Towards Representation Learning with Tractable Probabilistic Models

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Tractable Probabilistic Models

Density estimation is the unsupervised task of learning an estimator for the joint probability distribution $p(\mathbf{X})$ from a set of i.i.d. samples $\{\mathbf{x}_i\}_{i=1}^m$ over RVs $\mathbf{X}$

Once such a density estimator is learned, one uses it to answers probabilistic queries about configurations on $p(\mathbf{X})$, that is to do***inference***

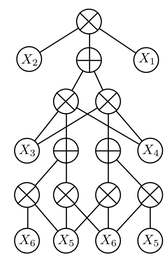
Operations that may be required to be efficient are
- $p(\mathbf{X} = \mathbf{x})$ (evidence)
- $p(\mathbf{E}), \mathbf{E} \subset \mathbf{X}$ (marginals)
- $p(\mathbf{Q}|\mathbf{E}), \mathbf{Q}, \mathbf{E} \subset \mathbf{X}, \mathbf{Q} \cap \mathbf{E} = \emptyset$ (conditionals)
- $\arg\max_{\mathbf{q} \sim \mathbf{Q}} p(\mathbf{q}|\mathbf{E})$ (MPE assignment)
- $Z = \sum_{\mathbf{x} \sim \mathbf{X}} \phi(\mathbf{x})$ (partition function)

Tractable Probabilistic Models (**TPMs**) are density estimators for which some kind of inference is *tractable*, i.e. polynomial in the number of r.v.s or their domains.

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 [3].

Representation Learning with TPMs

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 *[4]*; ***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.

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 *[5]*. 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.

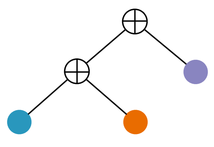
LearnSPN is too greedy and the resulting SPNs are overcomplex networks that may not generalize well. ***Structure quality desiderata***: *smaller* but *accurate*, *deeper* but not wider, SPNs.

Random query embedding extraction

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.



Input: a set of instances $\mathcal{D} = \{\mathbf{x}^i\}_{i=1}^m$ over r.v.s $\mathbf{X} = \{X_1, \ldots, X_n\}$, k as the number of features to generate
Output: a set of embeddings $\mathcal{E} = \{\mathbf{e}^i\}_{i=1}^m, \mathbf{e}^i \in \mathbb{R}^k$
$\theta \leftarrow$ learnDensityEstimator$(\mathcal{D})$
$\mathcal{E} \leftarrow \{\}$
for $j = 1, \ldots, k$ **do**
  $\mathbf{Q}_j \leftarrow$ selectRandomRVs$(\mathbf{X})$
  for $i = 1, \ldots, m$ **do**
    $e^i_j = p_\theta(\mathbf{x}^i_{\mathbf{Q}_j})$
  $\mathcal{E} \leftarrow \mathcal{E} \cup \{\mathbf{e}^i\}$
return $\mathcal{E}$

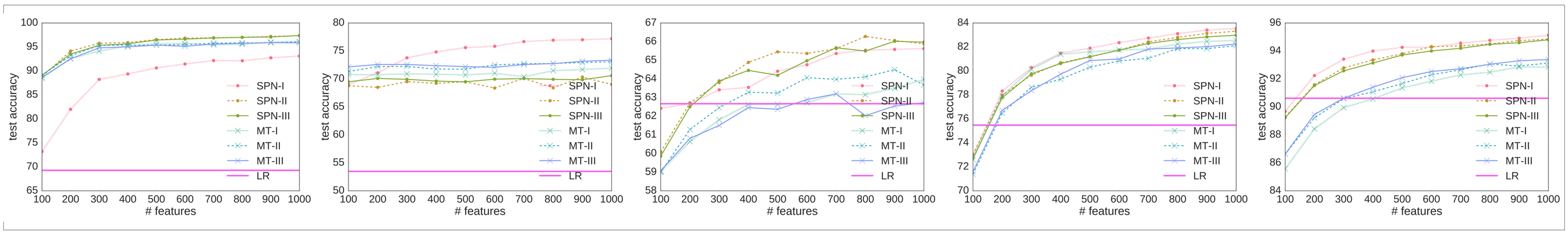
Input: a set of instances $\mathcal{D} = \{\mathbf{x}^i\}_{i=1}^m$ over r.v.s $\mathbf{X} = \{X_1, \ldots, X_n\}$, s as the number of patches to extract, d as the patch length,
Output: a set of embeddings $\mathcal{E} = \{\mathbf{e}^i\}_{i=1}^m, \mathbf{e}^i \in \mathbb{R}^k$
$\mathcal{R} \leftarrow \{\}$
for $i = 1, \ldots, s$ **do**
  $\mathbf{x}^{\text{rand}} \leftarrow$ selectRandomSample$(\mathcal{D})$
  $\mathbf{r}^i \leftarrow$ extractRandomPatch$(\mathbf{x}^{\text{rand}}, d)$
  $\mathcal{R} \leftarrow \mathcal{R} \cup \{\mathbf{r}^i\}$
$\theta \leftarrow$ learnDensityEstimator$(\mathcal{R})$
$\mathcal{E} \leftarrow \{\}$
for $i = 1, \ldots, m$ **do**
  $j \leftarrow 0$
  for each patch $\mathbf{q}^i, |\mathbf{q}^i| = d$ in $\mathbf{x}^i$ **do**
    $e^i_j = p_\theta(\mathbf{q}^i)$
    $j \leftarrow j + 1$
  $\mathcal{E} \leftarrow \mathcal{E} \cup \{\mathbf{e}^i\}$
return $\mathcal{E}$

Evaluation

Empirical evaluation of the random marginal query approach:
- 5 binary image datasets: rectangles (REC), convex (CON), ocr_letters (OCR), caltech101 (CAL), binary MNIST (BMN)
- OVR L2-reg logistic regressor for all representations, LR baseline

- 3 SPN models trained with LearnSPN-b [6] with $m \in \{500, 100, 50\}$ (SPN-I, SPN-II, SPN-III)
- 3 Mixture of trees models with $k \in \{3, 15, 30\}$ (MT-I, MT-II, MT-III)

- 1000 randomly generated marginal queries corresponding to adjacent pixels in a rectangular image patch having minimum sizes of 2 pixels and maximum of 7 pixels for OCR and 10 pixels for the remaining datasets



References

[1] Aaron Dennis and Dan Ventura. "Learning the Architecture of Sum-Product Networks Using Clustering on Varibles". In: *Advances in Neural Information Processing Systems 25*. Curran Associates, Inc., 2012, pp. 2033–2041.

[2] Robert Gens and Pedro Domingos. "Learning the Structure of Sum-Product Networks". In: *Proceedings of the ICML 2013*. 2013, pp. 873–880.

[3] James Martens and Venkatesh Medabalimi. "On the Expressive Efficiency of Sum Product Networks". In: *CoRR* abs/1411.7717 (2014).

[4] Robert Peharz, Bernhard Geiger, and Franz Pernkopf. "Greedy Part-Wise Learning of Sum-Product Networks". In: *ECML-PKDD 2013*. 2013.

[5] Amirmohammad Rooshenas and Daniel Lowd. "Learning Sum-Product Networks with Direct and Indirect Variable Interactions". In: *Proceedings of the 31st International Conference on Machine Learning*. 2014, pp. 710–718.

[6] Antonio Vergari, Nicola Di Mauro, and Floriana Esposito. "Simplifying, Regularizing and Strengthening Sum-Product Network Structure Learning". In: *ECML-PKDD 2015*. 2015.

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