Università degli Studi di Bari
Dipartimento di Informatica

LACAM
Machine Learning

Simplifying, Regularizing and Strengthening Sum-Product Network Structure Learning

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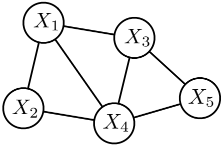
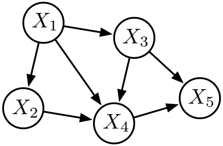
Summary

- Sum-Product Networks refresher
- Why and How Structure learning
- Simplifying by limiting splits
- Regulizing by effective early stopping
- Strengthening by model averaging
- Conclusions and further works

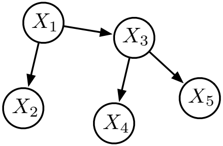
PGMs and Tractability



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



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



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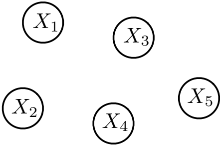

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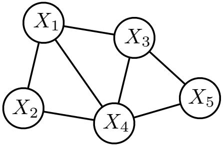
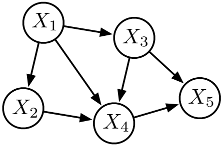


untractable



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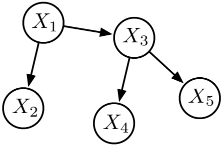
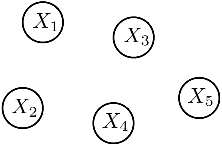
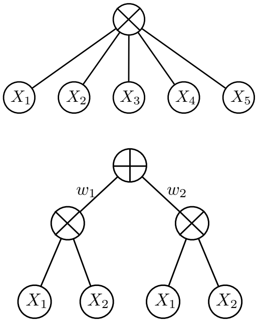


tractable



tractable

Sum-Product Networks (I)



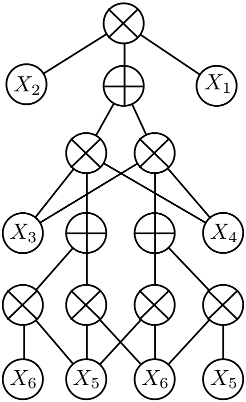
Compiling the partition function of a pdf into a ***deep*** architecture of **sum** and **product** nodes.

Product nodes define factorizations over independent vars, sum nodes mixtures.

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

Considering only valid SPNs of *alternated layers of sum and products*.

Sum-Product Networks (II)



Bottom-up evaluation of the network:

$$S_{X_i}(x_j) = P(X_i = x_j)$$
$$S_+(\mathbf{x}) = \sum_{i \in ch(+)} w_i S_i(\mathbf{x})$$
$$S_\times(\mathbf{x}) = \prod_{i \in ch(\times)} S_i(\mathbf{x})$$

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

- $Z = S(*)$
- $P(\mathbf{e}) = S(\mathbf{e})/S(*)$
- $P(\mathbf{q}|\mathbf{e}) = \frac{P(\mathbf{q},\mathbf{e})}{P(\mathbf{e})} = \frac{S(\mathbf{q},\mathbf{e})}{S(\mathbf{e})}$
- $MPE(\mathbf{q},\mathbf{e}) = \max_{\mathbf{q}} P(\mathbf{q},\mathbf{e}) = S^{max}(\mathbf{e})$

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

Tractability is guaranteed if the network size is polynomial in # vars.

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]

Overcomplex networks do 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:

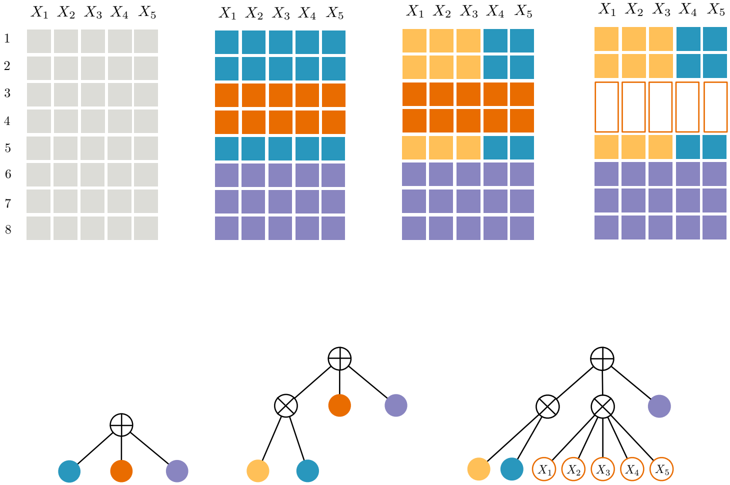
- splitting columns into pairs by a greedy ***G Test*** based procedure with threshold ρ:

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

- clustering instances with ***online Hard-EM*** with cluster penalty λ:

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

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



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

Symplifying by limiting node splits

LearSPN performs two interleaved ***greedy hierarchical*** divisive ***clustering*** processes (co-clustering).

Each 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.

Pros:

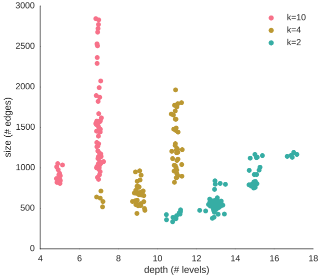
- not committing to complex structures too early
- same expressive power: successive splits allow for more node children
- reducing node out fan increases the depth
- same accuracy, smaller networks

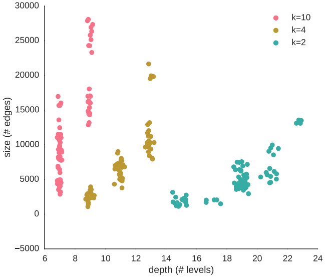
Experimental setting

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

- comparing the ***average log-likelihood*** on predicting instances from a test set
- 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)
- Model selection via *grid search* in the same parameter space:
  - $\lambda \in \{0.2, 0.4, 0.6, 0.8\}$,
  - $\rho \in \{5, 10, 15, 20\}$,
  - $m \in \{1, 50, 100, 500\}$,
  - $\alpha \in \{0.1, 0.2, 0.5, 1.0, 2.0\}$
- comparing our variants against LearnSPN, ID-SPN and MT [Meilă and Jordan 2000]

Depth VS Size





Regularizing by effective early stopping

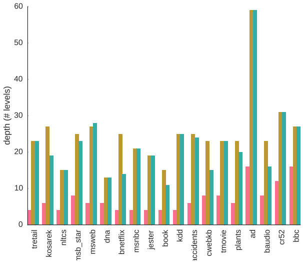
LearnSPN regularization is governed by α and m, however can be very ineffective:

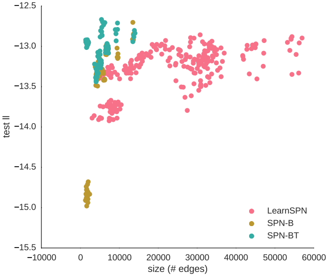
- naive factorizations are too strong assumptions
- best likelihood structures prefer smaller values for m to get accurate naive factorizations

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 multivariate distributions for marginals, conditionals and MPE
- same or higher accuracy for larger vlaues of m
- possibly reducing structure complexity even more

Early stopping exp





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).

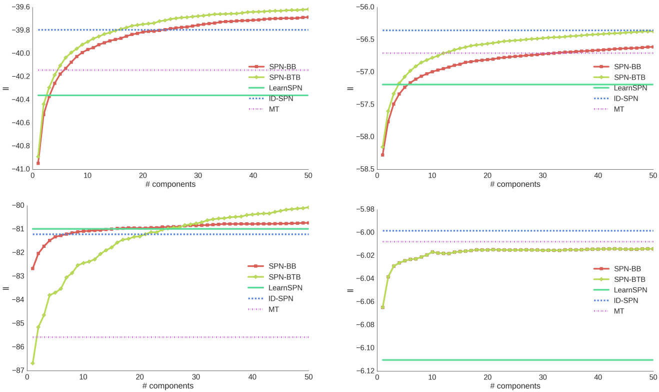
Two variants in the experiments: SPN-BB and SPN-BTB, whether Chow-Liu trees are employed or not.

LL exp

	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 : Average test log likelihoods for all algorithms.

Bagging exp



Conclusions and Further work

- 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

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