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 $\mathbf{X}$

Given such an estimator, one uses it to answers probabilistic queries about configurations on $\mathbf{X}$, i.e. to do ***inference***

Different kinds of inference query kinds:

- $p(\mathbf{X} = \mathbf{x})$ pointwise evidence (EVI)
- $p(\mathbf{E}), \mathbf{E} \subset \mathbf{X}$ marginals (MAR)
- $p(\mathbf{Q}|\mathbf{E}), \mathbf{Q}, \mathbf{E} \subset \mathbf{X}, \mathbf{Q} \cap \mathbf{E} = \emptyset$ conditionals (CON)
- $\arg\max_{\mathbf{q} \sim \mathbf{Q}} p(\mathbf{q}|\mathbf{E})$ MPE assignments (MPE)
- $Z = \sum_{\mathbf{x} \sim \mathbf{X}} \phi(\mathbf{x})$ partition function (Z)
- sampling: generate $\mathbf{x} \sim p(\mathbf{X})$ (SAM)

Good estimators guarantee *exact* and *efficient* inference.

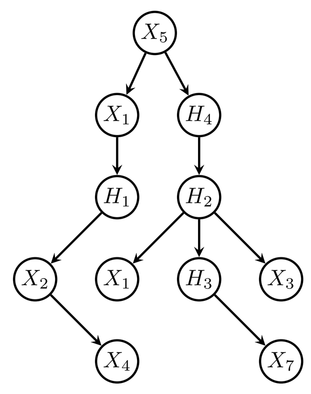
Tractable Probabilistic Models (**TPMs**) are density estimators for which some kind of inference is *tractable*, i.e. polynomial in the number of r.v.s or their domains.

Different TPMs guarantee different inference kinds to be tractable.

TPMs can be roughly classified into:

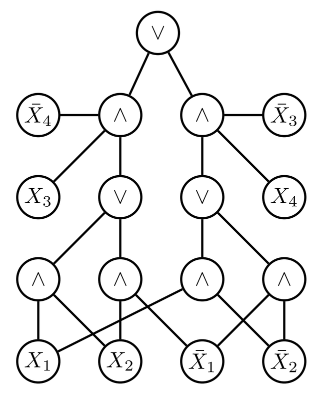
- ***low-treewidth*** Probabilistic Graphical Models (PGMs)(*)
- ***computational graphs*** compiling $p(\mathbf{X})$ ($^\times$)
- ***neural autoregressive*** models ($^+$)

Tree distributions [6] (*)



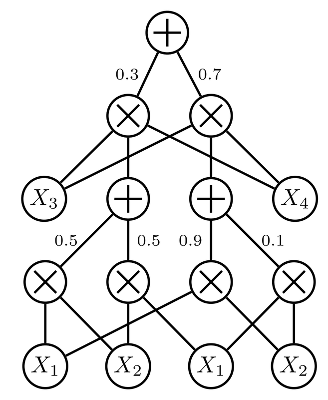
✓EVI, ✓SAM, ✓MAR, ✓CON, ✓MPE, ✓Z

d-DNNF [3] ($^\times$)



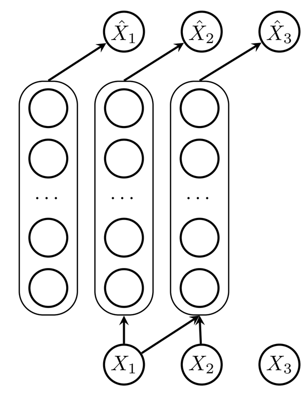
✓EVI, ✗SAM, ✓MAR, ✓CON, ✓MPE, ✓Z

Sum-Product Networks [7] ($^\times$)



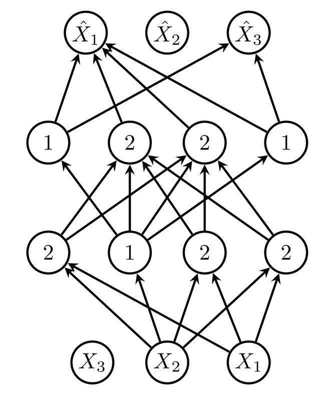
✓EVI, ✓SAM, ✓MAR, ✓CON, ✗MPE, ✓Z

NADEs [5] ($^+$)



✓EVI, ✓SAM, ✗MAR, ✗CON, ✗MPE, ✗Z

MADEs [4] ($^+$)



✓EVI, ✓SAM, ✗MAR, ✗CON, ✗MPE, ✗Z

Representation Learning with TPMs

Representation Learning deals with generating new representations for the initial data $\{\mathbf{x}^i\}_{i=1}^m$, e.g. ***embeddings*** $\{\mathbf{e}^i | \mathbf{e}^i \in \mathbb{R}^k\}_{i=1}^m$, k-dimensional continuous arrays. Once learned, one can employ them in new tasks such as supervised classification or clustering [2].

Given a TPM θ we want to generate an embedding such as:

$$\mathbf{e}^i = f_{p,\theta}(\mathbf{x}^i)$$

for each sample, with f being a transformation provided by θ estimating the probability distribution p.

Simple idea: exploit the *geometric space* induced by p, e.g. P-kernels, Fisher vectors... [8], but:

- model dependent extraction
- closed form analytical derivation needed

We argue that TPMs can be employed as *black box* embedding extractors, on a common ground, by answering generated templated queries.

We define two approaches exploiting a random query generator schema:

I templates are constructed by **random marginal queries**, i.e. generating subsets of r.v.s $\mathbf{Q}_j \subseteq \mathbf{X}, j = 1 \ldots, d$:

$$e_j^i = p_\theta(\mathbf{Q}_j = \mathbf{x}^i_{\mathbf{Q}_j})$$

II generating a dataset of random *patches* from samples, then training a TPM θ on it; embeddings are generated by evaluating θ a sliding "*window*" of size d along the samples

$$e_j^i = p_\theta(\mathbf{q}^i), \forall \mathbf{q}^i \sim \mathbf{x}^i, |\mathbf{q}^i| = d$$

Tractable inference is mandatory: for a congruous embedding size k, one has to perform $k \cdot m$ queries, e.g. on training split of BMNIST $k = 10^3, m = 5 \cdot 10^4 \rightarrow 5 \cdot 10^7$ evals for approach I

Experimental Design

Planning an extensive experimentation comprising at least two TPMs from each family class, on a wide range of query types

Empirical evaluation of approach I on five binary image datasets used for classification:

- rectangles (REC), 28×28 pixels, wide VS tall rectangles
- convex (CON), 28×28 pixels, convex VS concave shapes
- ocr_letters (OCR), 16×8 pixels, ten digits
- caltech101 (CAL), 28×28 pixels, 101 object shapes
- binary MNIST (BMN), 28×28 pixels, ten digits

Learning the structure of *differently regularized* TPMs on RVs $\mathbf{X}$ alone (unsupervised) to compare different *model capacities*:

- 3 SPN architectures trained with LearnSPN-b [9] with hyperparameters: $\rho = 15$ for OCR and $\rho = 20$ for all the rest, $m \in \{500, 100, 50\}$ ($\rightarrow$ SPN-I, SPN-II, SPN-III), then grid search on $\alpha \in \{0.1, 0.2, 0.5, 1.0, 2.0\}$
- 3 Mixture of trees models (MT) [6] with $k \in \{3, 15, 30\}$ components ($\rightarrow$ MT-I, MT-II, MT-III) trained with EM

Extracting embeddings, then training a linear classifier on top of them to predict Y (supervised):

- OVR L2-reg logistic regressor for all representations, grid search for regularization coefficient C value in $\{0.0001, 0.001, 0.01, 0.1, 1.0\}$
- baseline with initial representations ($\rightarrow$ LR)

Generating random queries:

- up to 1000 randomly generated marginal queries
- generating RVs over adjacent pixels in rectangular patches of min sizes of 2, max of 7 pixels for OCR and 10 pixels for the others

Random query embedding extraction

Approach I demands models for which marginals can be tractable

- more flexible: other kinds of inference kinds can be embedded, e.g. more complex query types [1]

Algorithm 1 randQueryEmbedding($\mathcal{D}$, k)

```
Input: a set of instances D = {x^i}_{i=1}^m over r.v.s
       X = {X_1, ..., X_n}, k as the number of features to generate
Output: a set of embeddings E = {e^i}_{i=1}^m, e^i ∈ R^k
θ ← learnDensityEstimator(D)
E ← {}
for j = 1, ..., k do
    Q_j ← selectRandomRVs(X)
    for i = 1, ..., m do
        e_j^i = p_θ(x^i_{Q_j})
    E ← E ∪ {e^i}
return E
```

Approach II requires only tractable pointwise evidence

- largely employable: many more models can answer pointwise queries in a tractable way

Algorithm 1 randPatchEmbedding($\mathcal{D}$, s, d)

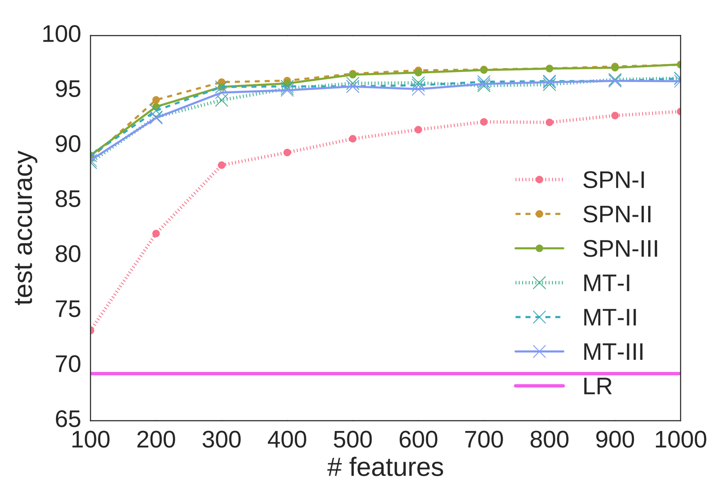
```
Input: a set of instances D = {x^i}_{i=1}^m over r.v.s X = {X_1, ..., X_n}, s
       as the number of patches to extract, d as the patch length,
Output: a set of embeddings E = {e^i}_{i=1}^m, e^i ∈ R^k
R ← {}
for i = 1, ..., s do
    x^rand ← selectRandomSample(D)
    r^i ← extractRandomPatch(x^rand, d)
    R ← R ∪ {r^i}
θ ← learnDensityEstimator(R)
E ← {}
for i = 1, ..., m do
    j ← 0
    for each patch q^i, |q^i| = d in x^i do
        e_j^i = p_θ(q^i)
        j ← j + 1
    E ← E ∪ {e^i}
return E
```

Results

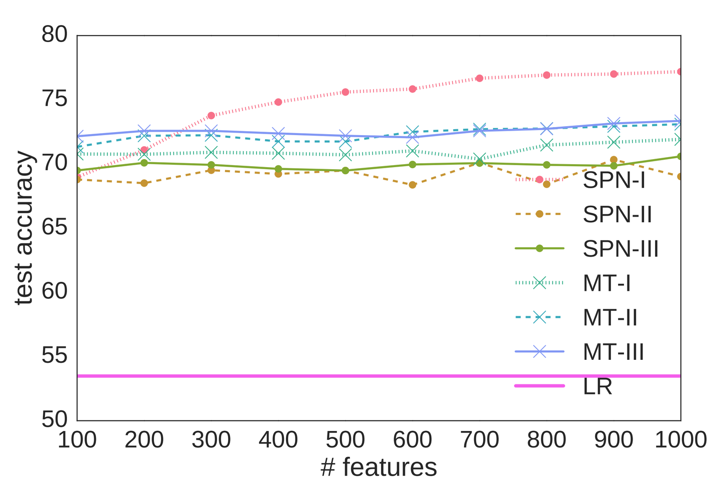
For all models, less than 300 features to beat the LR baseline
$\rightarrow$ the geometric space induced is meaningful/useful

SPN embeddings outperform **MT** ones all datasets, but CAL
$\rightarrow$ MT scoring best likelihoods on $\mathbf{X}$ but worst accuracies for Y

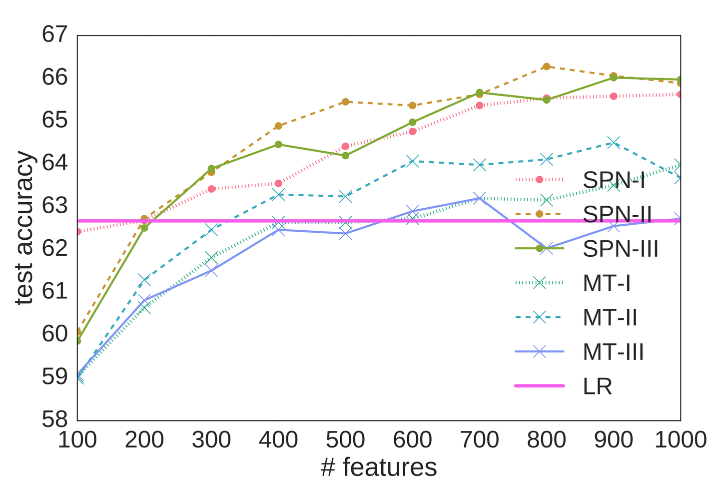
More regularized models perform better than specialized ones
$\rightarrow$



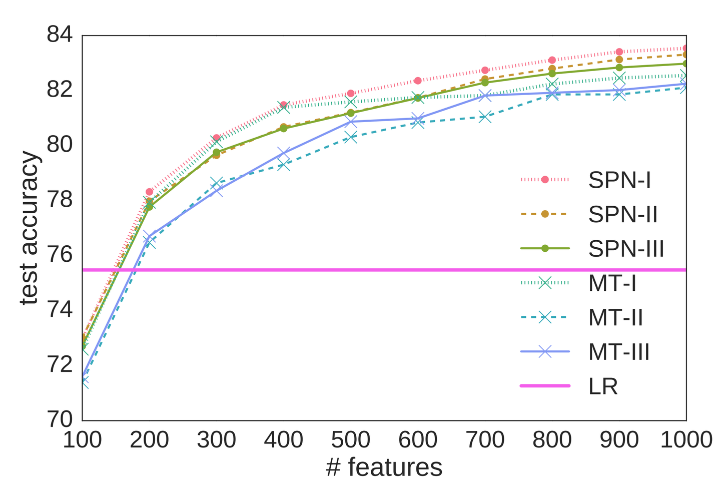
REC



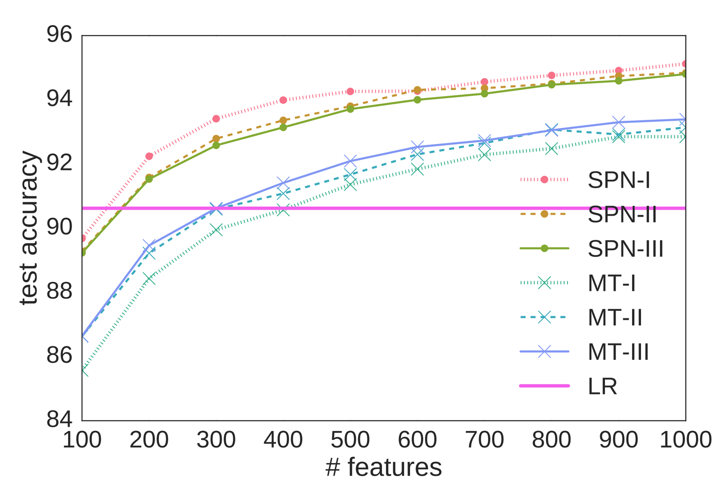
CON



OCR



CAL



BMN

References

[1] Jessa Bekker et al. "Tractable Learning for Complex Probability Queries". In: *Advances in Neural Information Processing Systems 28 (NIPS)*. 2015.
[2] Yoshua Bengio, Aaron C. Courville, and Pascal Vincent. "Unsupervised Feature Learning and Deep Learning: A Review and New Perspectives". In: *CoRR* abs/1206.5538 (2012).
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[4] Mathieu Germain et al. "MADE: Masked Autoencoder for Distribution Estimation". In: *CoRR* abs/1502.03509 (2015).
[5] Hugo Larochelle and Iain Murray. "The Neural Autoregressive Distribution Estimator". In: *International Conference on Artificial Intelligence and Statistics*. 2011, pp. 29–37.
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[8] John Shawe-Taylor and Nello Cristianini. *Kernel Methods for Pattern Analysis*. New York, NY, USA: Cambridge University Press, 2004. ISBN: 0521813972.
[9] Antonio Vergari, Nicola Di Mauro, and Floriana Esposito. "Simplifying, Regularizing and Strengthening Sum-Product Network Structure Learning". In: *ECML-PKDD 2015*. 2015.

Links

paper available at:
`https://arxiv.org/abs/1608.02341`
code available at:
`https://github.com/arranger1044/spyn-repr`
more references:
`https://github.com/arranger1044/awesome-spn`

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