





Automatic Bayesian **Density Analysis**

Antonio Vergari

Max-Plank-Institute IS

Zoubin Ghahramani University of Cambridge

Aleiandro Molina

TU Darmstadt

Kristian Kersting TI I Darmstadt

Robert Peharz University of Cambridge

Isabel Valera Max-Plank-Institute IS

31st January 2019 - AAAI19 Honolulu

In a nutshell

or why should you care about SPNs

A short tutorial on

Sum-Product Networks (SPNs) [Poon and Domingos 2011]

an appealing deep and tractable density estimator allowing exact inference

Plus, SPNs can be *interpreted* as *hierarchical latent variable* (LV) probabilistic models, *Multi-layer perceptrons*, and special kind of *Arithmetic Circuits* and even *Bayesian Networks*

Briefly reviewing representation capabilities, *inference* and *learning* schemes with SPNs

Ultimately touching some *applications*, extensions and research ideas

Notation

```
X, Y, Z, \ldots
                                                                                                        random variables (RVs)
\mathsf{val}(X)
                                                                                                                  support of RV X
x \sim X
                                                      x is drawn/distributed according to X or x \in \mathsf{val}(X)
\mathbf{X} = (X_1, X_2, \dots, X_n)
                                                                                                               ordered set of RVs
\mathbf{x} \sim \mathbf{X}, \mathbf{x} = \langle x_1, x_2, \dots, x_n \rangle
                                                                                                multivariate sample from X
                                                                               restriction of sample {f x} to RVs {f Y}\subset {f X}
\mathbf{x}_{|\mathbf{Y}}
                                                                                                       PMF or PDF over RVs X
p_{\mathbf{X}}, p
p_{\mathbf{X},\mathbf{Y}}(\mathbf{x},\mathbf{y}), p(\mathbf{x},\mathbf{y})
                                                                                             joint distribution over \mathbf{X} \cup \mathbf{Y}
p_{\mathbf{Y}|\mathbf{x}}(\mathbf{y}|\mathbf{x}), p(\mathbf{Y}|\mathbf{x})
                                                                                     conditional probability distribution
```

Density estimation

Unsupervisedly learning an estimator for the joint probability distribution $p(\mathbf{X})$ from a set of i.i.d. samples $\mathcal{D} = \{\mathbf{x}^i\}_{i=1}^m$ over random variables (RVs) $\mathbf{X} = \{X_1, \dots, X_n\}^3$

Given such an estimator, one uses it to **answer probabilistic queries** about configurations on X, i.e. to do **inference**. \Rightarrow most ML task can be reframed as probabilistic inference!

The inherent trade-off in density estimation: balancing

- ▶ the *representation expressiveness* of the model to learn
- ▶ the *cost of performing inference* on it
- ▶ and the **cost of learning** such a model

(Different kinds of) Inference

complete evidence (EVI)

 $p(\mathbf{X} = \mathbf{x})$

► marginals (MAR)

 $p(\mathbf{E} = \mathbf{e}), \quad \mathbf{E} \subset \mathbf{X}$

conditionals (CON)

 $p(\mathbf{Q}|\mathbf{E}), \quad \mathbf{Q}, \mathbf{E} \subset \mathbf{X}, \mathbf{Q} \cap \mathbf{E} = \emptyset$

Most Probable Explanation (MPE)

 $\arg \max_{\mathbf{q} \sim \mathbf{Q}} p(\mathbf{q}|\mathbf{E}), \quad \mathbf{Q} \cup \mathbf{E} = \mathbf{X}, \mathbf{Q} \cap \mathbf{E} = \emptyset$

Maximum A Posteriori (MAP)

- $rg \max_{\mathbf{q} \sim \mathbf{Q}} \sum_{\mathbf{h} \sim \mathbf{H}} p(\mathbf{q}, \mathbf{h} | \mathbf{E})$
- $\mathbf{Q} \cup \mathbf{H} \cup \mathbf{E} = \mathbf{X}, \mathbf{Q} \cap \mathbf{H} = \emptyset, \mathbf{Q} \cap \mathbf{E} = \emptyset, \mathbf{H} \cap \mathbf{E} = \emptyset$
- partition function computation

$$Z = \sum_{\mathbf{x}} \phi(\mathbf{x})$$

ightharpoonup sampling (SAM): generate independent samples from p

We strive for \emph{exact} inference, computable in $\emph{tractable}$ time, i.e. polynomial in $|\mathbf{X}|$

SPNs: exact and tractable inferences

Let \mathbf{S}^{\oplus} (resp. \mathbf{S}^{\otimes}) be the set of all sum (resp. product) nodes in an SPN S, then

- lacksquare S is complete iff $\forall n \in \mathbf{S}^{\oplus}, \forall c_1, c_2 \in \mathsf{ch}(n) : \mathsf{sc}(c_1) = \mathsf{sc}(c_2)$
- $lackbox{lack}$ is decomposable iff $orall n\in \mathbf{S}^\otimes, orall c_1, c_2\in \mathsf{ch}(n): \mathsf{sc}(c_1)\cap \mathsf{sc}(c_2)=\emptyset$

If S is complete and decomposable, it is valid, and it exactly computes, in time linear w.r.t. to its size $|S|^{45}$:

- ightharpoonup complete evidence $p(\mathbf{X} = \mathbf{x})$
- ightharpoonup marginals $p(\mathbf{Q} = \mathbf{q})$, conditionals $p(\mathbf{Q} = \mathbf{q} | \mathbf{e})$
- ightharpoonup partition function ${f Z}$

An SPN S is selective ⁶, iff $\forall \mathbf{x}^i \sim \mathbf{X}, \forall n \in \mathbf{S}^{\oplus} : |\{c \mid c \in \mathsf{ch}(n) : S_c(\mathbf{x}^i) > 0\}| \leq 1$

 \Rightarrow | S | *MPE inference, assignments* in time linear to $\left|S\right|^7$

 \Rightarrow caveat: |S| shall be polynomial in $|\mathbf{X}|$...

Trivia: Interpreting SPNs

An SPN encodes a *multi-linear function* in a compact data structure ⁸

 \Rightarrow a giant (network) polynomial over X!

SPNs are **not PGMs**! They are **computational graphs**

⇒ equivalent to Arithmetic Circuits for finite discrete domains ⁹

SPNs are hierarchical LV probabilistic

models

> one can think of them as the **deep version of mixture models**

SPNs are peculiar *feedforward neural networks*

> reparameterizable as sparse, constrained, fully-probabilistic MLPs 10

References I

- ⊕ Choi, Arthur and Adnan Darwiche (2017). "On Relaxing Determinism in Arithmetic Circuits". In: Proceedings of ICML, pp. 825–833.
- Darwiche, Adnan (2009). Modeling and Reasoning with Bayesian Networks. Cambridge.
- 🕀 Peharz, Robert, Robert Gens, and Pedro Domingos (2014). "Learning Selective Sum-Product Networks". In: Workshop on Learning Tractable Probabilistic Models. LTPM.
- Poon, Hoifung and Pedro Domingos (2011). "Sum-Product Networks: a New Deep Architecture". In: UAI 2011.
- Booshenas, Amirmohammad and Daniel Lowd (2014). "Learning Sum-Product Networks with Direct and Indirect Variable Interactions". In: Proceedings of ICML 2014.
- Wergari, Antonio, Nicola Di Mauro, and Floriana Esposito (2016). "Visualizing and Understanding Sum-Product Networks". In: preprint arXiv. URL: https://arxiv.org/abs/1608.08266.

