Simplifying, Regularizing and Strengthening Sum-Product Network Structure Learning

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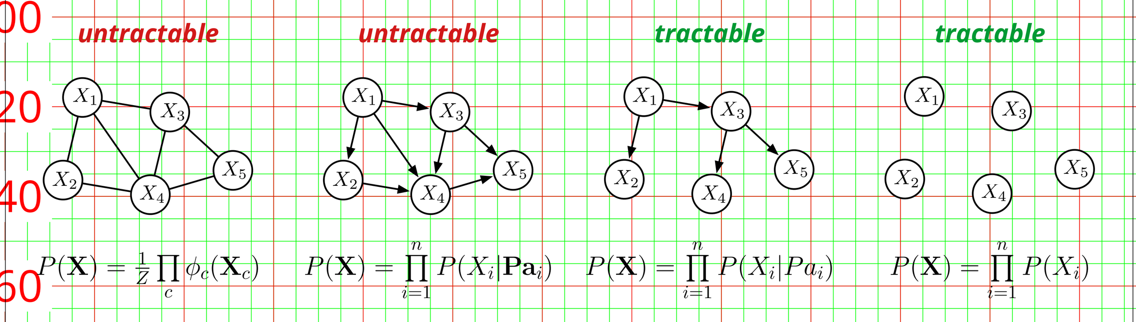
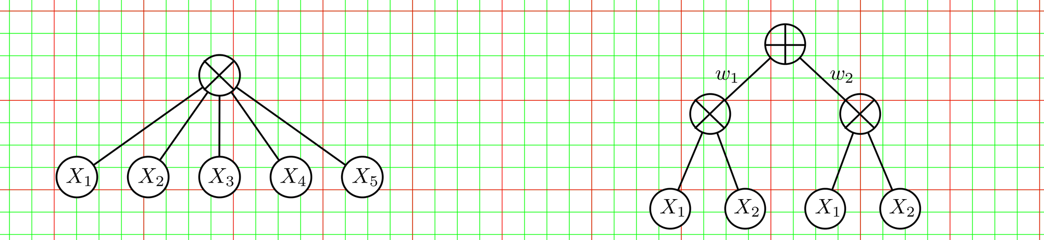
Sum-Product Networks and Tractable Models

Probabilistic Graphical Models (PGMs) provide a tool to compactly represent joint probability distributions $P(\mathbf{X})$.
However, ***inference***, the main task one may want to perform on a PGM, is generally ***untractable***.



To ensure polynomial inference, tractable models trade off expressiveness.

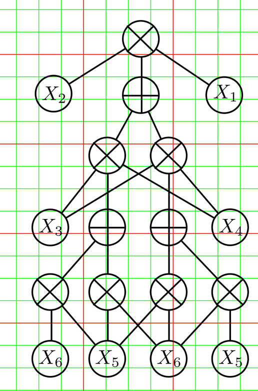
Sum-Product Networks (SPNs) are DAGs *compiling* a pdf $P(\mathbf{X})$ into a ***deep*** architecture of **sum** and **product** nodes over univariate distributions $X_1, \dots, X_n$ as leaves. The parameters of the network are the weights w_{ij} associated to sum nodes children edges.
Product nodes define factorizations over independent components, while sum nodes represent mixtures.
Products over nodes with different scopes (*decomposability*) and sums over nodes with same scopes (*completeness*) guarantee modeling a pdf (*validity*).



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*):

- $Z = S(*)$ (all leaves output 1)
- $P(\mathbf{e}) = S(\mathbf{e})/S(*)$
- $P(\mathbf{q}|\mathbf{e}) = \frac{P(\mathbf{q},\mathbf{e})}{P(\mathbf{e})} = \frac{S(\mathbf{q},\mathbf{e})}{S(\mathbf{e})}$
- $MPE(\mathbf{q}, \mathbf{e}) = \max_{\mathbf{q}} P(\mathbf{q}, \mathbf{e}) = S^{max}(\mathbf{e})$, turning sum nodes into max nodes

The ***depth of the network*** (# *layers*) determines expressive efficiency [4].

How and why to perform structure learning

SPN structure learning is a constraint-based search. Main ideas: to discover hidden variables for sum nodes and independences for product nodes by applying some form of clustering along matrix axis. Different variations: using K-Means on features *[1]*; merging features bottom-up with IB heuristics *[6]*; ***LearnSPN*** *[2]* is the first principled top-down greedy algorithm.

LearnSPN builds a tree-like SPN by recursively splitting the data matrix: columns in pairs by a greedy ***G Test*** based procedure with threshold ρ: $G(X_i, X_j) = 2\sum_{x_i \sim X_i}\sum_{x_j \sim X_j} c(x_i, x_j) \cdot \log\frac{c(x_i,x_j)\cdot|T|}{c(x_i)c(x_j)}$ (Figure 1.c); instances in $|C|$ clusters with ***online Hard-EM*** (Figure 1.b) with cluster number penalty λ: $Pr(\mathbf{X}) = \sum_{C_i \in \mathbf{C}} \prod_{X_j \in \mathbf{X}} Pr(X_j, C_i)$. Weights are the cluster proportions.

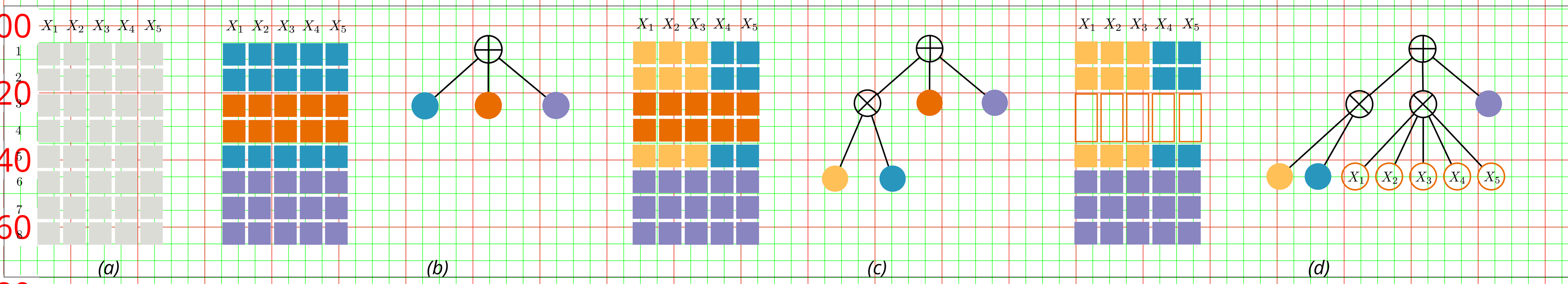


Figure 1. LearnSPN steps depiction: starting from a full data matrix *(a)*, clustering on rows *(b)*, then on columns *(c)*, and putting a naive factorization on leaves *(d)*.

If there are less than m instances, it puts a ***naive factorization*** over leaves (Figure 1.d). For each univariate distribution it gets its ***ML estimation*** smoothed by α. LearnSPN hyperparameter space is thus: $\{\rho, \lambda, m, \alpha\}$.

The state-of-the-art, in terms of test likelihood, is **ID-SPN**: it turns LearnSPN in log-likelihood guided expansion of sub-networks approximated by Arithmetic Circuits *[7]*. However it is overparametrized, and slower.

Tractability is guaranteed if the network size is polynomial in # vars. ***Structure quality matters*** as much as likelihood. Comparing network sizes is more solid than comparing inference times.

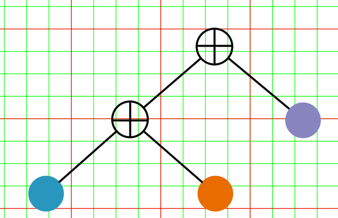
LearnSPN is too greedy and the resulting SPNs are overcomplex networks that may not generalize well. ***Structure quality desiderata***: *smaller* but *accurate*, *deeper* but not wider, SPNs.

Simplifying by limiting node splits

LearSPN performs two interleaved ***greedy hierarchical*** divisive ***clustering*** processes. Each process benefits from the other one improvements and similarly suffers from the 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 but doing only Binary splits for sum nodes children ($k = 2$) when clustering rows.

Objectives: not committing to complex structures too early while retaining same expressive power (right Figure is equivalent to the SPN in Figure 1.b); moreover, reducing the node out fan increases the network depth.
Plus, there is no need for λ anymore.



By increasingly limiting the max number of allowed splits the depth of the structures increases and the network size growth rate decreases.

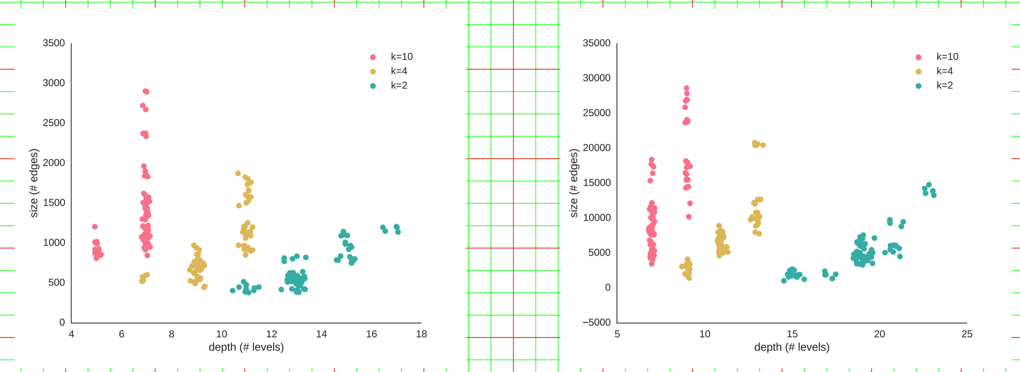


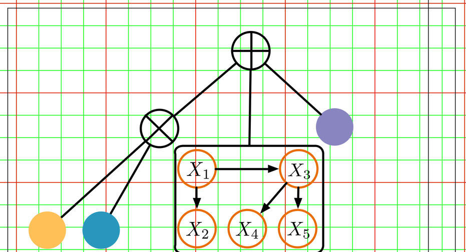
Figure 2. Comparing network sizes and depths while varying the max number of sum node children splits ($k \in \{10, 4, 2\}$). Each dot is an experiment in the grid search hyperparameter space performed by SPN-B on the datasets NLTCS (left) and Plants (right).

Regularizing by introducing tree distributions as leaves

LearnSPN regularization is is governed by the hyperparameters α and m, however using naive factorizations can be ineffective. In order to get accurate networks, the algorithm prefers smaller values for m, resulting in more complex networks

Idea: substitute naive factorizations with Bayesian trees as ***multivariate tractable tree distributions***. SPN-BT learns such Trees with the Chow-Liu algorithm when stopping the splitting process.

Objectives: represent more information allowing for larger values of m to be chosen, while preserving tractability for marginals, conditionals and MPE inference (still linear in the number of leaves).



SPN-BT reduces the size of the networks even more while preserving SPN-B accuracy. At larger values of m, when both SPN-B and LearnSPN accuracies tend to decrease, SPN-BT seems to preserve or improve its likelihood.

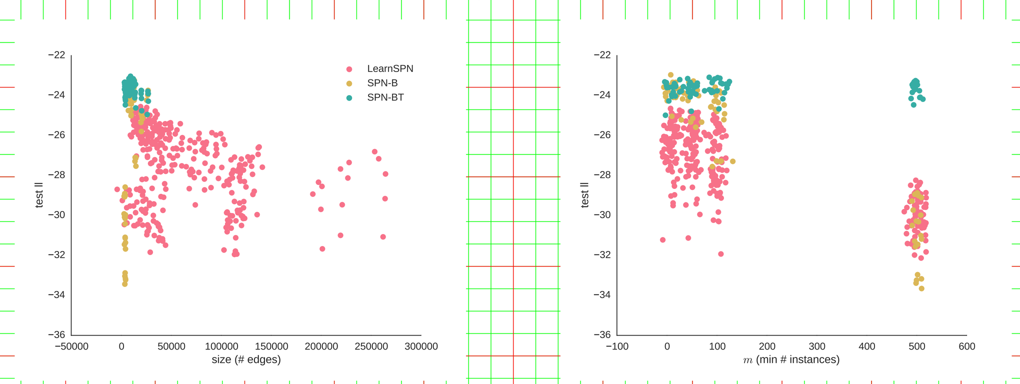


Figure 3. Comparing network sizes (left) and values for m against the average test log-likelihood obtained by LearnSPN, SPN-B and SPN-BT number of sum node children splits. Each dot is an experiment in the grid search performed for the dataset Pumsb-star.

Strengthening by model averaging

The structure building process can still be too greedy and the resulting networks not so accurate.

Idea: interpreting sum nodes as *general additive estimators* by leveraging classic statistical tools to learn them: ***bagging***.

We draw k bootstrapped samples from the data, then grow an SPN S_{B_i} on each one. Join them into a single SPN $\hat{S}$ with a sum node: $\hat{S} = \sum_{i=1}^{k}\frac{1}{k}S_{B_i}$.

Two new variants, SPN-BB and SPN-BTB, apply Bagging to SPN-B and SPN-BT.

Objectives: more robustness and less variance in the model. However, the number of nodes can grow exponential if we bootstrap k times *for each sum node*, thus we apply it once, at the root level only.

Both SPN-BB and SPN-BTB improve their respective variants accuracies considerably and beat ID-SPN on 14 datasets (see Table 1). Monitoring the test log-likelihood gain can help decide the proper number of components.

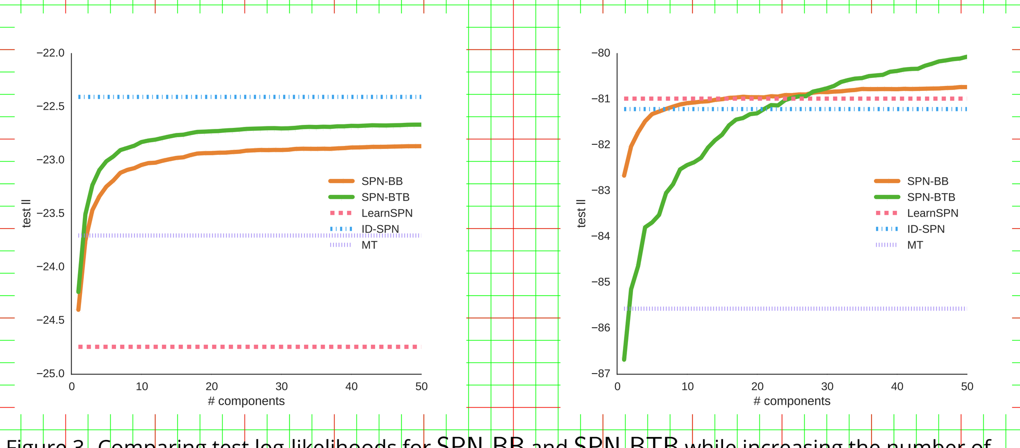


Figure 3. Comparing test log-likelihoods for SPN-BB and SPN-BTB while increasing the number of components against LearnSPN, MT and ID-SPN best models accuracies for Pumsb_star (left) and DNA (right).

Experiments

We devised our experiments in a classical setting for ***generative*** graphical models structure learning [2]: we used 19 binary datasets from classification, recommendation, frequent pattern mining domains [3] which are split into a training (∼75%), a validation (∼10%) and a test (∼15%) part to compare both the networks accuracies and their structure quality. We measured:

- ***average log-likelihood*** on predicting test instances
- network ***sizes*** (# edges)
- network ***depths*** (# alternated type layers)

We first compare LearnSPN against our variations, SPN-B using only Binary splits and SPN-BT with Binary splits and Trees as leaves, to measure the structure quality improvements and then we add SPN-BB combining Binary splits and Bagging and SPN-BTB including all variants in a comparison against the state-of-the-art in terms of log-likelihood: ID-SPN [7] and MT [5].
We perform a model selection via a *grid search* in the same parameter space for LearnSPN, SPN-B, SPN-BT:

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

The gain in network sizes is up to one order of magnitude with SPN-BT while very considerable depths are preserved.

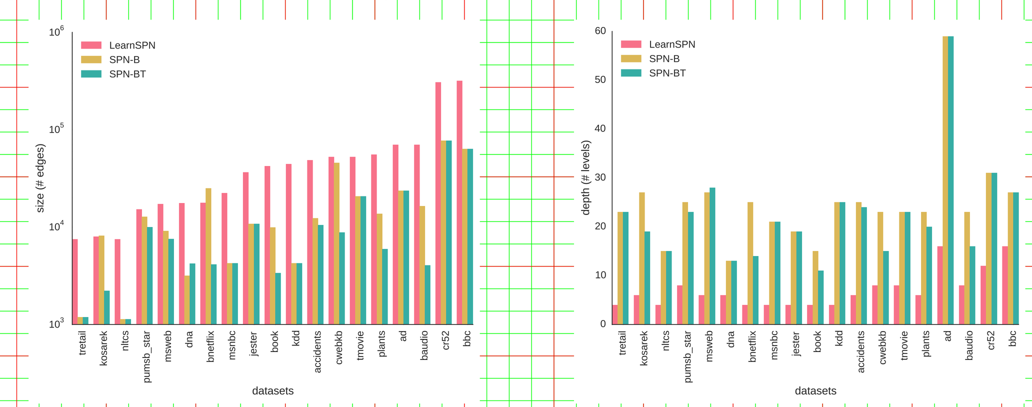


Figure 4. Comparing network sizes (left) and depths (right) for the networks scoring the best log-likelihoods in the grid search as obtained by LearnSPN, SPN-B and SPN-BT for each dataset.

For SPN-BB and SPN-BTB we simply use the best parameters found for SPN-B and SPN-BT using up to 50 bootstrapped components; while for ID-SPN and MT we reproduce the experiments as in [7].

Considering the test log-likelihoods, SPN-B improves LearnSPN values 6 times, and is surpassed by SPN-BT on 13 datasets; while SPN-BB and SPN-BTB score 11 and 13 wins against ID-SPN respectively.

	LearnSPN	SPN-B	SPN-BT	ID-SPN	SPN-BB	SPN-BTB	MT
NLTCS	-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 1. 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.

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http://www.di.uniba.it/~vergari/code/spyn.html