Università degli Studi di Bari
Dipartimento di Informatica

LACAM
Machine Learning

Simplifying, Regularizing and Strengthening Sum-Product Network Structure Learning

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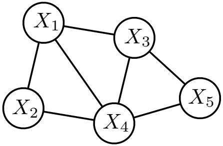
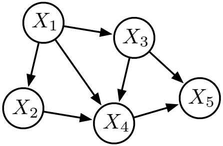
Summary

- 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

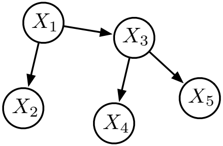
PGMs and Tractability



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



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



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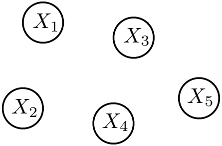

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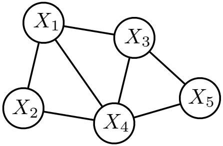
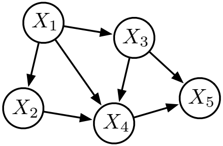
PGMs and Tractability



untractable



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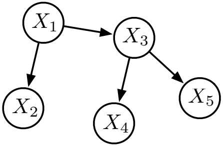
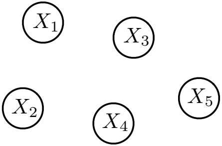
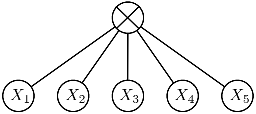


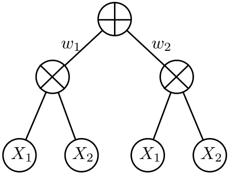
tractable



tractable

Sum-Product Networks (I)





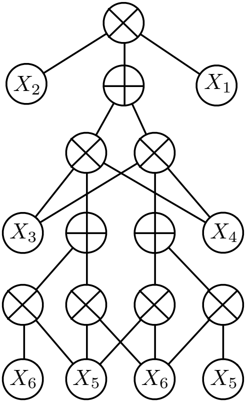
Compiling the partition function of a pdf into a ***deep*** architecture of **sum** and **product** nodes.

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:

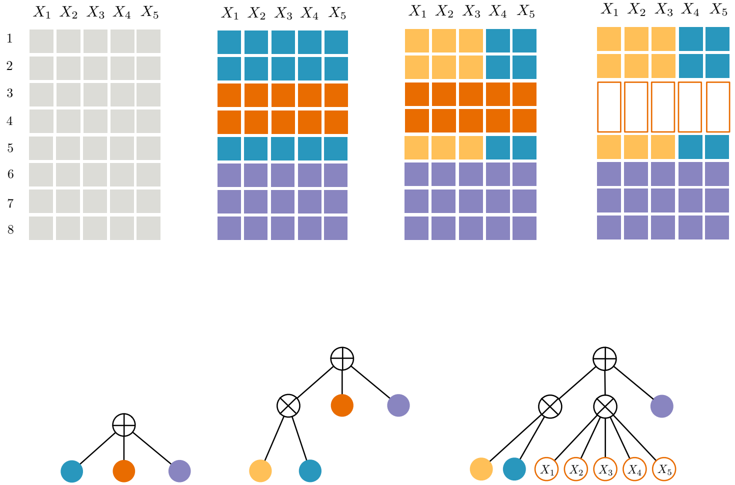
- splitting columns into pairs by a greedy ***G Test*** based procedure with threshold ρ:

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

- 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



X1 X2 X3 X4 X5
1
2
3
4
5
6
7
8
X1 X2 X3 X4 X5
X1 X2 X3 X4 X5
X1 X2 X3 X4 X5
X1 X2 X3 X4 X5

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:

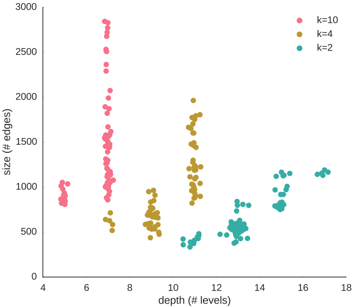
- not committing to complex structures too early
- same expressive power: successive splits allow for more node children
- reducing node out fan increases the depth
- same accuracy, smaller networks

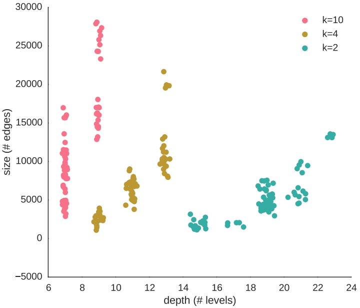
Experimental setting

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

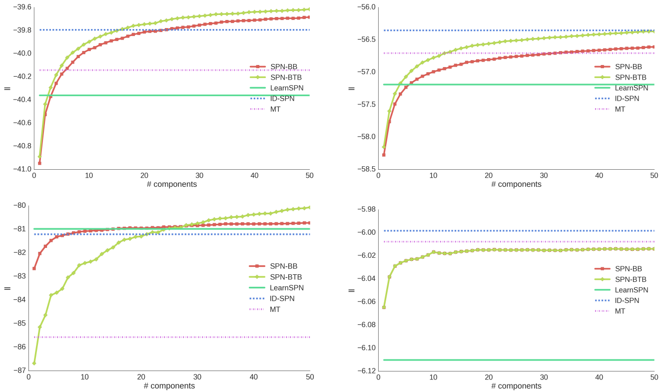
Interpreting sum nodes as general additive estimators. They can be learned as bagged estimators.

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

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