



Università degli Studi di Bari
Dipartimento di Informatica



LACAM
Machine Learning

Learning Sum-Product Networks

Nicola Di Mauro Antonio Vergari

September 2016

The need for SPN

Sum-Product Networks (SPNs) are a type of probabilistic model¹

- ▶ for Probabilistic Graphical Models (PGMs) there exist multi-purpose inference tools
 - ▶ the computational effort scales unproportional to the complexity of the graph
 - ▶ solution: using approximate inference

¹H. Poon and P. Domingos, *Sum-Product Network: a New Deep Architecture*, UAI 2011

The need for SPNs

Why should you work on SPNs?

- ▶ exact tractable inference
- ▶ NN for which structure learning is easy

SPNs represent probability distributions and a corresponding exact inference machine for the represented distribution at the same time

Representation

Density estimation

(Different kinds of) Inference

Different kinds of queries:

- ▶ $p(\mathbf{X})$ (evidence)
- ▶ $p(\mathbf{E}), \mathbf{E} \subset \mathbf{X}$ (marginals)
- ▶ $p(\mathbf{Q}|\mathbf{E}), \mathbf{Q}, \mathbf{E} \subset \mathbf{X}, \mathbf{Q} \cap \mathbf{E} = \emptyset$ (conditionals)
- ▶ $\arg \max_{\mathbf{q} \sim \mathbf{Q}} p(\mathbf{q}|\mathbf{E})$ (MPE assignment)
- ▶ complex queries

Tractable Probabilistic Models

Sum-Product Networks

Scopes

Structural Properties

Inference

Complete evidence

Marginal inference

MPE inference

Interpretation

Interpretation

- ▶ probabilistic model
- ▶ deep feedforward neural network

Network Polynomials

Arithmetic Circuits

Differences with ACs:

- ▶ probabilistic semantics
 - ▶ learning
 - ▶ sampling
- ▶ no shared weights

SPNs as NNs (I)

SPNs are a particular kind of ***labelled constrained*** and ***fully probabilistic*** neural networks.

Labelled: each neuron is associated a *scope*

Constrained: completeness and decomposability determine network topology.

Fully probabilistic: each valid sub-SPN is still a valid-SPN.

SPNs provide a direct encoding of the input space into a deep architecture → ***visualizing representations*** (back) into the ***input space***.

SPNs as NNs (II)

A classic MLP hidden layer computes the function:

$$h(\mathbf{x}) = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b})$$

SPNs can be reframed as *DAGs* of MLPs, each sum layer computing:

$$\mathbf{S}(\mathbf{x}) = \log(\mathbf{W}\mathbf{x})$$

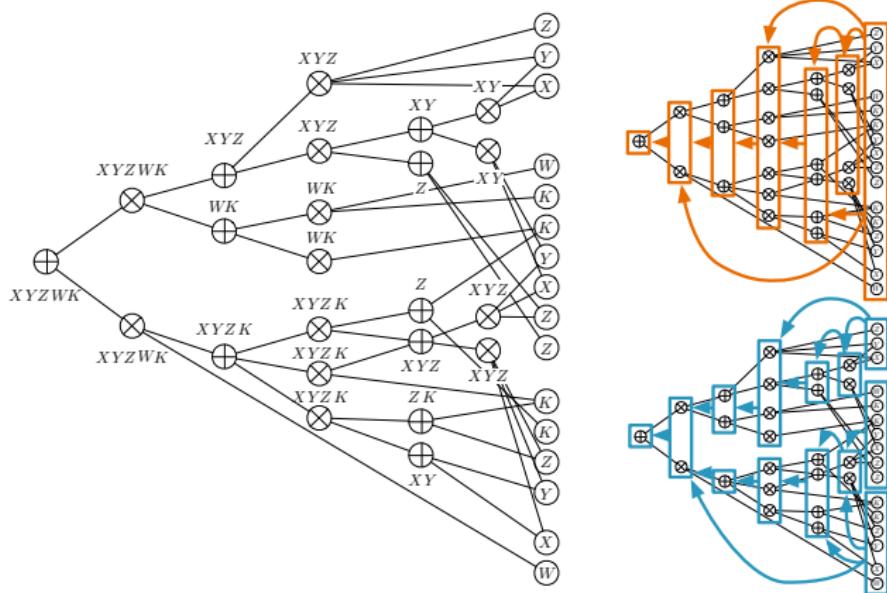
and product layers computing:

$$\mathbf{S}(\mathbf{x}) = \exp(\mathbf{P}\mathbf{x})$$

where $\mathbf{W} \in \mathbb{R}_+^{s \times r}$ and $\mathbf{P} \in \{0, 1\}^{s \times r}$ are the weight matrices:

$$\mathbf{W}_{(ij)} = \begin{cases} w_{ij} & \text{if } i \rightarrow j \\ 0 & \text{otherwise} \end{cases} \quad \mathbf{P}_{(ij)} = \begin{cases} 1 & \text{if } i \rightarrow j \\ 0 & \text{otherwise} \end{cases}$$

SPNs as NNs (III)



SPNs as NNs (IV): filters

Learned features as images maximizing neuron activations [Erhan et al. 2009]:

$$\mathbf{x}^* = \underset{\mathbf{x}, \|\mathbf{x}\|=\gamma}{\operatorname{argmax}} h_{ij}(\mathbf{x}; \boldsymbol{\theta}).$$

With SPNs, joint solution as an MPE assignment for all nodes (linear time):

$$\mathbf{x}_{|\text{sc}(n)}^* = \underset{\mathbf{x}}{\operatorname{argmax}} S_n(\mathbf{x}_{|\text{sc}(n)}; \mathbf{w})$$



→ scope length ($|\text{sc}(n)|$) correlates with feature abstraction level

SPNs as BNs I

Zhao and Poupart

SPNs as BNs II

Peharz

Myths about SPNs

SPNs are PGMs. false

SPNs are convolutional NNs. false

SPNs

Learning

Learning SPNs

Parameter learning: estimate \mathbf{w} from data considering an SPN as a latent RV model, or as a NN

Structure learning: build the network from data by assigning scores to tentative structures or by exploiting constraints

How to learn a “complete” SPN:

- ▶ handcrafted structure, then parameter learning [Gens and Domingos 2012; Poon and Domingos 2011]
- ▶ random structures, then parameter learning [Rashwan et al. 2016]
- ▶ structure learning, then parameter learning (fine tuning) [Zhao, Adel, et al. 2016]
- ▶ learn both weight and structure at the same time [Adel et al. 2015; Gens and Domingos 2013; Rooshenas and Lowd 2014; Antonio Vergari et al. 2015]...

Structure Learning

Score vs constraint based search. No closed form for likelihood scores, need heuristics [Rooshenas and Lowd 2014].

No need for it by exploiting the inner nodes probabilistic semantics

Learning graph vs tree structures: Easier to learn a tree SPN (sometimes SPT) with greedy approaches. Graph SPNs may be more compact and expressive efficient.

Top-down vs bottom-up approaches: iteratively cluster data matrix (top-down) or start by the marginal RVs (bottom-up)

LearnSPN [Gens and Domingos 2013] is a *greedy, top down, constraint based* learner for **tree** SPNs

- First principled top-down learner, inspired many algorithms and variations.
- Surprisingly simple and accurate.

LearnSPN (I)

Build a tree 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

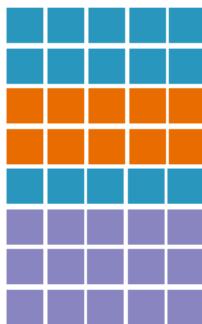
Hyperparameter space: $\{\rho, \lambda, m, \alpha\}$.

LearnSPN (II)

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

LearnSPN (II)

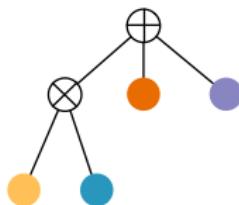
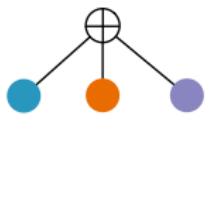
$X_1 \ X_2 \ X_3 \ X_4 \ X_5$



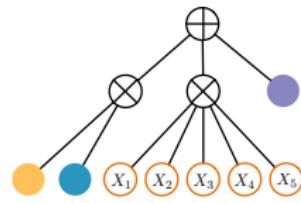
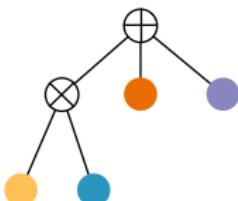
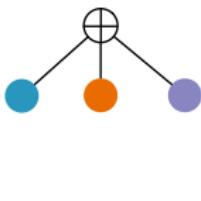
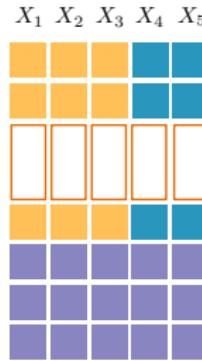
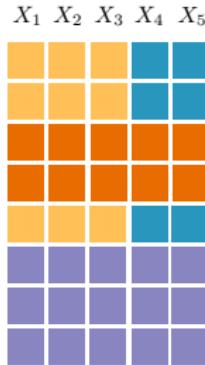
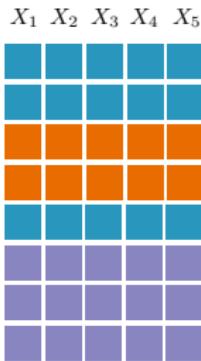
LearnSPN (II)

X_1	X_2	X_3	X_4	X_5
Blue	Blue	Blue	Blue	Blue
Blue	Blue	Blue	Blue	Blue
Orange	Orange	Orange	Orange	Orange
Orange	Orange	Orange	Orange	Orange
Blue	Blue	Blue	Blue	Blue
Purple	Purple	Purple	Purple	Purple
Purple	Purple	Purple	Purple	Purple

X_1	X_2	X_3	X_4	X_5
Yellow	Yellow	Yellow	Blue	Blue
Orange	Orange	Orange	Orange	Orange
Yellow	Yellow	Yellow	Blue	Blue
Purple	Purple	Purple	Purple	Purple
Purple	Purple	Purple	Purple	Purple



LearnSPN (II)



Tweaking LearnSPN

LearnSPN 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 → *slow down the two processes*

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 → *look for deeper networks*

Tractable leaf estimation. But too strong naive factorization independence assumptions, hard to regularize → *learn tree distributions as leaves*

ML estimations are effective. But they are not robust to noise, they can overfit the training set easily → *learn bagged sum nodes*

Why Structure Quality Matters

Tractable inference is guaranteed *if the network size is polynomial* in $|\mathbf{X}|$.

Network **size** influences inference complexity: smaller networks, faster inference!

→ Comparing network sizes is better than comparing inference times

Network **depth** influences *expressive efficiency* [Martens and Medabalimi 2014; Zhao, Melibari, et al. 2015].

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

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

LearnSPN-b

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

Idea: slow them down the processes by limiting the number of nodes to split to the minimum. LearnSPN-b, binary splitting $k = 2$.

- one hyperparameter less, λ .
- not committing to complex structures too early
- reducing node out fan increases the depth
- same expressive power as LearnSPN structures
- statistically same (or better) accuracy, smaller networks



LearnSPN-b: depth VS size

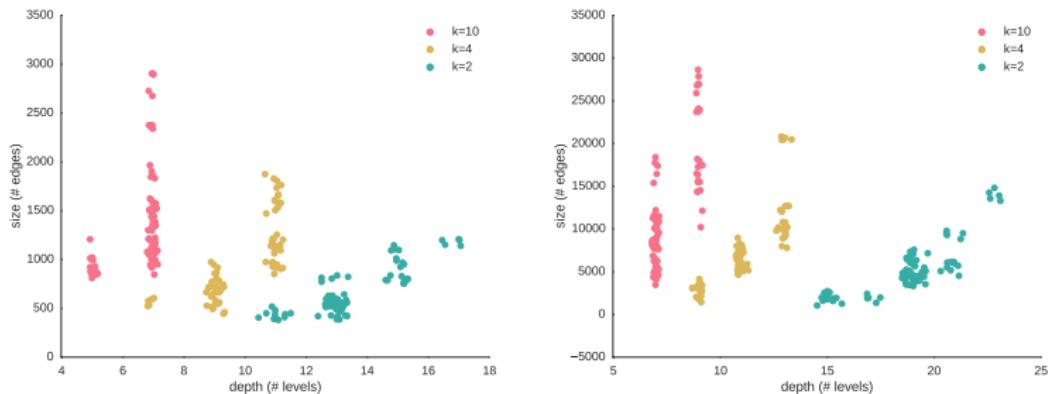


Figure : Network sizes VS depths while varying the max number of sum node children splits ($k \in \{10, 4, 2\}$). Each dot is an experiment in the grid search hyperparameter space performed by LearnSPN-b on NLTCS (left) and Plants (right).

LearnSPN-b: best II VS size

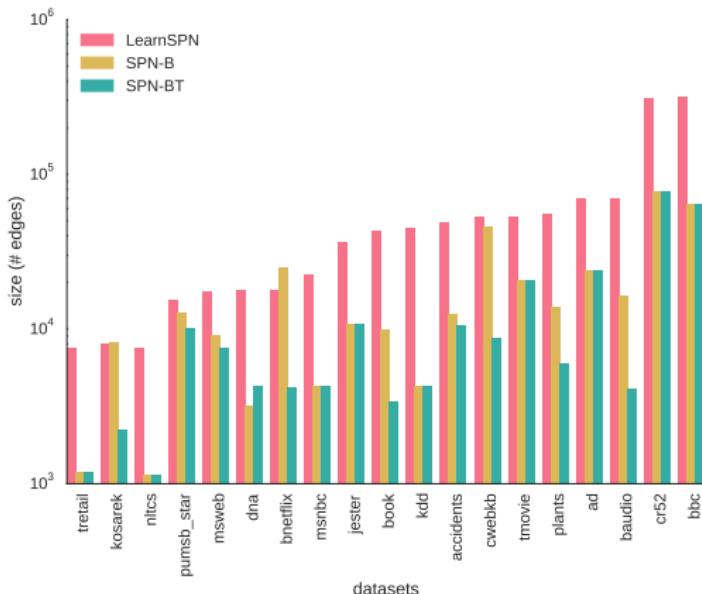


Figure : Comparing network sizes for the networks scoring the best log-likelihoods in the grid search as obtained by LearnSPN, LearnSPN-b and LearnSPN-bT for each dataset.

Other variations on LearnSPN

ACs modeling leaves by performing a greedy score search. **ID-SPN** best log-likelihood learner (but lots of hyperparameters).

Freely available in the Libra² toolkit. [Rooshenas and Lowd 2014]

Looking for **correlations instead of independencies** via matrix factorizations.

Splitting matrix rows and columns at the same time: SPN-SVD.

It can cope with continuous data [Adel et al. 2015]

Post-learning **merging sub-SPNs** that model “similar” distributions.

Reducing network sizes [Rahman and Gogate 2016].

Learning Relational SPNs on **first order data** represented in Tractable Markov Logic (TML), LearnRSPN [Nath and Domingos 2015].

²<http://libra.cs.uoregon.edu/>

Other Tendencies in Structure Learning

Learning deterministic structures which enable closed form log-likelihood and weight estimation.

Selective SPNs, enabling efficient Stochastic Local Search [Peharz, Gens, et al. 2014].

Mixing latent and deterministic mixtures as sum nodes (a Cutset Network is an SPN!). [Rahman and Gogate 2016]

Learning DAGs structures instead of trees.

Substituting sub-structures with more complex ones by cloning mixtures. [Dennis and Ventura 2015]

Template learning for sequence models. Stochastic local search over well defined constrained structures. Dynamic SPNs [Melibari et al. 2016] → PGM'16!

Parameter Learning

Non convex optimization, solvable with iterative methods like: GD, EM,...and their online variants

Use backpropagation (\rightarrow differential approach) to compute $\nabla_{\mathbf{w}} S(\mathbf{x})$

Hard/Soft gradients

Some issues:

- ▶ vanishing gradients
- ▶ hyperparameter choices

“Hard” gradients

Hard/Soft Parameter Learning

	soft	
Generative Gradient	$\frac{\partial S(\mathbf{x})}{\partial w_{pc}} = S_c(\mathbf{x}) \frac{\partial S(\mathbf{x})}{\partial S_p(\mathbf{x})}$	$\#\{w_{pc} \in \text{MPE-1}\}$
Discriminative Gradient	$\frac{1}{S(\mathbf{y} \mathbf{x})} \frac{\partial S(\mathbf{y} \mathbf{x})}{\partial w_{pc}} - \frac{1}{S(*) \mathbf{x})} \frac{\partial S(*) \mathbf{x})}{\partial w_{pc}}$	
Generative Posterior	$p(H_p = c \mathbf{x}) \propto \frac{1}{S(\mathbf{x})} \frac{\partial S(\mathbf{x})}{\partial S_p(\mathbf{x})} S_c(\mathbf{x}) w_{pc}$	$p(H_p)$

Bayesian Parameter Learning

Parameter Learning VS LearnSPN

	LearnSPN ³	LearnSPN-b ⁴	CVB-SPN ⁵	OBMM ⁶	SGD ⁷	EM ⁸	SEG ⁹
NLTCS	-6.11	-6.05	-6.08	-6.07	-8.76	-6.31	-6.85
MSNBC	-6.11	-6.04	-6.29	-6.03	-6.81	-6.64	-6.74
KDDCup2k	-2.18	-2.14	-2.14	-2.14	44.53	-2.20	-2.34
Plants	-12.98	-12.81	-12.86	-15.14	-21.50	-17.68	-33.47
Audio	-40.50	-40.57	-40.36	-40.70	-49.35	-42.55	-46.31
Jester	-53.48	-53.53	-54.26	-53.86	63.89	-54.26	-59.48
Netflix	-57.33	-57.73	-60.69	-57.99	64.27	-59.35	-64.48
Accidents	-30.04	-29.34	-29.55	-42.66	53.69	-43.54	-45.59
Retail	-11.04	-10.94	-10.91	-11.42	-97.11	-11.42	-14.94
Pumsb-star	-24.78	-23.31	-25.93	-45.27	-128.48	-46.54	-51.84
DNA	-82.52	-81.91	-86.73	-99.61	-100.70	-100.10	-105.25
Kosarek	-10.99	-10.72	-10.70	-11.22	34.64	-11.87	-17.71
MSWeb	-10.25	-9.83	-9.89	-11.33	-59.63	-11.36	-20.69
Book	-35.89	-34.30	-34.44	-35.55	-249.28	-36.13	-42.95
EachMovie	-52.49	-51.36	-52.63	-59.50	-227.05	-64.76	-84.82
WebKB	-158.20	-154.28	-161.46	-165.57	-338.01	-169.64	-179.34
Reuters-52	-85.07	-83.34	-85.45	-108.01	-407.96	-108.10	-108.42
20-Newsgrp	-155.93	-152.85	-155.61	-158.01	-312.12	-160.41	-167.89
BBC	-250.69	-247.30	-251.23	-275.43	-462.96	-274.82	-276.97
Ad	-19.73	-16.23	-19.00	-63.81	-638.43	-63.83	-64.11

³Gens and Domingos 2013.

Parameter Learning

Why learning parameters

Representation Learning

Extracting Embeddings

Exploiting SPNs as feature extractors

Given an SPN S , generate a dense vector

$$\mathbf{e}^i = f_S(\mathbf{x}^i)$$

Issues with SPNs as NNs:

- ▶ layer-wise extraction may be arbitrary
- ▶ power law distribution of nodes by scopes
- ▶ scope lengths as proxy for feature abstraction levels (see filter visualizations)

How to extract embeddings?

- ▶ from node outputs (one query)
 - ▶ all (non-leaf) nodes
 - ▶ sum/product nodes only
 - ▶ with a certain scope length
 - ▶ aggregating node outputs by scope
- ▶ from several queries evaluations (root outputs)

Supervised classification

Experimental settings

Embeddings (I)

Table : Test set accuracy scores for the embeddings extracted with the best SPN, RBM models and with the baseline LR model on all datasets. Bold values denote significantly better scores than all the others for a dataset.

	LR	SPN-I	SPN-II	SPN-III	RBM-5h	RBM-1k	RBM-5k
REC	69.28	77.31	97.77	97.66	94.22	96.10	96.36
CON	53.48	67.48	78.31	84.69	67.55	75.37	79.15
OCR	75.58	82.60	89.95	89.94	86.07	87.96	88.76
CAL	62.67	59.17	65.19	66.62	67.36	68.88	67.71
BMN	90.62	95.15	97.66	97.59	96.09	96.80	97.47

Embeddings (II)

Table : Test set accuracy scores for the embeddings extracted with SPN models and filtered by node type. Results for SPN-III embeddings filtered by Small , Medium and Large scope lengths are reported in columns 8-10. Bold values denote significantly better scores than all the others. ▲ indicates a better score than an RBM embedding with greater or equal size. ▽ indicates worse scores than an RBM embedding with smaller or equal size.

	SPN-I		SPN-II		SPN-III		SPN-III		
	sum	prod	sum	prod	sum	prod	S	M	L
REC	72.46	62.25	98.03▲	97.06▲	98.00▲	97.04▲	88.73	98.45▲	93.91
CON	62.36	64.03	77.13▲	76.07▲	83.59▲	82.06▲	70.51▽	77.18	83.32▲
OCR	74.19	81.58	89.73▲	88.78▲	90.02▲	89.32	87.22▽	89.29▲	88.19▲
CAL	38.19	56.95	62.64	64.80	66.58▽	66.40▽	63.37▽	66.23▽	66.10
BMN	93.50	94.75	97.67	96.90▽	97.80	97.20▽	96.02▽	97.42▽	97.38

Embeddings (III)

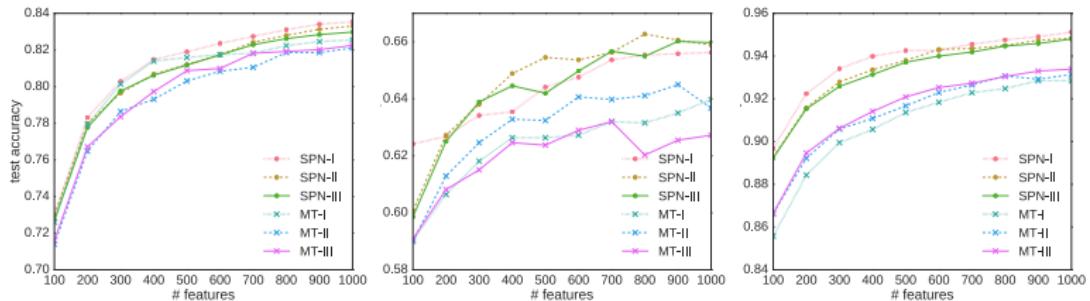
Table : Test set accuracy scores for the embeddings extracted with SPN models by aggregating node outputs with the same scope. Results for when leaves are not counted in the aggregation (no-leaves columns) are reported alongside the case in which they are considered (leaves columns). Bold values denote significantly better scores than all the others for each dataset. ▲ indicates a better score than an RBM embedding with greater or equal size. ▽ indicates worse scores than an RBM embedding with smaller or equal size.

	SPN-I		SPN-II		SPN-III	
	no-leaves	leaves	no-leaves	leaves	no-leaves	leaves
REC	72.47	75.92▽	97.94▲	97.99▲	97.94▲	98.02▲
CON	62.35	66.49▽	77.21▲	78.05	83.52▲	83.84▲
OCR	74.32	81.85	89.71▲	89.68▲	89.90▲	89.91▲
CAL	38.10	63.19▽	62.59	62.76▽	66.49▽	66.58▽
BMN	93.51	94.83▽	97.64▲	97.62▲	97.80	97.80

Random Marginal Queries

Generate embeddings by asking several random queries to a black box density estimator.

Eg. marginals: $e_j^i = P_\theta(\mathbf{Q}_j = \mathbf{x}_{\mathbf{Q}_j}^i)$, according to estimator θ where $\mathbf{Q}_j \subseteq \mathbf{X}, j = \dots, k$.



Encoding/Decoding Embeddings

MPN as autoencoders¹⁰.

¹⁰Vergari et al. Encoding and Decoding Representations with Sum-Product Networks, 2016, to appear

Applications

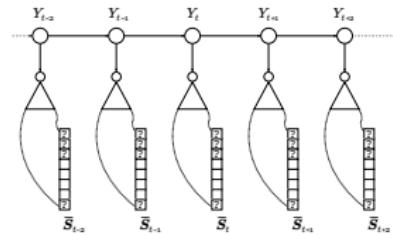
Applications I: computer vision

Applications II: language modeling

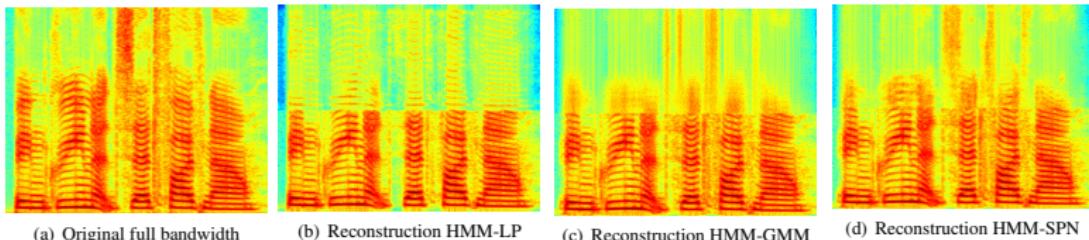
Applications III: activity recognition

Applications IV: speech

SPNs to model the joint pdf of observed RVs in HMMs (HMM-SPNs).



State-of-the-art high frequency reconstruction (MPE inference)



Trends & What to do next

Scalable structure learning Continuous RVs structure learning

End-to-end training with hybrid NN architectures

References

awesome-spn

A curated and structured list of resources about SPNs¹¹.

<https://github.com/arranger1044/awesome-spn>

¹¹ Inspired by the SPN page <http://spn.cs.washington.edu/> at the Washington University