Simplifying, Regularizing and Strengthening Sum-Product Network Structure Learning

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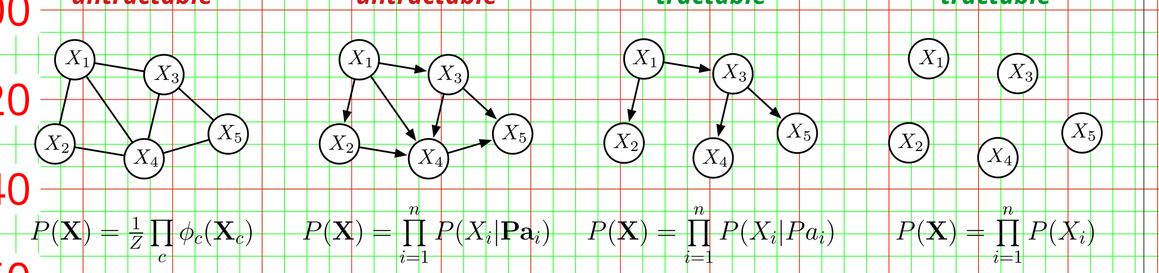
Machine Learning

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***.

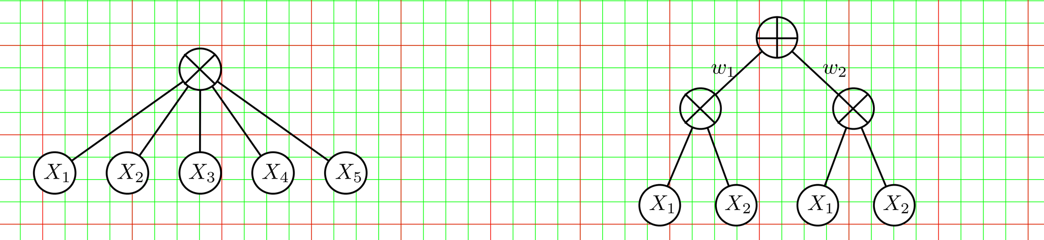


To guarantee polynomial inference, tractable models trade off model expressiveness.

Sum-Product Networks (SPNs) are DAGs *compiling* a pdf $P(\mathbf{X})$ into a ***deep*** architecture of **sum** and **product** nodes over univariate distributions $X_1, \ldots, X_n$ as leaves. The parameters of the network are the weights w_{ij} associated to sum nodes children edges.

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

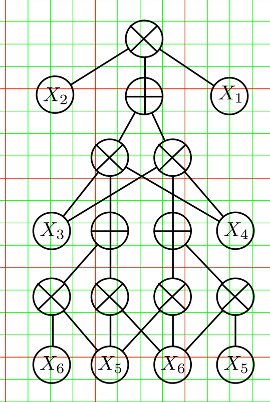
Products over nodes with different scopes (*decomposability*) and sums over nodes with same scopes (*completeness*) guarantee modeling a pdf (*validity*).



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 [5, 9]

How and why to perform structure learning

Fixed structures are hard to engineer and train (fully connected layers). Structure learning is more flexible and enables automatic latent features discovery.
Constraint-based search formulation. Discover hidden variables for sum node mixtures and independences for product node components:
- greedy top-down: KMeans on features *[1]*; alternating clustering on instances and independence tests on features, **LearnSPN** *[2]*
- greedy bottom up: merging feature regions by a *Bayesian-Dirichlet independence test*, and reducing edges by maximizing MI *[7]*
- **ID-SPN**: turning LearnSPN in log-likelihood guided expansion of sub-networks approximated by Arithmetic Circuits *[8]*

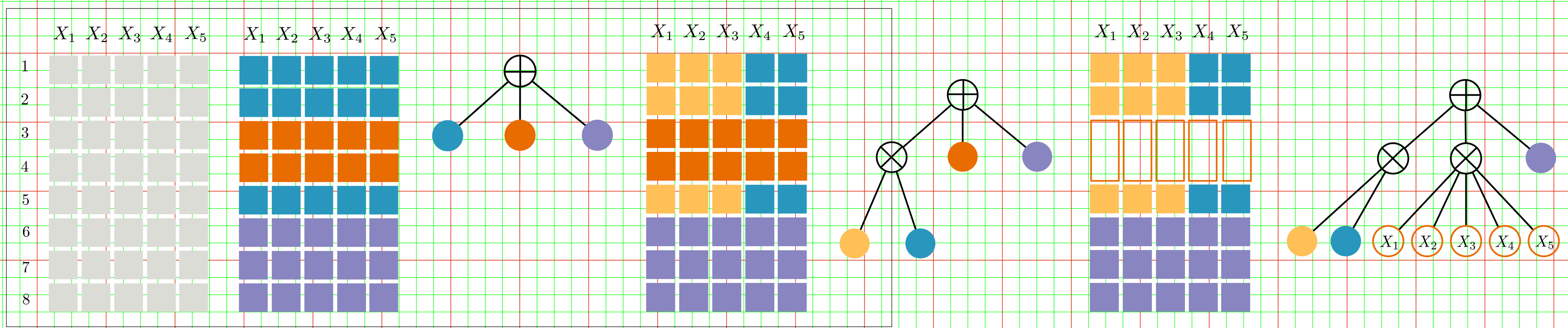
LearnSPN [2] builds a tree-like SPN by recursively split the data matrix:
- splitting columns in pairs by a greedy ***G Test*** based procedure with threshold ρ:

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

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

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

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



Simplifying by limiting node splits

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Regularizing by introducing tree distributions as leaves

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Strengthening by model averaging

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Experiments

Classical setting for ***generative*** graphical models structure learning [2]:
- 19 binary datasets from classification, recommendation, frequent pattern mining...[4] [3]
- Training 75% Validation 10% Test 15% splits (no cv)

Comparing both accuracy and structure quality:
- ***average log-likelihood*** on predicting test instances
- networks sizes (# edges)
- network depth (# alternated type layers)
- latent interactions captured (# number of parameters)

Comparing the state-of-the-art, LearnSPN, ID-SPN and MT [6], against our variations:
- SPN-B using only Binary splits
- SPN-BT with Binary splits and Trees as leaves
- SPN-BB combining Binary splits and Bagging
- SPN-BTB including all variants

Model selection via *grid search* in the same parameter space:
- $\lambda \in \{0.2, 0.4, 0.6, 0.8\}$,
- $\rho \in \{5, 10, 15, 20\}$,
- $m \in \{1, 50, 100, 500\}$,
- $\alpha \in \{0.1, 0.2, 0.5, 1.0, 2.0\}$

	# edges			# layers			# params		
	LearnSPN	SPN-B	SPN-BT	LearnSPN	SPN-B	SPN-BT	LearnSPN	SPN-B	SPN-BT
NLTCS	7509	1133	1133 (1125)	4	15	15	476	275	275
MSNBC	22350	4258	4258 (3996)	4	21	21	1680	1071	1071
KDDCup2k	44544	4272	4272 (4166)	4	25	25	753	760	760
Plants	55668	13720	5948 (1840)	6	23	20	3819	2397	490
Audio	70036	16421	4059 (478)	8	23	15	3389	2631	105
Jester	36528	10793	10793 (8587)	4	19	19	563	1932	1932
Netflix	17742	25009	4132 (203)	4	25	14	1499	4070	82
Accidents	48654	12367	10547 (6687)	6	25	26	5390	2708	1977
Retail	7487	1188	1188 (1153)	4	23	23	171	224	224
Pumsb-star	15247	12800	9984 (6175)	8	25	23	1911	2662	1680
DNA	17602	3178	4225 (2746)	6	13	12	947	884	1113
Kosarek	7993	8174	2216 (1311)	6	27	21	781	1462	242
MSWeb	17339	9116	7568 (6797)	6	27	34	620	1672	1446
Book	42491	9917	3503 (3485)	4	15	13	1176	1351	430
EachMovie	52693	20756	20756 (17861)	8	23	23	1010	2637	2637
WebKB	52498	45620	8796 (6874)	8	23	16	1712	6087	1128
Reuters-52	307113	77336	77336 (59197)	12	31	31	3641	8968	8968
BBC	318313	63723	63723 (41247)	16	27	27	1134	6147	6147
Ad	70056	23606	23606 (20079)	16	59	59	1060	1222	1222

Table : Structural quality results for the best validation models for LearnSPN, SPN-B and SPN-BT as the number of edges, layers and parameters. For SPN-BT are reported the number of edges considering those in the Chow-Liu leaves and without considering them (in parenthesis).

	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.

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