling* the partition function of a joint pdf into a **deep** architecture of **sum** and **product** nodes.

Product nodes define factorizations over independent components, sum nodes weighted mixtures. Leaves are tractable univariate distributions.



Products over nodes with different scopes (*decomposability*) and sums over nodes with same scopes (*completeness*) guarantee modeling a pdf (*validity*).



The **size** of the network is the number of *edges* in it.

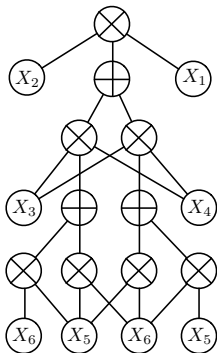
The **depth** of the network is the number of alternated *layers*.

Sum-Product Networks (II)

Bottom-up evaluation of the network:

$$S_{X_i}(x_j) = P(X_i = x_j)$$

$$S_+(\mathbf{x}) = \sum_{i \in ch(+)} w_i S_i(\mathbf{x}), \quad S_\times(\mathbf{x}) = \prod_{i \in ch(\times)} S_i(\mathbf{x})$$



Inferences linear in the size of the network (# edges):

- $\oplus Z = S(*)$
- $\oplus P(\mathbf{e}) = S(\mathbf{e})/S(*)$
- $\oplus P(\mathbf{q}|\mathbf{e}) = \frac{P(\mathbf{q},\mathbf{e})}{P(\mathbf{e})} = \frac{S(\mathbf{q},\mathbf{e})}{S(\mathbf{e})}$
- $\oplus MPE(\mathbf{q}, \mathbf{e}) = \max_{\mathbf{q}} P(\mathbf{q}, \mathbf{e}) = S^{max}(\mathbf{e})$
(by substituting sum nodes with *max* nodes)

How and Why Structure Learning

Fixed structures are hard to engineer and train (fully connected layers).

Automatic discovery of latent vars.

Constraint-based search formulation. Discover hidden variables for sum node mixtures and independences for product node components:

- ⊕ greedy top-down: KMeans on features [Dennis and Ventura 2012]; alternating clustering on instances and independence tests on features, **LearnSPN** [Gens and Domingos 2013]
- ⊕ greedy bottom up: merging feature regions by a *Bayesian-Dirichlet independence test*, and reducing edges by maximizing MI [Peharz, Geiger, and Pernkopf 2013]
- ⊕ **ID-SPN**: turning LearnSPN in log-likelihood guided expansion of sub-networks approximated by Arithmetic Circuits [Rooshenas and Lowd 2014]

Why Structure Quality Matters

Tractable inference is guaranteed *if the network size is polynomial* in # vars.

Smaller networks, faster inference (comparing network sizes is better than comparing inference times).

Deeper networks are possibly *more expressively efficient* [Martens and Medabalimi 2014; Zhao, Melibari, and Poupart 2015].

Structural simplicity as a bias: overcomplex networks may not generalize well.

Structure quality desiderata: **smaller** but **accurate**, **deeper** but not wider, SPNs.

LearnSPN (I)

Build a tree-like SPN by recursively split the data matrix:

- ⊕ splitting columns into pairs by a greedy **G Test** based procedure with threshold ρ :

$$G(X_i, X_j) = 2 \sum_{x_i \sim X_i} \sum_{x_j \sim X_j} c(x_i, x_j) \cdot \log \frac{c(x_i, x_j) \cdot |T|}{c(x_i)c(x_j)}$$

- ⊕ clustering instances into $|C|$ sets with **online Hard-EM** with cluster penalty λ :

$$Pr(\mathbf{X}) = \sum_{C_i \in \mathbf{C}} \prod_{X_j \in \mathbf{X}} Pr(X_j | C_i) Pr(C_i)$$

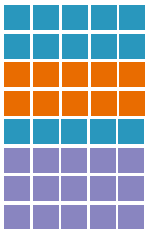
weights are estimated as cluster proportions

- ⊕ if there are less than m instances, put a **naive factorization** over leaves
- ⊕ each univariate distribution get **ML estimation** smoothed by α

Hyperparameter space: $\{\rho, \lambda, m, \alpha\}$.

	X_1	X_2	X_3	X_4	X_5
1					
2					
3					
4					
5					
6					
7					
8					

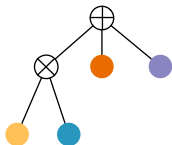
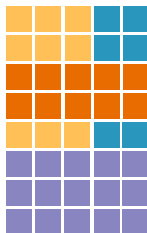
X_1 X_2 X_3 X_4 X_5



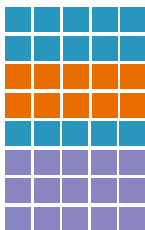
X_1 X_2 X_3 X_4 X_5



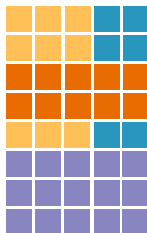
X_1 X_2 X_3 X_4 X_5



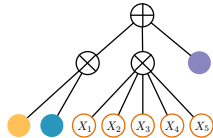
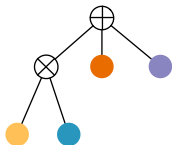
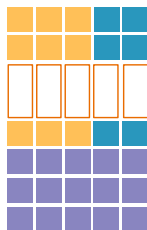
X_1 X_2 X_3 X_4 X_5



X_1 X_2 X_3 X_4 X_5



X_1 X_2 X_3 X_4 X_5



LearnSPN (II)

LearSPN performs two interleaved ***greedy hierarchical*** divisive ***clustering*** processes (co-clustering on the data matrix).

Fast and simple. But both processes never look back and are committed to the choices they take.

Online EM does not need to specify the number of clusters k in advance. But overcomplex structures are learned by exploding the number of sum node children.

Tractable leaf estimation. But naive factorization independence assumptions may be too strong.

ML estimations are effective. But they are not robust to noise, they can overfit the training set easily.

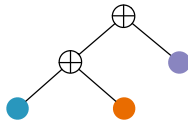
Simplifying by limiting node splits

Observation: each clustering process benefits from the other one improvements/highly suffers from other's mistakes.

Idea: slowing down the processes by limiting the number of nodes to split into. SPN-B, variant of LearnSPN that uses EM for mixture modeling with $k = 2$ to cluster rows. No need for λ anymore.

Objectives:

- ⊕ not committing to complex structures too early
- ⊕ same expressive power as LearnSPN
- ⊕ reducing node out fan increases the depth
- ⊕ same accuracy, smaller networks



SPN-B: depth VS size

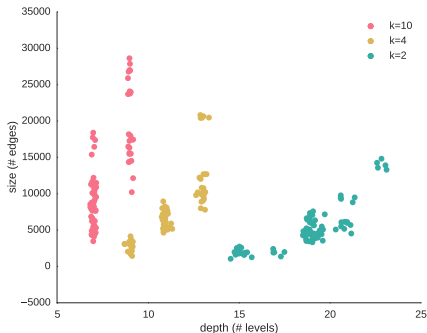


Figure : Comparing network sizes and depths while varying the max number of sum node children splits ($k \in \{10, 4, 2\}$). Each dot is an experiment in the grid search hyperparameter space performed by SPN-B on the dataset Plants.

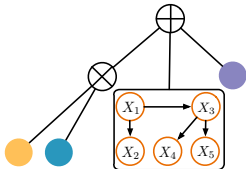
Regularizing by effective early stopping

LearnSPN regularization is governed by α and m , however can be very ineffective:

- ⊕ naive factorizations are too strong assumptions
- ⊕ best likelihood structures prefer smaller values for m to get accurate naive factorizations

Idea: substituting naive factorizations with Bayesian trees as leaf distributions

$$P(\mathbf{X}) = \prod_j P(X_j | Pa_j):$$



- ⊕ learnable with Chow-Liu algorithm
- ⊕ still tractable (linear) multivariate distributions for marginals, conditionals and MPE
- ⊕ same or higher accuracy
- ⊕ less complex structures for larger values of m

SPN-BT: preserving likelihoods

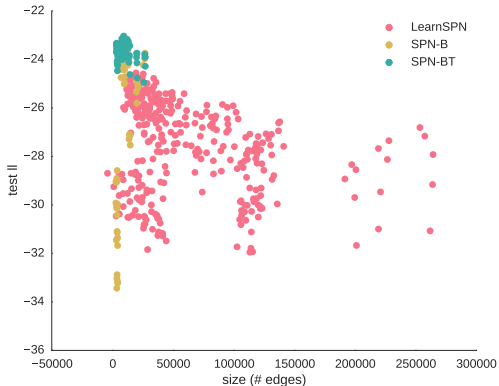


Figure : Comparing the network sizes against the average test log-likelihood obtained by LearnSPN, SPN-B and SPN-BT. Each dot is an experiment in the grid search performed for the dataset Pumsb-star.

SPN-BT: effective early stopping

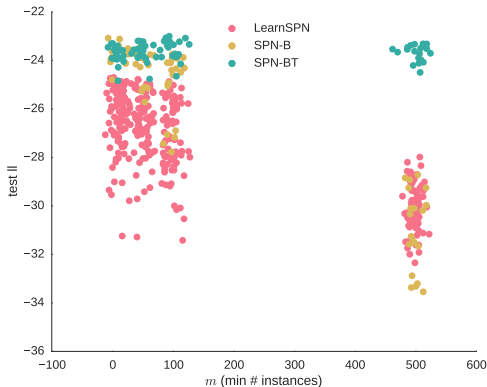


Figure : Comparing the values for m (10, 50, 100, 500) against the average test log-likelihood obtained by LearnSPN, SPN-B and SPN-BT. Each dot is an experiment in the grid search performed for the dataset Pumsb-star.

Strengthening by model averaging

Interpreting sum nodes as *general additive estimators*. Leveraging classic statistical tools to learn them: **bagging**.

Draw k bootstrapped samples from the data, then grow an SPN S_{B_i} on each of them. Join them into a single SPN \hat{S} with a sum node:

$$\hat{S} = \sum_{i=1}^k \frac{1}{k} S_{B_i}$$

More robustness and less variance in the model.

Exponential number of nodes if done for each sum node (bootstrapping only at the root).

Two variants in the experiments: SPN-BB and SPN-BTB, whether Chow-Liu trees are employed or not.

Bagging exp

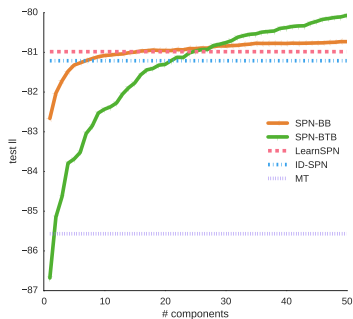
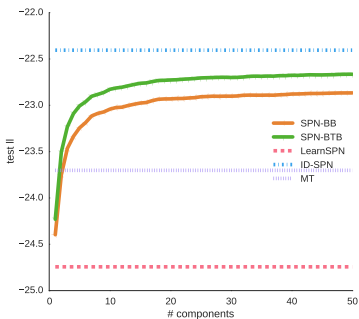


Table : Comparing test log-likelihoods for SPN-BB and SPN-BTB while increasing the number of components against LearnSPN, MT and ID-SPN best models accuracies for Pumsb_star (left) and DNA (right)

Experimental setting

Classical setting for **generative** PGMs structure learning [Gens and Domingos 2013]:

- ⊕ 19 binary datasets from classification, recommendation, frequent pattern mining... [Lowd and Davis 2010] [Haaren and Davis 2012]
- ⊕ Training 75% Validation 10% Test 15% splits (no cv)

Observing both structure quality parameters and the network accuracy:

- ⊕ test set **average log-likelihood**
- ⊕ network **size** (# edges) and network **depth** (# levels)

We perform a model selection via a *grid search* in the same parameter space for LearnSPN, SPN-B, SPN-BT:

- ⊕ $\lambda \in \{0.2, 0.4, 0.6, 0.8\}$, ⊕ $m \in \{1, 50, 100, 500\}$,
- ⊕ $\rho \in \{5, 10, 15, 20\}$, ⊕ $\alpha \in \{0.1, 0.2, 0.5, 1.0, 2.0\}$.

Up to 50 components and best grid parameters for SPN-BB and SPN-BTB.
Comparing ll against LearnSPN, ID-SPN and MT [Meilă and Jordan 2000].

Network sizes

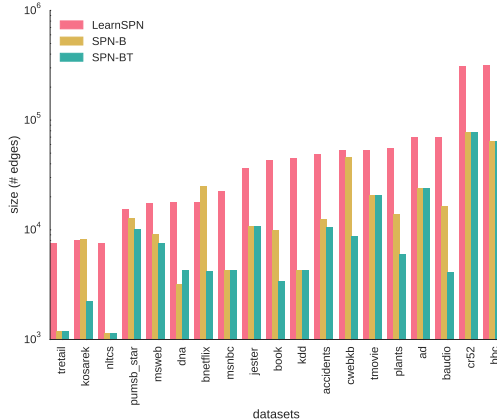


Figure : Comparing network sizes for the networks scoring the best log-likelihoods in the grid search as obtained by LearnSPN, SPN-B and SPN-BT for each dataset.

Network depths

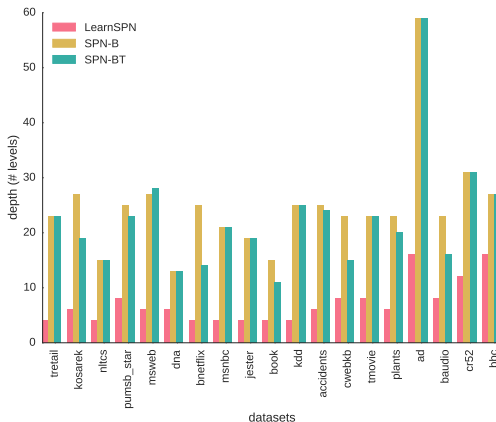


Figure : Comparing network depths for the networks scoring the best log-likelihoods in the grid search as obtained by LearnSPN, SPN-B and SPN-BT for each dataset.

Log-likelihoods

	LearnSPN	SPN-B	SPN-BT	ID-SPN	SPN-BB	SPN-BTB	MT
NLCS	-6.110	-6.048	-6.048	-5.998	-6.014	-6.014	-6.008
MSNBC	-6.099	-6.040	-6.039	-6.040	-6.032	-6.033	-6.076
KDDCup2k	-2.185	-2.141	-2.141	-2.134	-2.122	-2.121	-2.135
Plants	-12.878	-12.813	-12.683	-12.537	-12.167	-12.089	-12.926
Audio	-40.360	-40.571	-40.484	-39.794	-39.685	-39.616	-40.142
Jester	-53.300	-53.537	-53.546	-52.858	-52.873	-53.600	-53.057
Netflix	-57.191	-57.730	-57.450	-56.355	-56.610	-56.371	-56.706
Accidents	-30.490	-29.342	-29.265	-26.982	-28.510	-28.351	-29.692
Retail	-11.029	-10.944	10.942	-10.846	-10.858	-10.858	-10.836
Pumsb-star	-24.743	-23.315	-23.077	-22.405	-22.866	-22.664	-23.702
DNA	-80.982	-81.913	-81.840	-81.211	-80.730	-80.068	-85.568
Kosarek	-10.894	-10.719	-10.685	-10.599	-10.690	-10.578	-10.615
MSWeb	-10.108	-9.833	-9.838	-9.726	-9.630	-9.614	-9.819
Book	-34.969	-34.306	-34.280	-34.136	-34.366	-33.818	-34.694
EachMovie	-52.615	-51.368	-51.388	-51.512	-50.263	-50.414	-54.513
WebKB	-158.164	-154.283	-153.911	-151.838	-151.341	-149.851	-157.001
Reuters-52	-85.414	-83.349	-83.361	-83.346	-81.544	-81.587	-86.531
BBC	-249.466	-247.301	-247.254	-248.929	-226.359	-226.560	-259.962
Ad	-19.760	-16.234	-15.885	-19.053	-13.785	-13.595	-16.012

Table : Average test log likelihoods for the best networks learned by all algorithms on all datasets after the grid search. In bold the values that are statistically better than all the others according to a Wilcoxon signed rank test with p -value of 0.05.

Conclusions

- ⊕ Structure quality evaluation matters
- ⊕ Deeper networks by applying a simplicity bias when splitting
- ⊕ Regularized SPNs by introducing Chow-Liu trees as leaves
- ⊕ More robust and accurate SPNs with bootstrapped sum nodes

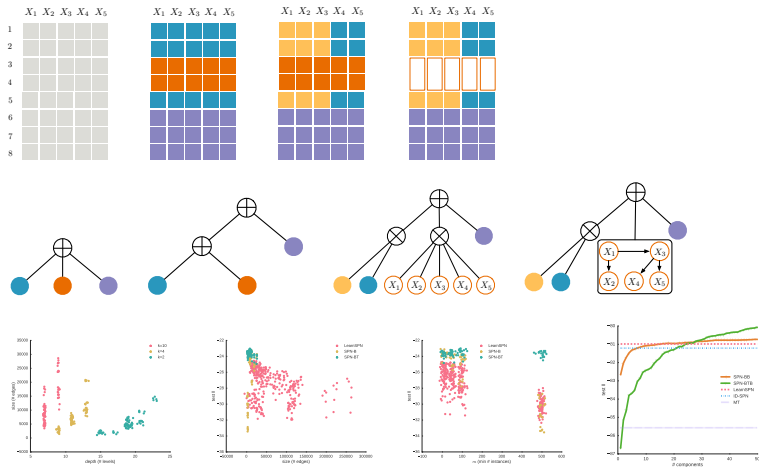
Further works

- ⊕ Are other sum node interpretations as gam effective?
- ⊕ Is it possible to compress learned structures?
- ⊕ How these variations influence representation learning?
- ⊕ How can these variations be generalized to other tractable PGMs?

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Discuss



Times

	LearnSPN	SPN-B	SPN-BT	ID-SPN	SPN-BB	SPN-BTB	MT
NLTCS	183	114	108	310	1004	1041	290
MSNBC	7354	5922	5774	46266	7963	8275	8645
KDDCup2k	5800	3946	4525	32067	10633	12148	39857
Plants	1156	1420	276	18833	7515	3023	7414
Audio	1146	1561	131	21009	10466	4113	6566
Jester	1289	789	687	10412	17753	8566	3064
Netflix	1331	2369	152	30294	14871	4768	11402
Accidents	839	1006	722	15472	9198	8280	14073
Retail	253	173	161	4041	2317	2505	320
Pumsb-star	230	1010	612	20952	7819	7790	18533
DNA	140	87	122	3040	2022	3049	228
Kosarek	225	1515	416	17799	16583	3642	18782
MSWeb	369	1711	1444	19682	16881	18273	36076
Book	457	832	389	61248	27473	16630	5918
EachMovie	307	939	946	118782	22506	29355	12100
WebKB	307	1960	490	45451	29265	34952	931
Reuters-52	2538	5256	4333	70864	36109	135970	15082
BBC	1136	2645	2479	61471	56271	121007	1324
Ad	668	1585	1356	87522	72632	58777	6850

Table : Times (in seconds) taken to learn the best models on each dataset for **LearnSPN**, **SPN-B**, **SPN-BT**, **SPN-BB**, **SPN-BTB** and **MT** and with default parameters values for **ID-SPN**. Experiments run on a 4-core Intel Xeon E312xx (Sandy Bridge) @2.0 GHz with 8Gb of RAM and Ubuntu 14.04.1, kernel 3.13.0-39.