

# **Scalable Learning of Probabilistic Circuits**

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# Resumo

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**Palavras-chave:** Circuitos probabilísticos. Aprendizado de máquina. Modelos probabilísticos.





# Abstract

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**Keywords:** Probabilistic circuits. Machine learning. Probabilistic models.





# **Nomenclature**

## **List of Symbols**

$\sigma$  Sigmoid function

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## Notation

We use the following notation throughout the work. Random variables are written in upper case (e.g.  $X$ ,  $Y$ ) and their values in lower case (e.g.  $x$ ,  $y$ ). We identify propositional variables with 0/1-valued random variables, and use them interchangeably. Sets of variables and their joint values are written in boldface (e.g.  $\mathbf{X}$ ,  $\mathbf{x}$ ). Given a Boolean formula  $f$ , we write  $\langle f \rangle$  to denote its semantics, i.e. the Boolean function represented by  $f$ . For Boolean formulas  $f$  and  $g$ , we write  $f \equiv g$  if they are logically equivalent, that is, if  $\langle f \rangle = \langle g \rangle$ ; we abuse notation and write  $\phi \equiv f$  to indicate that  $\phi = \langle f \rangle$  for a Boolean function  $\phi$ .



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# Chapter 1

## Introduction

When reasoning about the world, rarely can we find a realistic model that perfectly subsumes all of the needed relationships for flawless prediction. As such, the presence of a reliable uncertainty quantifier in intelligent systems is essential in developing performant yet diagnostible agents. This is made explicitly clear in the case of high-risk settings, such as autonomous vehicles or automated power plant systems, where a wrong prediction could cause disastrous consequences. A well known example in the case of the former is obstacle avoidance: while the agent should be capable of accurately identifying obstructions in its way during normal conditions, so should it be able to identify its own lack of confidence in high uncertainty situations like ones brought by environmental factors, such as severe blizzard or heavy rain. In these situations where predictions are highly unreliable, the safest option might be for the agent to first identify its uncertainty, and second to reach out for human help. Other interesting applications of uncertainty quantification include out-of-distribution detection, which in our previous example could be visualized as the agent identifying a human's driving as abnormally irregular (due to inebriation, infirmity, etc.) and appropriately taking control of the vehicle before a potential accident takes place.

One popular approach to quantifying uncertainty is through probability theory. By abstracting the world as a probability distribution with a finite number of observable random variables that encode a possibly incomplete knowledge of the environment, we are, in theory, able to answer a diverse set of complex queries as long as we have access to the (approximate) true data distribution. Practice is far different from theory, however, as most machine learning models either lie within a very limited range in the tractability spectrum in terms of inference (VERGARI, CHOI, PEHARZ, *et al.*, 2020) or are too simplistic for complex real-world problems. Besides, although the majority of recent advances in deep learning claim some probabilistic meaning from the model's output, they are often uncalibrated distributions, a result of focusing on maximizing predictive accuracy at the expense of predictive uncertainty (GUO *et al.*, 2017; OVADIA *et al.*, 2019; CHERNIKOVA *et al.*, 2019), ultimately producing overconfident and peculiar results (SZEGEDY *et al.*, 2013; WEI *et al.*, 2018; SU *et al.*, 2019; CHERNIKOVA *et al.*, 2019). Crucially, mainstream deep models (i.e. standard neural networks) usually optimize a conditional distribution over the to-be-predicted random variables – and are thus often called *discriminative* models – and

do not model the actual joint distribution of the data, limiting inference capabilities and uncertainty estimation.

In contrast, *generative* models seek to extract information from the joint (in varying capacities), and have lately seen a sharp rise in interest within deep learning. Despite this, most popular models do not admit either exact or tractable querying of key inference scenarios. For instance, although Generative Adversarial Networks (GANs) allow for efficient sampling (GOODFELLOW *et al.*, 2014), basic queries such as likelihood or marginals are outside of their capabilities. Similarly, Normalizing Flows (NF) also permit access to efficient sampling, with the added feature of computing likelihoods, but are severely limited by the base distribution when it comes to discrete data (REZENDE and MOHAMED, 2015; PAPAMAKARIOS *et al.*, 2021) albeit recent works on discretizing NFs have shown empirically good results (LIPPE and GAVVES, 2021; ZIEGLER and RUSH, 2019). Variational Auto-Encoders (VAEs) are (under certain conditions) a generalization of NFs (YU, 2020; GRITSENKO *et al.*, 2019) with known extensions for categorical data (ROLFE, 2017; VAHDAT, MACREADY, *et al.*, 2018; VAHDAT, ANDRIYASH, *et al.*, 2018), but only permit access to sampling and an upper-bound on the likelihood, with the latter available only after solving a complex optimization task (KINGMA and WELLING, 2014).

Despite the impressive achievements of the aforementioned generative models on realistically producing samples consistent with evidence, in none of the previous models are complex queries like structured prediction under partial observations, *maximum a posteriori* (MAP), conditional or marginal probabilities tractable. An obvious alternative would be Probabilistic Graphical Models (PGMs), although they too suffer from intractability when dealing with high treewidth networks (R. DECHTER, 1998; KOLLER and FRIEDMAN, 2009), severely limiting expressivity. Instead, we draw our attention to an expressive class of models that subsumes several families of probabilistic models with tractable inference capabilities.

Probabilistic Circuits (PCs) define a superclass of probabilistic models distinctly specified by recursive compositions of distributions through graphical formalisms. Vaguely speaking, PCs are computational graphs akin to neural networks, but whose network structure and computational units abide by special constraints. Within these specific conditions span a wide range of subclasses, each establishing a distinct set of restrictions on their structure in order to enable different segments within the tractability spectrum. As an example, Sum-Product Networks (SPNs, POON and P. DOMINGOS, 2011) are usually loosely defined over a couple of constraints: namely *smoothness* and *decomposability*, which in turn enables likelihood, marginal and conditional computations. Arithmetic Circuits (ACs, DARWICHE, 2003) add *determinism* to the mix, allowing for tractable computation of MAP probabilities. Similarly, Cutset Networks (C Nets, RAHMAN *et al.*, 2014) employ the same constraints as ACs, but accept more expressive distributions as part of their computational units. Probabilistic Sentential Decision Diagrams (PSDDs, KISA *et al.*, 2014), Probabilistic Decision Graphs (PDGs, JAEGER, 2004) and And/Or-Graphs (AOGs, RINA DECHTER and MATEESCU, 2007) all require *smoothness* and *determinism*, but also call for a stronger version of *decomposability*, permitting all queries previously mentioned as well as computation of the Kullback-Leibler divergence and expectation between two circuits (CHOI *et al.*, 2020). Usually, PCs represent the joint distribution of the data, although they are sufficiently expressive for generative *and* discriminative modeling (KHOSRAVI *et al.*, 2019; RASHWAN

*et al.*, 2018; ROOSHENAS and LOWD, 2016; GENS and P. DOMINGOS, 2012; SHAO *et al.*, 2020). In this dissertation though, we shall focus on the generative side of PCs.

While inference is usually straightforward, as we shall see in ??, learning the structure of PCs so that they obey the needed structural restrictions requires either careful handcrafted architectures (POON and P. DOMINGOS, 2011; CHENG *et al.*, 2014; NATH and P. M. DOMINGOS, 2016) or usually involves running costly (in)dependence tests over most (if not all) variables (GENS and P. DOMINGOS, 2013; JAINI *et al.*, 2018; VERGARI, MAURO, *et al.*, 2015; DI MAURO *et al.*, 2017), which can become prohibitive in higher dimension data. Alternatively, some learning algorithms resort to structure preserving iterative methods to grow a PC that already initially satisfies desired constraints, adding complexity to the underlying distribution at each iteration (LIANG, BEKKER, *et al.*, 2017; DANG *et al.*, 2020). However, these can take several iterations until visible improvement and often take several minutes for each iteration when the circuit is big. Common techniques used in deep learning for generating scalable architectures for neural network also pose a problem, as the nature of the needed structural constraints make for sparse computational graphs. To circumvent these issues, work on scaling PCs to higher dimensions has focused mainly on random architectures, with competitive results (PEHARZ, VERGARI, *et al.*, 2020; MAURO *et al.*, 2021; GEH and MAUÁ, 2021; PEHARZ, LANG, *et al.*, 2020). Apart from the scalability side of random structure generation, usual structure learning algorithms often require grid-search for hyperparameter tuning to achieve top quality performance, which is usually not the case for random algorithms. For the usual data scientist or machine learning practitioner, hyperparameter tuning can become exhaustive, especially if the goal is to analyze and infer from large data, and not to achieve top tier performance on benchmark datasets.

In this dissertation, we propose two scalable structural learning algorithms for probabilistic circuits that are especially suited for large data and fast deployment. They both take advantage of random network generation to quickly construct PCs with little to no need for hyperparameters. The first is effective for constructing PCs from binary data with a highly constrained structure, and thus appropriate when complex querying is needed. The second builds less constrained random PCs, but supports both discrete and continuous data.

## 1.1 Contributions and Dissertation Outline

We organize this dissertation as follows. We begin [Chapter 2](#) by formally defining probabilistic circuits, conducting a review of some of the structural constraints that we might impose on PCs, as well as what we may gain from them in terms of tractability. We then list existing formalisms that may be viewed as instances of PCs, and what their structure entail in terms of inference power. In [Chapter 3](#), we address existing PC structure learning algorithms, and which guarantees in terms of tractability each give. We cover the two new structure learners in [Chapter 4](#), providing empirical results on their performance. The final chapter is dedicated to summarizing our research contributions and pointing to potential future work in learning PCs.

Our contributions in this dissertation address the following research topics.

### Scalably learning PCs directly from background knowledge

In [GEH and MAUÁ \(2021\)](#), we provide a learning algorithm for PSDDs that learns a PC directly from background knowledge in the form of logical constraints. The algorithm samples a structure from a distribution of possible PSDDs that are weakly consistent with the logical formula. How weak consistency is depends on a parameter that trades permission of false statements as non zero probability events with circuit complexity. We provide the algorithm and empirical results in Section 4.??.

### Using ensembles to strengthen consistency

The PC sampler given by [GEH and MAUÁ \(2021\)](#) produces competitive probabilistic models (in terms of likelihood), albeit weak logical models in the sense that it possibly assigns non-zero probability to false variable assignments – as we discuss in Section 4.??, it never assigns zero probability to true statements. By producing many weak models, we not only gain in terms of data fitness, but also consistency: if any one component in the ensemble returns an assignment to be impossible, the whole model should return false.

### Random projections to efficiently learn PCs

Usual methods often employ clustering algorithms for constructing convex combinations of computational units. These can take many iterations to converge or require space quadratic in the number of data points. Instead, in Section 4.?? we present linear alternatives based on random projections ([FREUND \*et al.\*, 2008](#); [DASGUPTA and FREUND, 2008](#)).

# Chapter 2

## Probabilistic Circuits

As we briefly mentioned in the last chapter, Probabilistic Circuits (PCs) are conceptualized as computational graphs under special conditions. In this chapter, [Section 2.1](#) to be more precise, we formally define PCs and give an intuition on their syntax, viewing other probabilistic models through the lenses of the PC framework. In [Section 2.2](#), we describe the special structural constraints that give PCs their inference power over other generative models and state which queries (as far as we know) are enabled from each constraint.

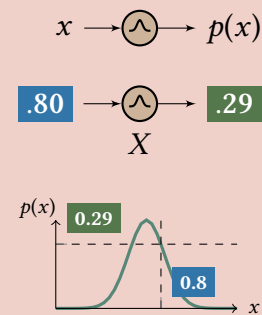
### 2.1 Distributions as Computational Graphs

Probabilistic circuits are directed acyclic graphs usually recursively defined in terms of their computational units. In its simplest form, a PC is a single unit corresponding to some tractable distribution. These can range from univariate or multivariate exponential distributions to complex non-parametric models, and are the foundational units of PCs. We shall refer to these computational units as *leaf nodes*, as no edges come out of them. To simplify notation, in this dissertation, unless specified, leaf nodes will denote univariate distributions. Let  $\mathcal{L}_p$  a PC leaf node and denote  $p$  as its inherent probability distribution. By definition, any query  $f : \mathcal{X} \rightarrow \mathcal{Y}$  which is tractable on  $p$  is tractable on  $\mathcal{L}_p$ . We shall denote  $\mathcal{L}_p(\mathbf{X}) = p(\mathbf{X})$ , and often omit  $p$  when its explicit form is not needed.

#### Example 2.1.1: Gaussians as probabilistic circuits

Let  $\mathcal{L}_p$  a leaf node and  $p(X) = \mathcal{N}(X; \mu, \sigma^2)$  a univariate Gaussian distribution. Computing any query on  $\mathcal{L}_p$  is straightforward: any query on  $\mathcal{L}_p$  directly translates to  $p$ . As an example, suppose  $\mu = 0$  and  $\sigma^2 = 1$  and we wish to compute  $\mathcal{L}_p(x = 0.8)$ . The probability of this leaf shall then be

$$\mathcal{L}_p(x = 0.8) = \mathcal{N}(x = 0.8; \mu = 0, \sigma^2 = 1) = 0.29.$$



Evidently, a single leaf node lacks the expressivity for modeling complex models, otherwise we would have just used the leaf distribution as a standalone model. The expressiveness of PCs comes from recursively combining distributions into complex functions. This can be done through computational units that either compute convex combinations or products of their children. Let us first look at convex combinations, known in the literature as *sum nodes*.

### Remark 2.1.1: On operators and tractability

Throughout this work we consider only products and convex combinations (apart from the implicit operations contained within leaf nodes) as potential computational units. The question of whether any other operator could be used to gain expressivity without loss of tractability is without a doubt an interesting research question, and one that is actively being pursued. However, this is certainly out of the scope of this dissertation, and so we restrict discussion on this topic and only give a brief comment on tractability here, pointing to existing literature in this area of research.

A. FRIESEN and P. DOMINGOS (2016) formalize the notion of operator generalization in PCs by looking at any commutative semiring, giving results on the conditions for marginalization to be tractable. They provide examples of common semirings and to which known formalisms they correspond to. Two such examples are PCs under the Boolean semiring ( $\{0, 1\}, \vee, \wedge, 0, 1$ ) for logical inference, which are equivalent to Negation Normal Form (NNF, BARWISE, 1982) and constitute an instance of Logic Circuits (LCs), of which Sentential Decision Diagrams (SDDs, DARWICHE, 2011) and Binary Decision Diagrams (BDDs, AKERS, 1978) are a part of; and PCs under the real min-sum semiring ( $\mathbb{R}_\infty, \min, +, \infty, 0$ ) for nonconvex optimization (A. L. FRIESEN and P. DOMINGOS, 2015).

Recently, VERGARI, CHOI, LIU, *et al.* (2021) extensively covered tractability conditions and complexity bounds for convex combinations, products, exp (and more generally powers in both naturals and reals), divisions and logarithms, even giving results for complex information-theoretic queries, such as entropies and divergences.

Up to now, we have only considered summations with nonnegative weights. Indeed, in most literature the sum node is defined as a convex combination. However, negative weights have appeared in Logistic Circuits (LIANG and VAN DEN BROECK, 2019) for discriminative modeling; and in Probabilistic Generating Circuits (ZHANG *et al.*, 2021), a superset of tractable probabilistic models that subsume PCs.

Other works on

Note how these second nonlinearity, the first being leaf nodes

## 2.2 Deciding What to Constraint

referenced structural constraints in passing



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