Scalable Learning of Probabilistic Circuits

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Abstract

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The rising popularity of generative models together with the growing need for flexible and exact inferences has motivated the machine learning community to look for expressive yet tractable probabilistic models. Probabilistic circuits (PCs) are a family of tractable probabilistic models capable of answering a wide range of queries exactly and in polynomial time. Their operational syntax in the form of a computational graph and their principled probabilistic semantics allow their parameters to be estimated by the highly scalable and efficient optimization techniques used in deep learning. Importantly, tractability is tightly linked to constraints on their underlying graph: by enforcing certain structural assumptions, queries like marginals, *maximum a posteriori* or entropy become linear time computable while still retaining great expressivity. While inference is usually straightforward, learning PCs that both obey the needed structural restrictions and exploit their expressive power has proven a challenge. Current state-of-the-art structure learning algorithms for PCs can be roughly divided into three main categories. Most learning algorithms seek to generate a usually tree-shaped circuit from recursive decompositions on data, often through clustering and costly statistical (in)dependence tests, which can become prohibitive in higher dimensional data. Alternatively, other approaches involve constructing an intricate network by growing an initial circuit through structural preserving iterative methods. Besides depending on a sufficiently expressive initial structure, these can possibly take several minutes per iteration and many iterations until visible improvement. Lastly, other approaches involve randomly generating a probabilistic circuit by some criterion. Although usually less performant compared to other methods, random PCs are orders of magnitude more time efficient. With this in mind, this dissertation aims to propose fast and scalable random structure learning algorithms for PCs from two different standpoints: from a logical point of view, we efficiently construct a highly structured binary PC that takes certain knowledge in the form of logical constraints and scalably translate them into a probabilistic circuit; from the viewpoint of data guided structure search, we propose hierarchically building PCs from random hyperplanes. We empirically show that either approach is competitive against state-of-the-art methods of the same class, and that their performance can be further boosted by simple ensemble strategies.

Keywords: Probabilistic circuits. Machine learning. Probabilistic models.

Resumo

Renato Lui Geh. **Aprendizado Escalável de Circuitos Probabilísticos**. Dissertação (Mestrado). Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, 2021.

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

Nomenclature

List of Symbols

σ 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 ϕ. We use the notation $[\![a, b]\!]$, with $b \geq a$ to denote the integer set $\{a, a+1, \ldots, b\} \subset \mathbb{Z}$. Similarly, we use $[\![b]\!]$ as an equivalent for $[\![1, b]\!]$. For independence, we use $\perp\!\!\!\perp$ to indicate that two variables X and Y are statistically independent, i.e. $X \perp\!\!\!\perp Y$.

Contents

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 distincly 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 (CNets, 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, Ghose, *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 Denis Deratani 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 practicioner, 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 Denis Deratani 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 Denis Deratani 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.

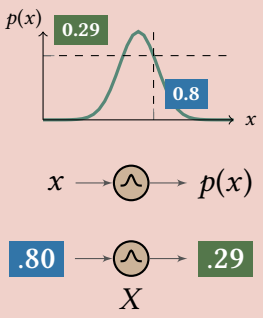
2.1 Distributions as Computational Graphs

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 with no outgoing edges whose value corresponds to the result of a function. These are often called *input* nodes, and can take any form as long as its value is tractably computable. More concretely, input nodes typically represent probability density (or mass) functions, although they also support inputs as joint probability density functions of complex non-parametric models as well. To simplify notation, from here on out we shall use the term distribution and probability density (resp. mass) function interchangeably and argue that the input node represents a probability distribution.

Example 2.1.1: Gaussians as probabilistic circuits

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

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



Let L_p a PC input node and denote p as its inherent probability distribution. By definition, any query $f : \mathcal{X} \to \mathcal{Y}$ which is tractable on p is tractable on L_p. We shall denote $\mathrm{L}_p(\mathbf{X}) = p(\mathbf{X})$, and often omit p when its explicit form is not needed. Evidently, a single input node lacks the expressivity for modeling complex models, otherwise we would have just used the input 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.

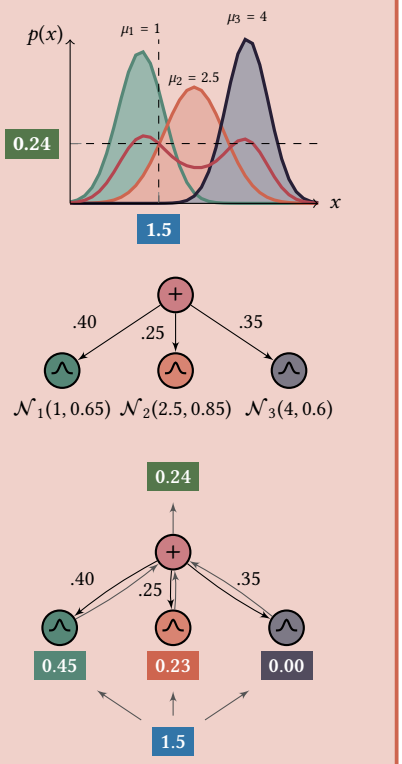
Let S be a PC sum node, and denote by Ch(S) the children nodes of S. For every edge $\overrightarrow{\mathrm{SC}}$ coming out of S and going to C, we attribute a weight $w_{\mathrm{S,C}} > 0$, such that $\sum_{\mathrm{C}\in\mathrm{Ch(S)}} w_{\mathrm{S,C}} = 1$. A sum node semantically defines a mixture model over its children, essentially acting as a latent variable over the component distributions (Poon and P. Domingos, 2011; Peharz, Gens, *et al.*, 2016). Its value is the weighted sum of its children $p_{\mathrm{S}}(\mathbf{X} = \mathbf{x}) = \sum_{\mathrm{C}\in\mathrm{Ch(S)}} w_{\mathrm{S,C}} \cdot p_{\mathrm{C}}(\mathbf{X} = \mathbf{x})$. To simplify notation, we shall use $\mathrm{N}(\mathbf{X} = \mathbf{x})$ as an alias for $p_{\mathrm{N}}(\mathbf{X} = \mathbf{x})$, that is, the probability function given by the N's induced distribution.

Example 2.1.2: Gaussian mixture models as probabilistic circuits

A Gaussian Mixture Model (GMM) defines a mixture over Gaussian components. Say we wish to compute the probability of $X = x$ for a GMM $\mathcal{G}$ with three components $\mathcal{N}_1(\mu_1 = 1, \sigma_1^2 = 0.65)$, $\mathcal{N}_2(\mu_2 = 2.5, \sigma_1^2 = 0.85)$ and $\mathcal{N}_3(\mu_3 = 4, \sigma_3^2 = 0.6)$, and suppose we have weights set to $\phi = (0.4, 0.25, 0.35)$. Computing the probability of G amounts to the weighted summation

$$\mathcal{G}(X = x) = 0.4 \cdot \mathcal{N}_1(x; \mu_1, \sigma_2^2) + 0.25 \cdot \mathcal{N}_2(x; \mu_2, \sigma_2^2) + 0.35 \cdot \mathcal{N}_3(x; \mu_3, \sigma_3^2),$$

which is equivalent to a computational graph (i.e. a PC) with a sum node whose weights are set to ϕ and children are the components of the mixture. The figure on the right shows $\mathcal{G}$ (top) and its corresponding PC (middle). Given $x = 1.5$ (in blue), input nodes are computed following the inference flow (bottom, gray edges) up to the root sum node (in red), where a weighted summation is computed to output the probability (in green).



Before we address products as computational units in PCs, we first need to discuss the concept of scope of a PC node. Denote by Sc(N) the set of all variables that appear in N. We inductively compute the scope of circuit by a bottom-up approach: the scope of an input node L_p is the set of variables that appear in p's distribution, and the scope of any other node is the union of all of its childrens' scopes. The notion of a node's scope is

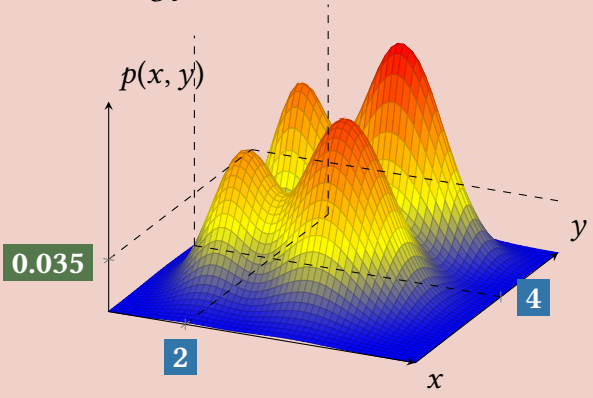
essential to the structural constraints seen in Section 2.2.

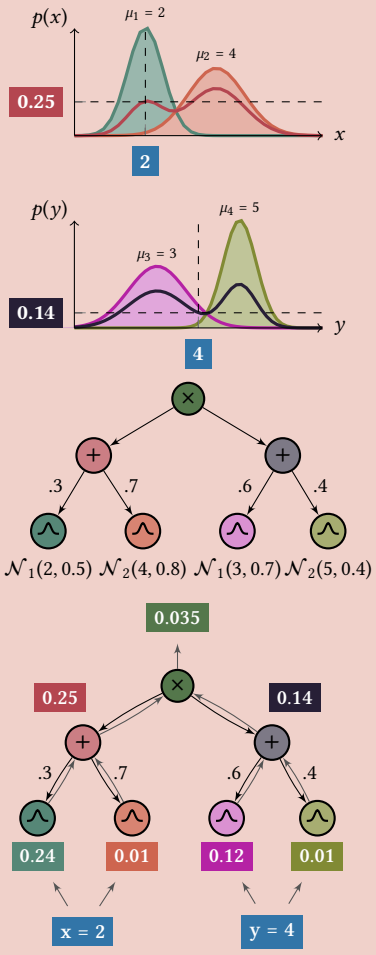
So far, the only nonlinearities present in PCs come from the internal computations of input nodes. In fact, a PC that only contains sums inputs can always be reduced to a sum node rooted PC with a single layer, i.e. a mixture model (see Theorem A.1.1). Adding *product nodes* as another form of nonlinearity increases expressivity sufficiently for PCs to be capable of representing any (discrete) probability distribution (Darwiche, 2003; Martens and Medabalimi, 2014; Peharz, Tschiatschek, *et al.*, 2015). More importantly, products semantically act as factorizations of their children, indicating an independence relationship between variables from different children. In practice, product nodes are simply products of their childrens' distribution: if P is a PC product node, then its value is given by $\mathrm{P}(\mathbf{X} = \mathbf{x}) = \prod_{\mathrm{C} \in \mathrm{Ch(P)}} \mathrm{C}(\mathbf{X} = \mathbf{x})$.

Example 2.1.3: Factors as probabilistic circuits

Say we have two GMMs $\mathcal{G}_1$ and $\mathcal{G}_2$. The first is a mixture model over variable X, with component weights $\phi_1 = (0.3, 0.7)$ and gaussians $\mathcal{N}_1(\mu_1 = 2, \sigma_1 = 0.5)$ and $\mathcal{N}_2(\mu_2 = 4, \sigma_2 = 0.8)$. The second is composed of $\mathcal{N}_3(\mu_3 = 3, \sigma_2 = 0.7)$ and $\mathcal{N}_4(\mu_4 = 5, \sigma_2 = 0.4)$, both distributions over variable Y and with weights $\phi_2 = (0.6, 0.4)$.

Suppose $X \perp\!\!\!\perp Y$, yet we wish to compute the joint probability of both x and y. If $X \perp\!\!\!\perp Y$, then $p(x, y) = p(x)p(y) = \mathcal{G}_1(x)\mathcal{G}_2(y)$, which corresponds to a factoring of mixtures. This is represented as a product node (in green) over the two mixture models (in red and purple). The resulting joint of this circuit is shown below.





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 input 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 operator tractability here, pointing to existing literature in this area of research.

A. Friesen and P. Domingos (2016) formalize the notion of replacing sums and products in PCs with any pair of operators in a 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. One such example 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. Another less common semiring in PCs is 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), quotients and logarithms, even giving results for complex information-theoretic queries, such as entropies and divergences. Notably, they analyze whether structural constraints (and thus, in a sense, tractability) under these conditions are preserved.

Up to now, we have only considered summations as nonnegative weighted sums. 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 class of tractable probabilistic models that subsume PCs. Denis D. Mauá *et al.* (2017) extend (nonnegative) weights in sum nodes with probability intervals, effectively inducing a credal set (Cozman, 2000) for measuring imprecision.

Other works include PCs with quotients (Sharir and Shashua, 2018), transformations (Pevný *et al.*, 2020), max (Melibari *et al.*, 2016), and einsum (Peharz, Lang, *et al.*, 2020) operations.

2.2 Deciding What to Constraint

referenced structural constraints in passing

Appendix A

Appendix

A.1 Proofs

Theorem A.1.1. *Let $\mathcal{C}$ a probabilistic circuit whose first l layers are composed solely of sum nodes. Call* $\mathbf{N}$ *the set of all nodes in layer $l+1$. $\mathcal{C}$ is equivalent to a PC $\mathcal{C}'$ whose root is a sum node with* $\mathbf{N}$ *as children.*

Proof. We adapt a similar proof due to Jaini, Poupart, *et al.* (2018). Every sum node is of the form

$$\mathrm{S}(\mathbf{x}) = \sum_{\mathrm{C} \in \mathrm{Ch}(\mathrm{S})} w_{\mathrm{S},\mathrm{C}} \cdot \mathrm{C}(\mathbf{x}).$$

Particularly, every child C in a sum node in layer $1 \leq i \leq l-1$, is a sum node, and so for the first layer we have that

$$\begin{aligned}\mathrm{S}(\mathbf{x}) &= \sum_{\mathrm{C}_1 \in \mathrm{Ch}(\mathrm{S})} w_{\mathrm{S},\mathrm{C}_1} \sum_{\mathrm{C}_2 \in \mathrm{Ch}(\mathrm{C}_1)} w_{\mathrm{C}_1,\mathrm{C}_2}\, \mathrm{C}_2(\mathbf{x}) \\ &= \sum_{\mathrm{C}_1 \in \mathrm{Ch}(\mathrm{S})} \sum_{\mathrm{C}_2 \in \mathrm{Ch}(\mathrm{C}_1)} w_{\mathrm{S},\mathrm{C}_1} w_{\mathrm{C}_1,\mathrm{C}_2}\, \mathrm{C}_2(\mathbf{x}).\end{aligned}$$

Define a one-to-one mapping that takes a tuple $(\mathrm{C}_1, \mathrm{C}_2)$ where $\mathrm{C}_1 \in \mathrm{Ch}(\mathrm{S})$ and $\mathrm{C}_2 \in \mathrm{Ch}(\mathrm{C}_1)$ and returns a (unique) path from S to every grandchild C_2 of S. Call $\mathbf{K}$ the set of all paths, and $w_{\mathrm{S},\mathrm{C}_1}$ and $w_{\mathrm{C}_1,\mathrm{C}_2}$ the weights for one such path. We can merge these two weights into a single weight $w'_{\mathrm{S},\mathrm{C}_2} = w_{\mathrm{S},\mathrm{C}_1} \cdot w_{\mathrm{C}_1,\mathrm{C}_2}$, yielding

$$\mathrm{S}(\mathbf{x}) = \sum_{(w_{\mathrm{S},\mathrm{C}_1}, w_{\mathrm{C}_1,\mathrm{C}_2}) \in \mathbf{K}} w'_{\mathrm{S},\mathrm{C}_2}\, \mathrm{C}_2(\mathbf{x}).$$

This ensures that two consecutive sum layers can be collapsed into a single layer. Particularly, for the first (root) and second layers, the above transformation generates a circuit with one fewer layer and whose root has $\mathcal{O}(nm)$ edges, where n and m are the number of edges coming from the original root and its children respectively. We can apply this

procedure until there are no more consecutive sum nodes. This results in a PC of the form

$$\mathrm{S}(\mathbf{x}) = \sum_{\mathrm{C} \in \mathrm{Ch}(S)} w_{\mathrm{S,C}}\, \mathrm{N}(\mathbf{x}),$$

where $\mathrm{N} \in \mathbf{N}$. The number of children of the resulting root sum node will be exponential on the number of edges of its children. □

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