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 write $\mathcal{X}$ as the sample space and for independence we use $\perp\!\!\!\perp$ to indicate that two variables X and Y are statistically independent, i.e. $X \perp\!\!\!\perp Y$. 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 $[1..b]$. We denote the Iverson bracket as $[\![\phi]\!]$, i.e. a function that returns 1 if ϕ is true and 0 otherwise. In the context of graph theory, we use sans serif letters for graph nodes (e.g. N, S, P, L) and bold variants for sets of nodes (e.g. $\mathbf{N}$, $\mathbf{S}$, $\mathbf{P}$, $\mathbf{L}$). We call $\mathrm{Ch}(\mathsf{N})$ the set of all children of a node N, $\mathrm{Pa}(\mathsf{N})$ as the set of all parents, and $\mathrm{Desc}(\mathsf{N})$ the set of all descendants.

Contents

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 quantifier on the aleatoric uncertainty of 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 and other situations where a system faces unusual and perhaps never before seen evidence, predictions might prove unreliable, and the safest option might be for the agent to first identify its uncertainty, and second to reach out for human help. Conversely, in a case of anomaly detection, the agent might identify a human's driving as abnormally irregular (due to inebriation, infirmity, etc.) and appropriately take 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 (Y. Choi, Vergari, and Van den Broeck, 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 (data) 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.

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, Kothalkar, *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 (Y. Choi, Vergari, and Broeck, 2020). Usually, PCs represent the joint distribution of the data, although they are sufficiently expressive for generative *and* discriminative modeling (Khosravi, Liang, *et al.*, 2019; Rashwan, Poupart, *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 Section 2.2, 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, Vergari, *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; R. L. Geh and Denis Deratani Mauá, 2021b; 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 (Section 2.1), 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 (Section 2.2). 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 dividing them into three classes: divide-and-conquer learning (Section 3.1), incremental learning (Section 3.2) and random learning (Section 3.3). For each, we give a brief analysis on their complexity and discuss their advantages and disadvantages. 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 R. L. Geh and Denis Deratani Mauá (2021b), 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 R. L. Geh and Denis Deratani Mauá (2021b) 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).

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.

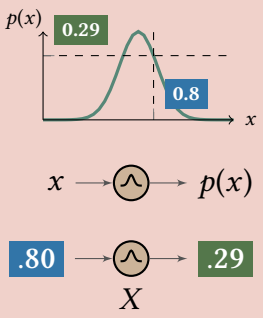
2.1 Distributions as Computational Graphs

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: 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 $\mathsf{L}_p(x = 0.8)$. The probability of this input shall then be

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



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 $\mathsf{L}_p(\mathbf{X}) = p(\mathbf{X})$, 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.

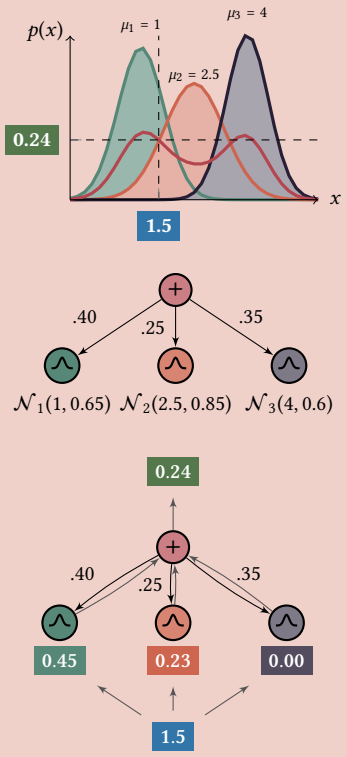
Let S be a PC sum node, and denote by $\mathrm{Ch}(\mathsf{S})$ the children nodes of S. For every edge $\overrightarrow{\mathsf{S}\,\mathsf{C}}$ coming out of S and going to C, we attribute a weight $w_{\mathsf{S},\mathsf{C}} > 0$, such that $\sum_{\mathsf{C}\in\mathrm{Ch}(\mathsf{S})} w_{\mathsf{S},\mathsf{C}} = 1$. 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, Pernkopf, *et al.*, 2016). Its value is the weighted sum of its children $p_{\mathsf{S}}(\mathbf{X} = \mathbf{x}) = \sum_{\mathsf{C}\in\mathrm{Ch}(\mathsf{S})} w_{\mathsf{S},\mathsf{C}} \cdot p_{\mathsf{C}}(\mathbf{X} = \mathbf{x})$. To simplify notation, we shall use $\mathsf{N}(\mathbf{X} = \mathbf{x})$ as an alias for $p_{\mathsf{N}}(\mathbf{X} = \mathbf{x})$, that is, the probability function given by N's induced distribution. We often omit the variable assignment $\mathbf{X} = \mathbf{x}$ to $\mathbf{x}$ if the notation is unambiguous.

Example 2.2: 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).



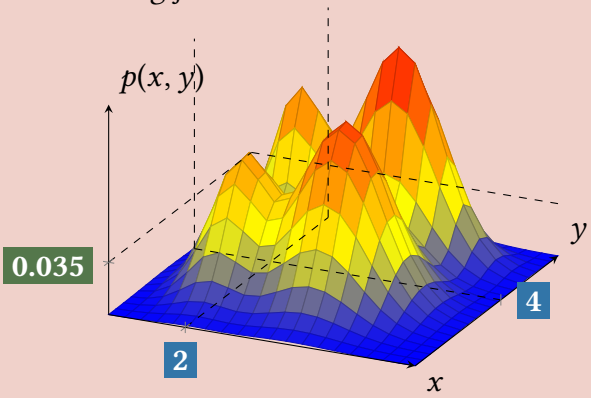
So far, the only nonlinearities present in PCs come from the internal computations of input nodes. In fact, a PC that only contains sums inputs can always be reduced to a sum node rooted PC with a single layer, i.e. a mixture model (see Theorem A.1.1). Adding *product nodes* as another form of nonlinearity increases expressivity sufficiently for PCs

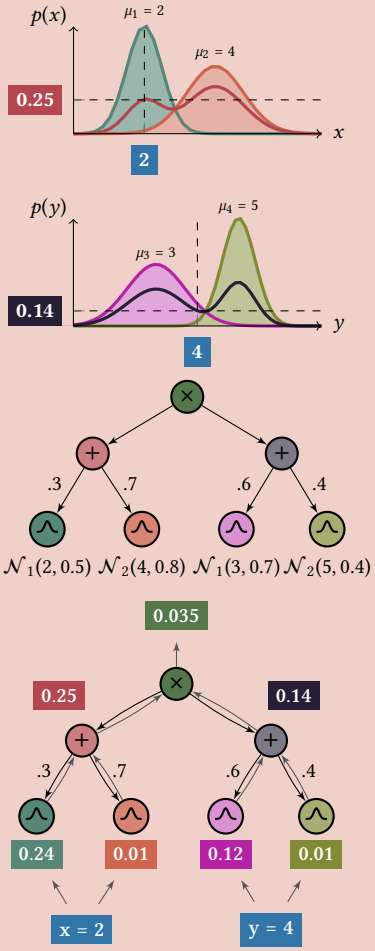
to be capable of representing any (discrete) probability distribution (Darwiche, 2003; Martens and Medabalimi, 2014; Peharz, Tschiatschek, *et al.*, 2015). More importantly, products semantically act as factorizations of their children, indicating an independence relationship between variables from different 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 2.3: 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.





Now that we have introduced the three most important computational units in PCs, we are finally ready to formally define probabilistic circuits.

Definition 2.1.1 (Probabilistic circuit)**.** *A* probabilistic circuit *$\mathcal{C}$ is a rooted connected DAG whose nodes compute any tractable operation of their children, usually either convex combinations, known as* sum *nodes, or* products*. Nodes with no outgoing edges, i.e.* input *nodes, are tractable nonnegative functions whose integrals exist and equal to one. Computing a value from $\mathcal{C}$ amounts to a bottom-up feedforward pass from input nodes to root.*

While we assume that *tractable* operation or function is acceptable, we are usually interested in $\mathcal{O}(1)$ time computable operations, and often assume the same of input functions to simplify analysis. Further, in this dissertation we are only interested in convex combinations and products, and as such only these operations are considered. When a

probabilistic circuit C contains no consecutive sums or products (i.e. for every sum all of its children are either inputs or products and respectively for products) then it is said to be a *standard* form circuit. Any PC can be transformed into a *standardized* circuit, a process we call *standardization* (see Theorem A.1.2).

Remark 2.1: 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 (Abram L. Friesen and P. Domingos, 2015).

Recently, Vergari, Y. Choi, *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) and Mattei, Antonucci, *et al.* (2020a) extend (nonnegative) weights in sum nodes with probability intervals, effectively inducing a credal set (Fabio G. Cozman, 2000) for measuring imprecision.

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

Before we address the key components that make PCs interesting tractable probabilistic models, we must first discuss some important concepts that often come up in PC literature.

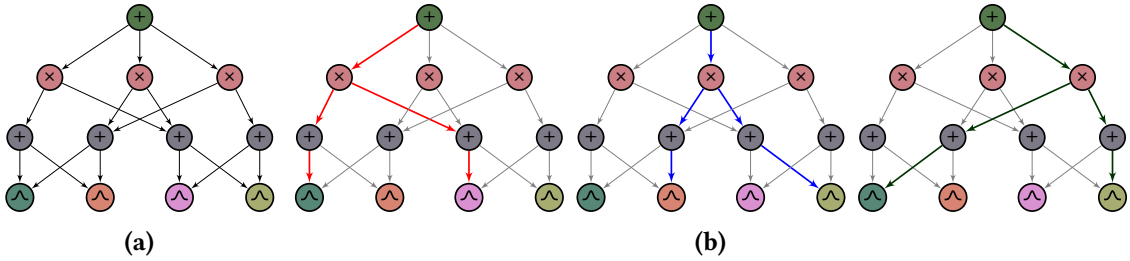


Figure 2.1: *A probabilistic circuit (a) and 3 of the 12 possible induced subcircuits (b).*

Mainly, we are interested in defining two notions here: the scope of a unit and induced subcircuits.

In simple terms, the scope of a computational unit N of a PC is merely the set of all variables that appear in the descendants of N. More formally, 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[1], and the scope of any other node is the union of all of its childrens' scopes. The notion of scope is essential to the structural constraints seen in Section 2.2.

As an example, take the circuit from Example 2.3. The scope of input nodes and are Sc() = Sc() = $\{X\}$, while Sc() = Sc() = $\{Y\}$. Consequentially, their parent sum nodes will have the same scope as their children Sc() = $\{X\}$ and Sc() = $\{Y\}$, yet the root node's scope is Sc() = $\{X, Y\}$, since its childrens' scopes are distinct. The size of a probabilistic circuit is the number of nodes and edges of its computational graph. We use $|\mathcal{C}|$ to denote the size of a probabilistic circuit $\mathcal{C}$.

Let $\mathcal{C}$ a probabilistic circuit and node $\mathsf{N} \in \mathcal{C}$. We say that $\mathcal{S}_\mathsf{N}$ is a subcircuit of $\mathcal{C}$ rooted at N if $\mathcal{S}_\mathsf{N}$'s root is N, all nodes and edges in $\mathcal{S}_\mathsf{N}$ are also in $\mathcal{C}$ and $\mathcal{S}$ is also a probabilistic circuit. We now introduce the concept of induced subcircuits (Chan and Darwiche, 2006; Dennis and Ventura, 2015; Peharz, Gens, and P. Domingos, 2014).

Definition 2.1.2 (Induced subcircuit)**.** *Let $\mathcal{C}$ a probabilistic circuit. An induced subcircuit $\mathcal{S}$ of $\mathcal{C}$ is a subcircuit of $\mathcal{C}$ rooted at $\mathcal{C}$'s root such that all edges coming out of product nodes in $\mathcal{C}$ are also in $\mathcal{S}$, and of all edges coming out of sum nodes in $\mathcal{C}$, only one is in $\mathcal{S}$.*

Examples of induced subcircuits are visualized in Figure 2.1. When the induced subcircuit is a tree, as is the case in Figure 2.1, they are referred to as induced tree (H. Zhao, Melibari, *et al.*, 2015; H. Zhao, Adel, *et al.*, 2016).

So far, by Definition 2.1.1 a PC does not yet necessarily represent a probability distribution with tractable (marginal) inference. In the next section, we formally define sufficient conditions for tractability in the form of structural constraints that we have only previously mentioned in passing.

[1] Although we previously defined input nodes as mere functions, here we are explicitly associating a random variable to a *probability* function. Indeed, if we are being rigorous, we should define input nodes as a pair of random variable and function. To save space we instead assume, as previously stated, that the function is seen as both the probability (density) function as well as the distribution itself, and thus its scope is the scope of its distribution, i.e. the random variables that come into play in a probability distribution.

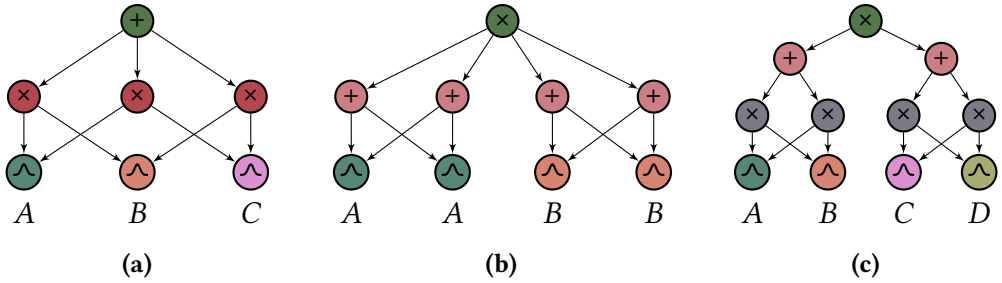


Figure 2.2: *Decomposable but non-smooth (a), smooth but non-decomposable (b), and smooth and decomposable (c) circuits.*

2.2 Deciding What to Constraint

In this section we are interested in studying how the structural constraints in PCs enable different inference tasks. We shall first cover the more basic queries, namely *probability of evidence* (EVI), *marginal probability* (MAR), *conditional probability* (CON) and *maximum a posteriori probability* (MAP). After that we briefly address more complex queries such as mutual information, entropies and *expectation* (EXP).

2.2.1 Basic Queries

The most basic inference task we are interested in computing is the probability of evidence. To unlock this, we must introduce two structural constraints known as *smoothness* and *decomposability*.

Definition 2.2.1 (Smoothness)**.** *A probabilistic circuit $\mathcal{C}$ is said to be* smooth *if for every sum node S in $\mathcal{C}$,* $\mathrm{Sc}(C_1) = \mathrm{Sc}(C_2)$ *for* $C_1, C_2 \in \mathrm{Ch}(S)$.

Definition 2.2.2 (Decomposability)**.** *A probabilistic circuit $\mathcal{C}$ is said to be* decomposable *if for every product node P in $\mathcal{C}$,* $\mathrm{Sc}(C_1) \cap \mathrm{Sc}(C_2) = \emptyset$ *for* $C_1, C_2 \in \mathrm{Ch}(P)$.

When a PC is *decomposable*, all of its induced subcircuits are induced trees. For any *smooth* and *decomposable* PC, computing EVI is done in linear time in the number of edges. In fact this is true for MAR and CON as well. To compute marginals, it is sufficient to compute the corresponding marginals with respect to each input node and proceed to propagate values bottom-up. For conditionals, we simply compute two passes: one where we marginalize the conditional variables and the other any other variables that are not present in our query. These procedures are formalized in the theorem below.

Theorem 2.2.1 (Poon and P. Domingos, 2011; Y. Choi, Vergari, and Van den Broeck, 2020; Vergari, Y. Choi, *et al.*, 2021)**.** *Let $\mathcal{C}$ a* smooth *and* decomposable *PC. Any one of EVI, MAR or CON can be computed in linear time (in the number of edges of $\mathcal{C}$).*

Importantly, EVI and CON are both special cases of MAR in the sense that they are marginalizations over different intervals (see page 71). More specifically, EVI is a marginalization over an empty set and CON is simply the quotient between two marginalization passes. Algorithmically, this means that the only distinction between these three queries is on what to do on the input nodes. We say that a variable assignment $\mathbf{x}$ for circuit $\mathcal{C}$ is *complete* if for every variable $X \in \mathrm{Sc}(\mathcal{C})$, $\mathbf{x}$ assigns a value to X; otherwise it is said to be a

Algorithm 1 EVI

Input A probabilistic circuit $\mathcal{C}$ and complete assignment $\mathbf{x}$
Output Probability $\mathcal{C}(\mathbf{x})$

Let v a hash function mapping a node to its probability
for each N in reverse topological order **do**
    if N is an input **then** $v_{\mathsf{N}} \leftarrow \mathsf{N}(\mathbf{x})$
    else if N is a sum **then** $v_{\mathsf{N}} \leftarrow \sum_{\mathsf{C} \in \mathrm{Ch}(\mathsf{N})} w_{\mathsf{N},\mathsf{C}}\, v_{\mathsf{C}}$
    else if N is a product **then** $v_{\mathsf{N}} \leftarrow \prod_{\mathsf{C} \in \mathrm{Ch}(\mathsf{N})} v_{\mathsf{C}}$
return v_R, where R is $\mathcal{C}$'s root

Algorithm 2 MAR

Input A probabilistic circuit $\mathcal{C}$ and partial assignment $\mathbf{x}$
Output Probability $\int \mathcal{C}(\mathbf{x}, \mathbf{y})\, \mathrm{d}\mathbf{y}$

Let v a hash function mapping a node to its probability
for each N in reverse topological order **do**
    if N is an input **then** $v_{\mathsf{N}} \leftarrow \int \mathsf{N}(\mathbf{x}, \mathbf{y})\, \mathrm{d}\mathbf{y}$
    else if N is a sum **then** $v_{\mathsf{N}} \leftarrow \sum_{\mathsf{C} \in \mathrm{Ch}(\mathsf{N})} w_{\mathsf{N},\mathsf{C}}\, v_{\mathsf{C}}$
    else if N is a product **then** $v_{\mathsf{N}} \leftarrow \prod_{\mathsf{C} \in \mathrm{Ch}(\mathsf{N})} v_{\mathsf{C}}$
return v_R, where R is $\mathcal{C}$'s root

partial assignment. Algorithm 1 and Algorithm 2 show the exact algorithmic procedures to extract EVI and MAR queries from $\mathcal{C}$. For CON, it suffices to run two MARs.

Because EVI, MAR and CON are the most basic forms of querying in PCs, we shall refer to these as *base queries*. Although smoothness and decomposability are sufficient conditions for tractable base queries, they are not necessary conditions. As a matter of fact, decomposability can be replaced with a third weaker constraint known as *consistency*. Denote by Desc(N) the set of all descendants of N.

Definition 2.2.3 (Consistency)**.** *A probabilistic circuit $\mathcal{C}$ is said to be* consistent *if for any product node P in $\mathcal{C}$, it holds that for every two children $C_1, C_2 \in \mathrm{Ch}(P)$ there does not exist two input nodes $L_p^1 \in \mathrm{Desc}(C_1)$ and $L_q^2 \in \mathrm{Desc}(C_2)$ whose scope is the same and $p(\mathbf{x}) \neq q(\mathbf{x})$ for any $\mathbf{x} \in \boldsymbol{\mathcal{X}}$.*

In Peharz, Tschiatschek, *et al.* (2015), the authors show that although smooth and consistent PCs are more succinct (Darwiche and Marquis, 2002) compared to smooth and decomposable circuits, the gain is only mild, further proving that any smooth and consistent PC can be polynomially translated to a decomposable equivalent. In practice, because constructing decomposable circuits (and verifying decomposability) is much easier compared to doing the same with consistency, we instead focus on smooth and decomposable PCs.

Suppose we wish to compute the most probable assignment of a variable, say for classification or image reconstruction. To do so, we must compute the conditional query

$$\max_{\mathbf{y}} p(\mathbf{y}|\mathbf{x}) = \max_{\mathbf{y}} \frac{p(\mathbf{y}, \mathbf{x})}{p(\mathbf{x})} = \frac{\max_{\mathbf{y}} p(\mathbf{y}, \mathbf{x})}{p(\mathbf{x})}, \tag{2.1}$$

Algorithm 3 MAP

Input A probabilistic circuit $\mathcal{C}$ and evidence assignment $\mathbf{x}$
Output Probability $\max_{\mathbf{y}} \mathcal{C}(\mathbf{y}|\mathbf{x})$

Let v a hash function mapping a node to its probability
for each N in reverse topological order **do**
    if N is an input **then** $v_{\mathsf{N}} \leftarrow \max_{\mathbf{y}} \mathsf{N}(\mathbf{y}, \mathbf{x})$
    else if N is a sum **then** $v_{\mathsf{N}} \leftarrow \max_{\mathsf{C} \in \mathrm{Ch}(\mathsf{N})} w_{\mathsf{N},\mathsf{C}}\, v_{\mathsf{C}}$
    else if N is a product **then** $v_{\mathsf{N}} \leftarrow \prod_{\mathsf{C} \in \mathrm{Ch}(\mathsf{N})} v_{\mathsf{C}}$
return $v_R/\mathcal{C}(\mathbf{x})$, where R is $\mathcal{C}$'s root

Algorithm 4 ARGMAP

Input A probabilistic circuit $\mathcal{C}$ and evidence assignment $\mathbf{x}$
Output The most probable state $\arg\max_{\mathbf{y}} \mathcal{C}(\mathbf{y}|\mathbf{x})$

Compute $\max_{\mathbf{y}} \mathcal{C}(\mathbf{y}|\mathbf{x})$ and store values in v
$\mathbf{N} \leftarrow$ MaxInducedTree($\mathcal{C}$, v)
Call $\mathbf{y}$ the set of initially empty arg max states
for each input node $\mathsf{L} \in \mathbf{N}$ **do**
    $\mathbf{y} \leftarrow \mathbf{y} \cup \arg\max_{\mathbf{z}} \mathsf{N}(\mathbf{z}, \mathbf{x})$
return $\mathbf{y}$

often called the *maximum a posteriori* (MAP) probability. For this dissertation, we shall only consider the case of full MAP, as computing partial MAP is provably hard in most PCs (Peharz, Gens, Pernkopf, *et al.*, 2016; De Campos, 2011). Unless explicitly stated, MAP shall mean full MAP, i.e. when $\mathbf{x} \cup \mathbf{y}$ forms a complete assignment of the scope. Full MAP also goes by the name of *most probable explanation* (MPE) in literature. Although at first it seems like MAP is no harder than computing a CON, it turns out that for smooth and decomposable PCs, MAP is unfortunately intractable (Conaty *et al.*, 2017; Mei *et al.*, 2018). To unlock access to MAP we must make the circuit *deterministic*.

Definition 2.2.4 (Determinism)**.** *A probabilistic circuit $\mathcal{C}$ is said to be* deterministic *if for every sum node $S \in \mathcal{C}$ only one child of S has nonnegative value at a time for any complete assignment.*

At this point, we must introduce a graphical notation for *indicator* nodes. An indicator node is an input node whose function is the characteristic function $f(x) = [\![x = k]\!]$, i.e. a degenerate function with all of its mass on k and zero anywhere else. A special case is when X is binary and $k = 1$, in which case we say the input node is a literal node, denoting by the usual propositional notation X for when $k = 1$ and $\neg X$ for $k = 0$. Graphically, we shall use ◎ for indicators and the textual propositional notation for literals.

With determinism, we now have access to MAP.

Theorem 2.2.2 (Peharz, Gens, Pernkopf, *et al.*, 2016)**.** *Let $\mathcal{C}$ a smooth, decomposable and* deterministic *PC. MAP is computable in linear time (in the number of edges of $\mathcal{C}$).*

When a PC is smooth, decomposable and deterministic, the MAP is easily computable by simply replacing sum nodes with a max operation and performing a feedforward

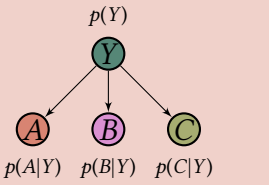
EVI pass. This is commonly called the Max-Product algorithm, shown more formally in Algorithm 3. To find the states that maximize Equation (2.1) in a given circuit $\mathcal{C}$, we first compute the MAP probabilities through the usual bottom-up pass, and then find the maximum (in terms of probability) induced tree $\mathcal{M}$ rooted at $\mathcal{C}$. This maximum induced tree can be retrieved by a top-down pass selecting the most probable sum child nodes according to the probabilities set by MAP. Since $\mathcal{C}$ is decomposable, there cannot exist a node in $\mathcal{M}$ with more than one parent, meaning it is by construction a tree whose leaves are input nodes with scopes whose union is the scope of $\mathcal{C}$. This reduces the problem to a divide-and-conquer approach where each input node is individually maximized (see Algorithm 4 and page 72 for a formal proof on its validity).

Example 2.4: Naïve Bayes as probabilistic circuits

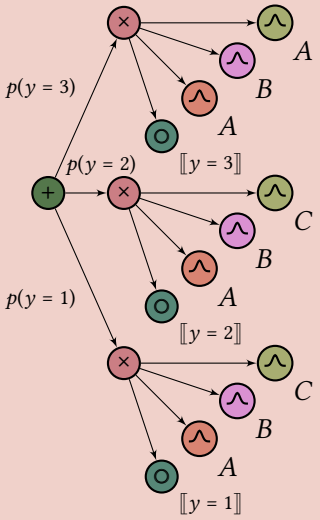
Suppose we have samples of per capita census measurements on three different features, say age A, body mass index B and average amount of cheese consumed daily C from three different cities Y. Assuming A, B and C are independent, given a sample $x = (a, b, c)$ we can use Gaussian naïve Bayes to predict x's class

$$p(y|a, b, c) = p(y)p(a|y)p(b|y)p(c|y).$$

In PC terms, $p(y)$ are the prior probabilities, i.e. sum weights, for each class and $p(z|y)$ are Gaussian input nodes corresponding to the distributions of each feature in each city. To make sure that these are in fact conditional distributions, we introduce indicator variables "selecting" Y's state. Since the PC resulting is deterministic, we can compute the MAP for classification in linear time by simply replacing the root node with a max, which is exactly equivalent to finding the highest likelihood of x for each city y.



Gaussian naïve Bayes



Equivalent PC

2.2.2 Complex Queries

Although base queries cover most of the needs of the usual data scientist, more complex tasks involving information-theoretic measures, logical queries or distributional divergences are also (tractably) computable under the right conditions. Particularly, we are interested in a key component for tractability in all these tasks: the notion of *vtrees* and *structure decomposability*, a stronger variant of decomposability where variable partitionings on product nodes follow a hierarchy. This hierarchy is easily visualized through a *vtree* (variable tree), a data structure that defines a (partial) ordering of variables.

Definition 2.2.5 (Vtree). *A variable tree $\mathcal{V}$, or* vtree, *over a set of variables* $\mathbf{X}$ *is a binary*

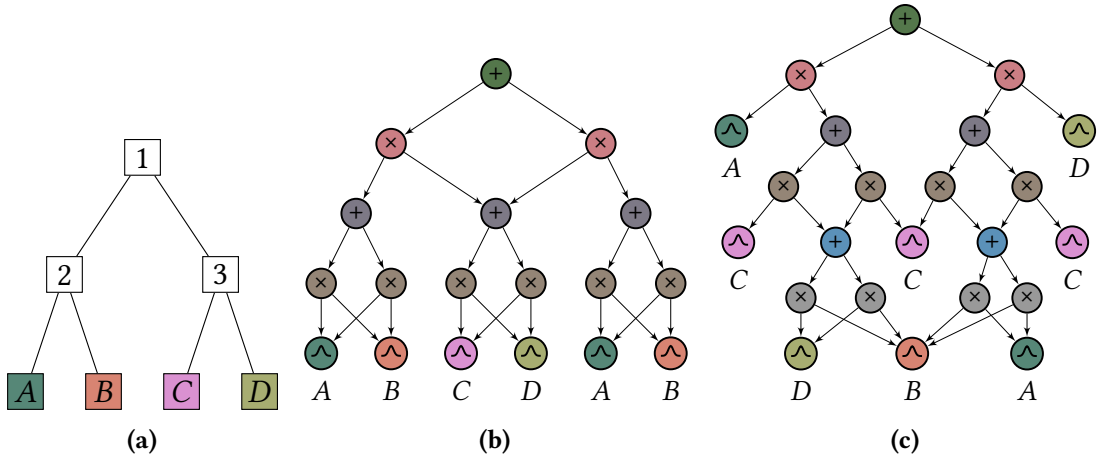


Figure 2.3: *A vtree (a) defining an order* (A, B, C, D)*, a 2-standard structure decomposable probabilistic circuit that respects the vtree (b), and a 2-standard decomposable probabilistic circuit that does not (c).*

tree whose leaf nodes have a one-to-one and onto mapping $\phi_{\mathcal{V}}$ *with* $\mathbf{X}$.

We shall adopt the same scope definition and notation $\mathrm{Sc}(\cdot)$ for vtrees as in PCs. Let v a vtree node from a vtree $\mathcal{V}$. If v is a leaf node, its scope is $\phi_{\mathcal{V}}(v)$, i.e. the leaf's assigned variable; otherwise its scope is the union of the scope of its children. For an inner node v, we shall call its left child $v^{\leftarrow}$ and right child $v^{\rightarrow}$. Every inner node v of a vtree $\mathcal{V}$ defines a variable *partitioning* of the scope $(\mathrm{Sc}(v^{\leftarrow}), \mathrm{Sc}(v^{\rightarrow}))$, while the leaves of $\mathcal{V}$ define a partial ordering of $\mathrm{Sc}(\mathcal{V})$. We are especially interested in the scope partitioning aspect of vtrees.

Definition 2.2.6. *A product node* P respects *a vtree node* v *if* P *contains only two children* $\mathrm{Ch}(P) = \{C_1, C_2\}$*, and* $\mathrm{Sc}(C_1) = \mathrm{Sc}(v^{\leftarrow})$ *and* $\mathrm{Sc}(C_2) = \mathrm{Sc}(v^{\rightarrow})$.

Obviously, the above definition is vague with regards to which child (i.e. graphically, left or right) of P should respect the scope of which v child. We therefore assume a fixed order for P's children and say that the (graphically) left child is called the *prime* and (graphically) right child the *sub*, and refer to P as an *element*. This ultimately means that the scope of the prime (resp. sub) of P must be the same as the scope of the left (resp. right) child of v. Although the graphical concept of left and right is needed for easily visualizing the scope partitioning of a product with respect to a vtree node, we do not use it strictly. In fact, when the situation is unambiguous, we compactly represent the computational graph without adhering to the left-right convention in favor of readability.

We say that a vtree is linear, if either it is left-linear or right-linear. A left- (resp. right) linear vtree is a vtree whose inner nodes all have leaf nodes on their right (resp. left) child. Similarly, a vtree is said to be left- (resp. right) leaning if the number of leaf nodes as right (resp. left) children is much higher then left (resp. right) children. Otherwise, it is a balanced vtree. The variable order of a vtree is the sequence of leaf nodes (i.e. variables) read from left to right. Figure 2.3a shows a balanced vtree with order (A, B, C, D).

Now that we understand what a vtree is, we can properly introduce *structure decomposability*, a stronger variant of decomposability. We say that a PC is 2-standard if it is standard and all of its product nodes have exactly two children.

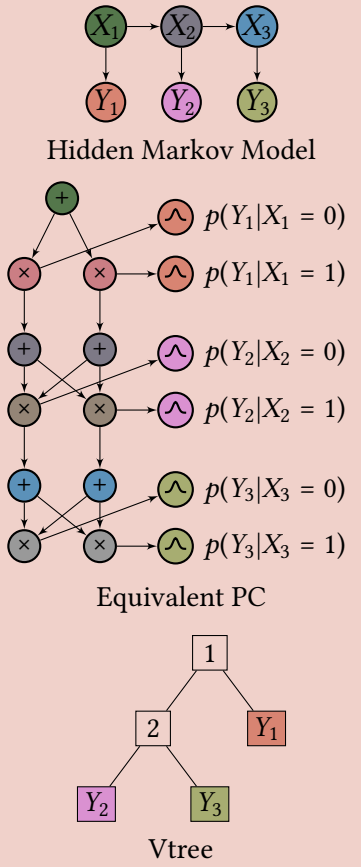
Definition 2.2.7 (Structure decomposability)**.** *Let $\mathcal{C}$ a 2-standard probabilistic circuit and $\mathcal{V}$ a vtree with same scope as $\mathcal{C}$. $\mathcal{C}$ is said to be* structure decomposable *if every i-th product layer of $\mathcal{C}$ respects every i-th inner node layer of $\mathcal{V}$.*

Example 2.5: Hidden Markov models as probabilistic circuits

Say we wish to model a temporal structured dependence between three latent binary variables, for example the presence of a subject X_1, verb X_2 and object X_3 in a natural language phrase. Each observation Y_i is a fragment (of X_i) taken from a complete sentence $\mathbf{y} = (y_1, y_2, y_3)$. The first-order Hidden Markov Model (HMM) (on the right) models the joint probability of sentences

$$p(X_{1..3}, Y_{1..3}) = p(X_1) \prod_{i=2}^{3} p(X_i|X_{i-1}) \prod_{i=1}^{3} p(Y_i|X_i).$$

This is computationally equivalent to the PC on the right. Each input node $p(Y_i|X_i)$ is a conditional distribution model (possibly another PC) for each assignment (here two) of X_i, meaning that if $p(Y_i|X_i = 0) > 0$, then $p(Y_i|X_i = 1) = 0$ and vice-versa. Root weights are exactly $p(X_1)$, and each $p(X_i|X_{i-1})$ translates into the other matched color sum weights. Further, every product (except for the redundant ⊗ nodes) follows the partitionings imposed by the vtree. This means that this PC is not only smooth, but structure decomposable and deterministic.



Although we assume a *2-standard* PC in Definition 2.2.7, its assumption was only for convenience, and does not imply in a loss of expressivity. As a matter of fact, any PC can be 2-standardized, i.e. to standardize the circuit such that every product node only has two children (see Theorem A.1.3). Intuitively, structure decomposability merely states that every two product nodes whose scopes are the same must partition their scopes (between their two children) exactly the same (and according to their corresponding vtree node). Semantically speaking, a vtree's inner node v defines an independence relationship between $\mathrm{Sc}(v^{\leftarrow})$ and $\mathrm{Sc}(v^{\rightarrow})$ under the distribution encoded by its PC.

Figure 2.3 shows a vtree $\mathcal{V}$ and two probabilistic circuits, say $\mathcal{C}_1$ for the one in the middle and $\mathcal{C}_2$ for the one on the right. Notice how $\mathcal{C}_1$ respects $\mathcal{V}$, as each ⊗ respects the split at vtree node 1 (namely $\{A, B\}$). The primes are then ⊕ whose scopes are $\{A, B\}$, while the sub is the one with two parents and scope $\{C, D\}$. For each of these, their children ⊗ also respect $\mathcal{V}$: they either encode he same split as 2 or as 3, depending on whether they are descendants from the sub or prime of 1. Although $\mathcal{C}_2$ is decomposable, it does *not* respect $\mathcal{V}$, as ⊗ encode different variable partionings $((\{A\}, \{B, C, D\})$ and $(\{A, B, C\}, \{D\}))$. In fact, it is not structure decomposable, as it does not respect any vtree.

Despite our structure decomposability definition relying on a vtree, there is at least one alternative definition that defines it in terms of *circuit compatibility*. Essentially, a circuit $\mathcal{C}_1$ is *compatible* with $\mathcal{C}_2$ if they can be 2-standardized and rearranged such that any two products with same scope, one from $\mathcal{C}_1$ and the other $\mathcal{C}_2$, partition the scope the same way (Vergari, Y. Choi, *et al.*, 2021). A structure decomposable PC is then defined as a PC that is compatible with a copy of itself. In summary, the two definitions of structure decomposability are equivalent, except compatibility implicitly assumes an arrangement of product scopes that is analogous to a vtree.

The notion of a vtree (or compatibility for that matter) is key to more complex queries. For instance, given two probabilistic circuits $\mathcal{C}_1$ and $\mathcal{C}_2$, computing cross entropy between the two is $\mathcal{O}(|\mathcal{C}_1||\mathcal{C}_2|)$ as long as both have the same vtree and at least the circuit that needs to be log-computable is also deterministic. Likewise, computing the Kullback-Leibler (KL) divergence between $\mathcal{C}_1$ and $\mathcal{C}_2$ requires that the two share the same vtree and both be deterministic. Mutual Information (MI), in turn, calls for the circuit to be smooth, structure decomposable and an even stronger version of determinism known as *marginal determinism* where sums can only have one nonnegative valued child for any *partial* assignment at a time. In fact, when a PC is smooth, decomposable and marginal deterministic, marginal MAP, i.e. MAP over partial assignments becomes linear time computable. For a more detailed insight on the tractability of these (and other) queries, as well as proofs on these results, we point to the comprehensive study of Vergari, Y. Choi, *et al.* (2021).

A particularly interesting class of queries that becomes tractable when circuits are structure decomposable is expectation (EXP). One notable example from this class is computing the probability of logical events. This leads us to logic circuits, a parallel version of probabilistic circuits for logical reasoning.

2.3 Probabilistic Circuits as Knowledge Bases

We superficially mentioned in Remark 2.1 that PCs under a Boolean semiring with conjunctions and disjunctions as operators are known as Logic Circuits (LCs). In this section, we formally yet briefly define LCs and more precisely show the connection between PCs and LCs.

2.3.1 From Certainty...

Logic circuits are computational graphs just like PCs, but whose input are always Booleans (and as such the scope is over propositional variables) and computational units define either a conjunction, disjunction or literal of their inputs. While the computational graph in PCs encodes uncertainty as a probability distribution, in LCs their computational graph encodes certain knowledge as a propositional language. Similar to PCs, computing the satisfiability of an assignment is done by a bottom-up feedforward evaluation of the circuit. In terms of notation, we shall use ⋃ for disjunction nodes, ⋂ for conjunction nodes, and X and $\neg X$ for literal nodes.

Definition 2.3.1 (Logic circuit)**.** *A logic circuit $\mathcal{L}$ is a rooted connected DAG whose nodes compute either a conjunction or a disjunction of their children. Nodes with no outgoing*

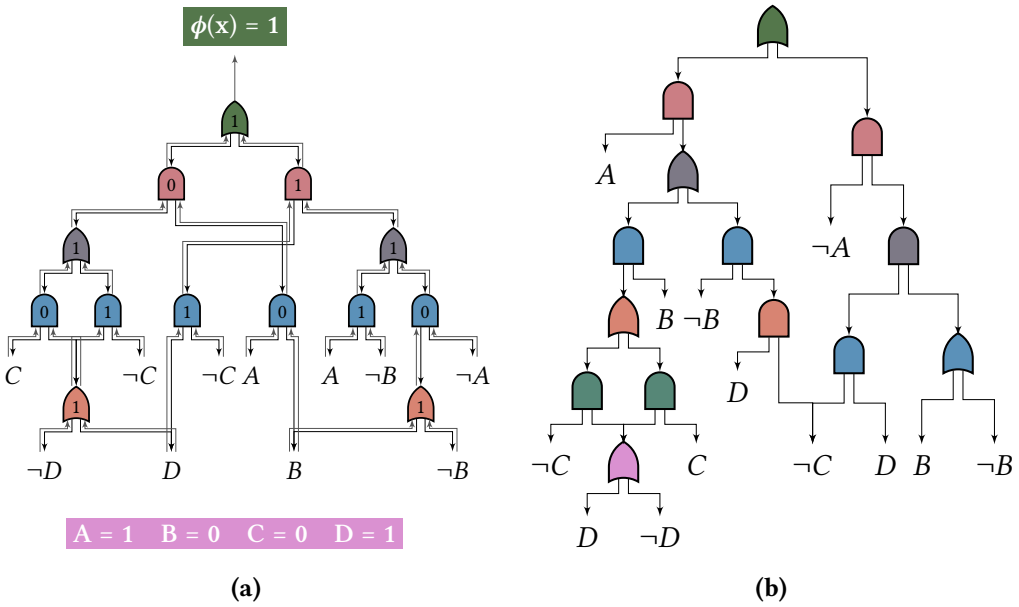


Figure 2.4: *Two smooth, structure decomposable and deterministic logic circuits encoding the same logic constraint $\phi \equiv (A \wedge B) \vee (\neg C \wedge D)$ for a balanced (a) and a right-linear (b) vtree. In (a), a circuit evaluation for an assignment, with each node value in the bottom-up evaluation pass shown inside nodes.*

edges, i.e. literal *nodes, are indicator functions of either a positive (true) or negative (false) assignment. Computing the satisfiability of $\mathcal{L}$ amounts to a bottom-up feedforward pass from literal nodes to root.*

Evidently, logic circuits are closely related to probabilistic circuits. The strikingly similar definitions are not coincidence: much of the literature on PCs have their origins on LCs. In fact, most structural constraints in PCs are the exact same (up to even their names[2]) as their LC analogues. In this dissertation, we are particularly interested in the specific subset of smooth, structure decomposable and deterministic LCs, known as Sentential Decision Diagrams (SDDs, Darwiche, 2011). Figure 2.4 shows two SDDs encoding the same knowledge base but under different vtrees. The one on the left respects a balanced vtree and the one on the right a right-linear vtree.

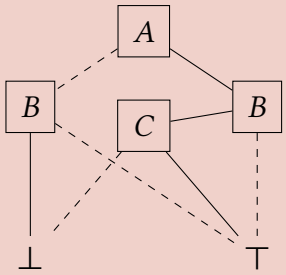
Logic circuits have appeared in literature under the name of Negated Normal Form (NNF) (Darwiche, 2001; Darwiche, 1999), a superset of other propositional compilation languages such as Binary Decision Diagrams (BDDs, Bryant, 1986), Propositional DAGs (PDAGs, Wachter and Haenni, 2006), Sentential Decision Diagrams (SDDs, Darwiche, 2011), DNFs and CNFs. Although no structural constraint is required for correctly evaluating satisfiability in logic circuits, the same properties defined in past sections have come up in LCs to enable other more complex queries like equivalence, implicates, sentential entailment and model counting, as well as transformations such as closed conditionings, forgetting, conjunctions and disjunctions (Darwiche and Marquis, 2002). The succinctness (i.e. expressive efficiency) of LCs are also impacted by these structural restrictions

[2] There are some exceptions. Smoothness is sometimes referred to as *completeness* in PCs, while determinism has the alternative name of *selectivity*.

(Gogic *et al.*, 1995; Papadimitriou, 1994; Darwiche and Marquis, 2002). See Darwiche and Marquis (2002) and Darwiche (2020) for more on logic circuits.

Example 2.6: BDDs as logic circuits

A Binary Decision Diagram (BDD, Bryant, 1986) defines a Boolean function over binary variables as a rooted DAG. BDDs are a subset of smooth, structure decomposable and deterministic LCs (i.e. SDDs) whose vtrees are always right-linear.



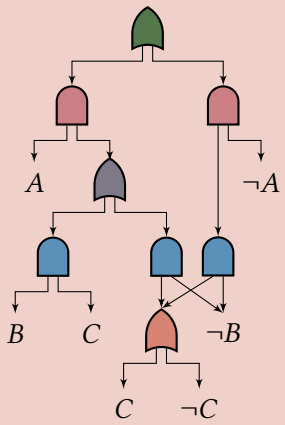
In their usual notation, inner nodes are variables and leaves are constants $\bot$ and $\top$. Evaluating an assignment $\mathbf{x} \subseteq \{0,1\}^n$ is equivalent to a path from the root to a leaf where each variable X determines a decision to go through the dashed line when $x = 0$ or solid line when $x = 1$. If the path ends at a $\top$, the function returns 1, otherwise it must end at a $\bot$ and therefore returns 0. The BDD above encodes the following logic formula

$$\phi(A, B, C) = (A \vee \neg B) \wedge (\neg B \vee C),$$

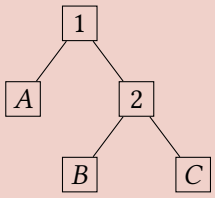
also shown as a truth table on the right, together with a logic circuit that encodes the same truth table and its vtree.

A	B	C	$\phi(\mathbf{x})$
0	0	0	1
1	0	0	1
0	1	0	0
1	1	0	0
0	0	1	1
1	0	1	1
0	1	1	0
1	1	1	1

Truth Table



Equivalent LC



Vtree

2.3.2 ...to Uncertainty

Logic circuits are easily extensible to probabilistic circuits. In fact, if we think of an LC as the support of a PC the connections between the two come naturally. Suppose a 2-standard smooth, structure decomposable and deterministic probabilistic circuit $\mathcal{C}$ over binary variables. We can construct an identically structured logic circuit (up to input nodes) $\mathcal{L}$ with same vtree as $\mathcal{C}$ whose underlying Boolean function encodes $\phi(\mathbf{x}) = [\![\mathcal{C}(\mathbf{x}) > 0]\!]$. Since sums act exactly like disjunctions and products like conjunctions under the Boolean semiring, products in $\mathcal{L}$ are replaced with conjunctions in $\mathcal{L}$, and sums with disjunctions. Input nodes from $\mathcal{C}$ are replaced with a literal node if the function is degenerate, or with a disjunction over positive and negative literals otherwise. This makes sure $\mathcal{L}$ acts as the

support of $\mathcal{C}$, as each disjunction node $S_{\mathcal{L}}$ of $\mathcal{L}$ defines

$$S_{\mathcal{L}}(\mathbf{x}) = \bigvee_{C \in \mathrm{Ch}_{\mathcal{C}}(S_{\mathcal{L}})} [\![C_p(\mathbf{x}) > 0]\!] \wedge [\![C_s(\mathbf{x}) > 0]\!],$$

where $\mathrm{Ch}_{\mathcal{C}}(S)$ retrieves the children of S's corresponding sum node in $\mathcal{C}$, with $C_p(\mathbf{x})$ and $C_s(\mathbf{x})$ the probabilities of C's prime and sub respectively. The corresponding sum node $S_{\mathcal{C}}$ in $\mathcal{C}$ then only attributes a weight (i.e. probability) to each positive element as usual

$$S_{\mathcal{C}}(\mathbf{x}) = \sum_{C \in \mathrm{Ch}(S_{\mathcal{C}})} w_{S_{\mathcal{C}},C} \cdot C_p(\mathbf{x}) \cdot C_s(\mathbf{x}).$$

When a deterministic sum (resp. disjunction) node has the above form, then this composition of a weighted sum (resp. disjunction) is known in PC and LC literature as a *partition*.

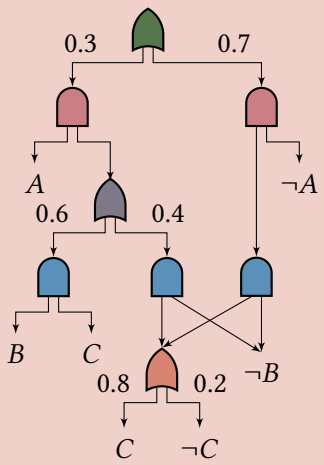
Example 2.7: Embedding certain knowledge in probabilistic circuits

Recall the logic circuit $\mathcal{L}$ from Example 2.6. Imagine we wish to model the uncertainty coming from all assignments where $\mathcal{L}(\mathbf{x}) = 1$. In other words, we want to assign a positive probability to all true entries in the previous example's truth table, turning it into a probability table. The table on the right shows the chosen probabilities for each instance. Naturally, they all sum to one, with logically impossible assignments set to zero.

A	B	C	$\phi(\mathbf{x})$	$p(\mathbf{x})$
0	0	0	1	0.140
1	0	0	1	0.024
0	1	0	0	0.000
1	1	0	0	0.000
0	0	1	1	0.560
1	0	1	1	0.096
0	1	1	0	0.000
1	1	1	1	0.180

Probability Table

Compiling an LC into a PC is straightforward: replace conjunctions with product nodes and disjunctions with sum nodes. Input nodes are left untouched, as literal nodes are just degenerate probability distributions. Sum weights are what ultimately define the probabilities in the probability table. The PC on the right is the result of the compilation of $\mathcal{L}$ into a probabilistic circuit whose distribution is defined by the probability table above it. When we mean to say that a PC has its support defined by its underlying LC, then we use the logic gate notation with the added weights on edges coming out from ⌓ nodes.



Probabilistic Circuit

This compatibility between logic and probabilistic circuits allows certain knowledge to be embedded into an uncertain model by constructing a computational graph whose underlying logic circuit correctly attributes positive values only to the support of the distribution. When such a computational graph is also smooth, structure decomposable and deterministic, then it belongs to a special subclass of PCs called Probabilistic Sentential Decision Diagrams (PSDDs, Kisa *et al.*, 2014). An alternative use case for logic circuits

Algorithm 5 EXP

Input A smooth, structure decomposable PC $\mathcal{C}$ and LC $\mathcal{L}$ both with vtree $\mathcal{V}$
Output The expectation $\mathbb{E}_{\mathcal{C}}[\mathcal{L}] = \int \mathcal{C}(\mathbf{x})\mathcal{L}(\mathbf{x})\,\mathrm{d}\mathbf{x}$

1: Let v a hash function mapping a pair of nodes to an expectation
2: **for** each pair of nodes $(\mathsf{N}_{\mathcal{C}}, \mathsf{N}_{\mathcal{L}})$ in reverse topological order **do**
3: **if** $\mathsf{N}_{\mathcal{C}}$ is an input **then** $v_{\mathsf{N}_{\mathcal{C}},\mathsf{N}_{\mathcal{L}}} \leftarrow \mathbb{E}_{\mathsf{N}_{\mathcal{C}}}[\mathsf{N}_{\mathcal{L}}]$
4: **else if** $\mathsf{N}_{\mathcal{C}}$ is a product **then** $v_{\mathsf{N}_{\mathcal{C}},\mathsf{N}_{\mathcal{L}}} \leftarrow \prod_{\mathsf{C}\in\mathrm{Ch}(\mathsf{N}_{\mathcal{C}})} v_{\mathsf{C}_{\mathcal{C}},\mathsf{C}_{\mathcal{L}}}$
5: **else if** $\mathsf{N}_{\mathcal{C}}$ is a sum **then** $v_{\mathsf{N}_{\mathcal{C}},\mathsf{N}_{\mathcal{L}}} \leftarrow \sum_{\mathsf{C}'\in\mathrm{Ch}(\mathsf{N}_{\mathcal{C}})} \sum_{\mathsf{C}''\in\mathrm{Ch}(\mathsf{N}_{\mathcal{L}})} w_{\mathsf{S},\mathsf{C}'} \cdot v_{\mathsf{C}',\mathsf{C}''}$
6: **return** v_R, where R is $\mathcal{C}$'s root

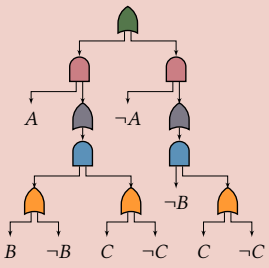
within the context of probabilistic reasoning is querying for the probability of logical events, i.e. the expectation of a logic query with respect to a distribution. This kind of query is enabled by the following result.

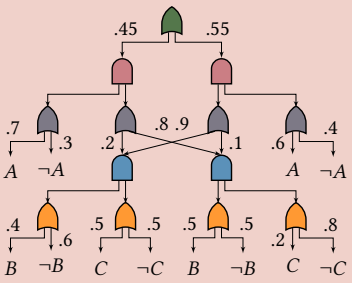
Theorem 2.3.1 (Y. Choi, Vergari, and Broeck, 2020). *If $\mathcal{C}$ is a smooth and structure decomposable probabilistic circuit with vtree $\mathcal{V}$, and $\mathcal{L}$ a structure decomposable logic circuit also respecting $\mathcal{V}$, then $\mathbb{E}_{\mathcal{C}}[\mathcal{L}]$ is polynomial time computable (in the number of edges).*

Let $\mathcal{C}$ a smooth and structure decomposable circuit with vtree $\mathcal{V}$, and $\mathcal{L}$ a logic circuit representing a logical query whose vtree is also $\mathcal{V}$. Computing the probability of $\mathcal{L}$ with respect to the distribution encoded by $\mathcal{C}$ is done by a bottom-up evaluation over both circuits at the same time. Algorithm 5 shows the procedure algorithmically. Importantly, the procedure relies on evaluating the expectation for each node in a reverse topological fashion according to line 2. This paired reverse topological sorting is done by a recursive assignment. For product nodes, primes are paired with primes, and subs with subs; for sums, each combination of PC child with LC child is paired up.

Example 2.8: Computing the probability of logical events

Say we have a PC encoding the distribution shown in the table on the right. Suppose we wish to compute the probability of a logical event, say $\phi \equiv A \vee \neg B$. A naïve approach would be to go over each assignment $\mathbf{x}$ where $\phi(\mathbf{x}) = 1$, and compute their sum. This is obviously exponential on the number of variables. Instead, we may compile ϕ into the logic circuit above and run the EXP algorithm to (in polynomial time) compute this otherwise intractable marginalization. Running the EXP gives us a probability of $0.6415 = 1.0 - (0.1365 + 0.2220)$, which is exactly the desired probability.





A	B	C	$\phi(\mathbf{x})$	$p(\mathbf{x})$
0	0	0	1	.1000
1	0	0	1	.0580
0	1	0	0	.1365
1	1	0	1	.0805
0	0	1	1	.1860
1	0	1	1	.0970
0	1	1	0	.2220
1	1	1	1	.1195

Remark 2.2: On applications of probabilistic circuits

So far, we have not yet addressed real-world applications of probabilistic circuits. Although their usage has not yet gained popularity among the data science crowd, they have been successfuly employed in a multitude of interdisciplinary tasks. Here, we give a brief survey on the different use cases of probabilistic circuits present in literature.

Computer vision is perhaps the most popular application for deep learning, and this could not be different for probabilistic circuits. PCs have been used for image classification (Gens and P. Domingos, 2012; Sguerra and F. G. Cozman, 2016; Llerena and Deratani Mauá, 2017; R. Geh and D. Mauá, 2019; Peharz, Vergari, *et al.*, 2020), image reconstruction and sampling (Poon and P. Domingos, 2011; Dennis and Ventura, 2017; Peharz, Lang, *et al.*, 2020; Cory J Butz *et al.*, 2019), image segmentation and scene understanding (Abram L Friesen and P. Domingos, 2017; Yuan *et al.*, 2016; Abram L Friesen and P. M. Domingos, 2018; Rathke *et al.*, 2017), and activity recognition (J. Wang and G. Wang, 2018; Amer and Todorovic, 2012; Nourani *et al.*, 2020; Amer and Todorovic, 2016).

Probabilistic circuits have also been used for sequential data (Melibari, Poupart, Doshi, and Trimponias, 2016), such as speech recognition and reconstruction (Peharz, Kapeller, *et al.*, 2014; Ratajczak *et al.*, 2014; Ratajczak *et al.*, 2018) and natural language processing (Cheng *et al.*, 2014).

Remarkably, probabilistic circuits have seen a recent boom in hardware-aware research (Shah, Isabel Galindez Olascoaga, *et al.*, 2019; Olascoaga *et al.*, 2019) and dedicated hardware for PCs in embedded systems (Sommer *et al.*, 2018; Shah, Olascoaga, Meert, *et al.*, 2020; Shah, Olascoaga, S. Zhao, *et al.*, 2021).

Some other applications include robotics (Sguerra and F. G. Cozman, 2016; R. Geh and D. Mauá, 2019; Zheng *et al.*, 2018; Pronobis *et al.*, 2017), biology (Cory J. Butz, Santos, *et al.*, 2018; Abram L. Friesen and P. Domingos, 2015), probabilistic programming (Stuhlm"uller and Goodman, 2012; Saad *et al.*, 2021), and fault localization (Nath and P. M. Domingos, 2016).

Now that we have addressed the (arguably) most important aspects of probabilistic circuits, we are now ready to understand how to build them in a principled way.

Example 2.9: Density estimation trees as probabilistic circuits

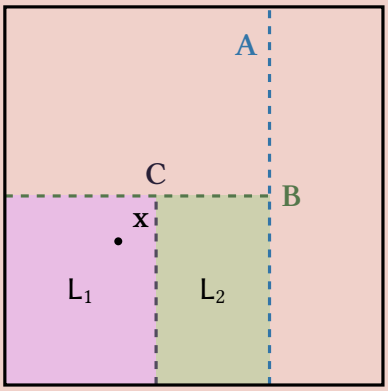
A density estimation tree is a decision tree for the task of density estimation (Ram and Gray, 2011). Briefly, a decision tree $\mathcal{T}$ partitions the data space (usually $\mathbb{R}^d$) into cells by laying out hyperplanes usually orthogonal to the axes, creating a latent variable for each node that essentially determines in which edge an observation should fall into. The density function of a tree $\mathcal{T}$ given a dataset $\mathbf{D}$ of dimension d is defined as the piecewise function

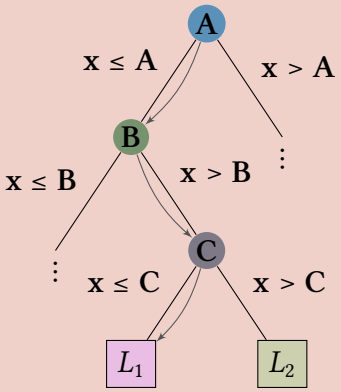
$$p_{\mathcal{T}}(\mathbf{x}) = \sum_{\mathsf{L} \in \text{Leaves}(\mathcal{T})} \frac{1}{\text{Vol}(\mathsf{L})} \cdot \frac{|\mathbf{D} \in \mathsf{L}|}{|\mathbf{D}|} \cdot [\![\mathbf{x} \in \mathsf{L}]\!],$$

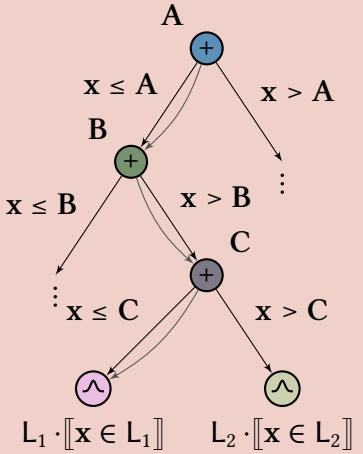
where $|\mathbf{D} \in \mathsf{L}|$ indicates the number of assignments $\mathbf{x}$ in the training dataset $\mathbf{D}$ which fall inside the cell determined by leaf L, and $\text{Vol}(\mathsf{L})$ retuns the volume of the d-dimensional cell L. The top figure on the right shows a two-dimensional data space being partitioned, with the corresponding decision tree below it. Each node in the tree is a (hyper)plane partitioning data, with every edge determining which cell the observation falls into.

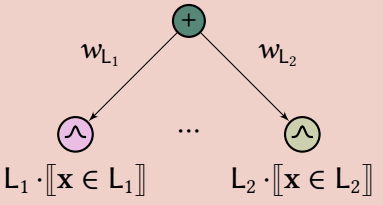
Equivalently, a sum node in a PC that determines the on-off state of a latent variable partitioning the data space configures the same semantics as a density estimation tree. Instead of delegating an observation's probability to the tree's leaves, a PC spreads out this density to both weights in sum nodes and density in input nodes. Let $\mathcal{C}$ a PC whose nodes are all sum nodes which encode such latent partitions and whose input nodes are truncated to follow these latent variables (i.e. their support is only over the space determined by the partitionings); collapse all layers (and weights) into a shallow PC with a single sum layer. Its value is then

$$p_{\mathcal{C}}(\mathbf{x}) = \sum_{\mathsf{L} \in \text{Inputs}(\mathcal{C})} w_{\mathsf{L}} \cdot \mathsf{L}(\mathbf{x}) \cdot [\![\mathbf{x} \in \mathsf{L}]\!].$$









3

Learning Probabilistic Circuits

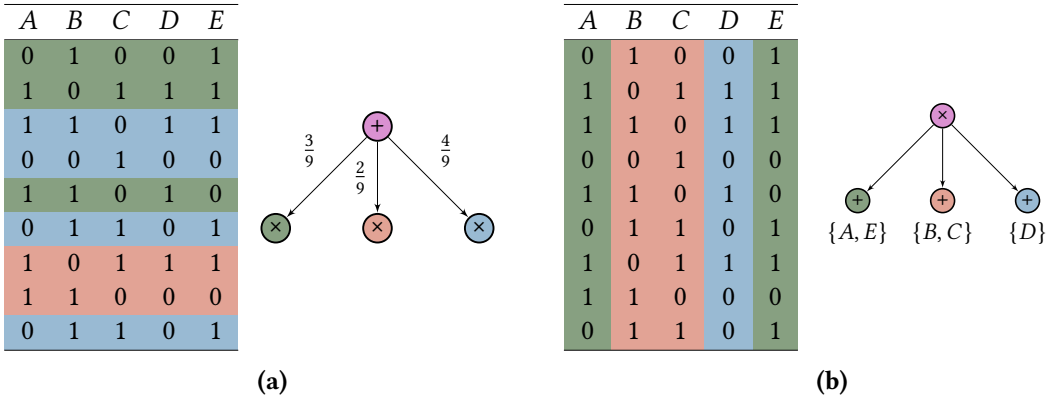
As we have seen in Chapter 2, inference in probabilistic circuits is, for the most part, straightforward. This is not so much the case when *learning* PCs. Despite the uncomplicated syntax, learning sufficiently expressive PCs in a principled way is comparatively harder to, say the usual neural network. For a start, we are usually required to comply with smoothness and decomposability to ensure marginalization at the least. This restriction excludes the possibility of adopting any of the most popular neural network patterns or architectures used in deep learning today. To make matters worse, constructing a PC graph more often than not involves costly statistical tests that make learning their structure a challenge for high dimensional data.

In this chapter, we review the most popular PC structure learning algorithms, their pros and cons, and more importantly, what can we learn from them to efficiently build scalable probabilistic circuits. We broadly divide existing structure learners into three main categories: divide-and-conquer (`DIV`, Section 3.1), incremental methods (`INCR`, Section 3.2) and random approaches (`RAND`, Section 3.3).

3.1 Divide-and-Conquer Learning

Arguably the most popular approach to learning the structure of probabilistic circuits are algorithms that follow a *divide-and-conquer* scheme. This class of PC learning algorithms, which here we denote by `DIV`, are characterized by recursive calls over (usually mutually exclusive) subsets of data in true divide-and-conquer fashion. This kind of procedure is more clearly visualized by LearnSPN, the first, most well-known, and perhaps most archetypal of its class.

Before we start however, we must first address how we denote data. Data is commonly represented as a matrix where rows are assignments (of all variables), and columns are the values that each variable takes at each assignment. Let $\mathbf{D} \in \mathbb{R}^{n \times m}$ a matrix with n rows and m columns. We use $\mathbf{D}_{i,j}$ to access an element of $\mathbf{D}$ at the i-th row, j-th column of matrix $\mathbf{D}$. We denote by $\mathbf{D}_{\mathbf{i},\mathbf{j}}$, where $\mathbf{i} \subseteq [1..n]$ and $\mathbf{j} \subseteq [1..m]$ are sets of indices, a submatrix from the extraction of the $\mathbf{i}$ rows and $\mathbf{j}$ columns of $\mathbf{D}$. We use a colon as a shorthand for selecting all rows or columns, e.g. $\mathbf{D}_{:,:} = \mathbf{D}$, $\mathbf{D}_{:,j}$ is the j-th column and $\mathbf{D}_{i,:}$ is the i-th row.



(a) **(b)**

Figure 3.1: *LearnSPN assigns either rows (a) or columns (b) for sum and product nodes respectively. For sums, their edge weights are set proportionally to the assignments. For product children, scopes are defined by which columns are assigned to them.*

Algorithm 6 LearnSPN

Input Data $\mathbf{D}$, whose columns are indexed by variables $\mathbf{X}$
Output A smooth and decomposable probabilistic circuit learned from $\mathbf{D}$

if $|\mathbf{X}| = 1$ **then return** an input node learned from $\mathbf{D}$
else
  Find scope partitions $\mathbf{X}_1, \dots, \mathbf{X}_t \subseteq \mathbf{X}$ st $\mathbf{X}_i \perp\!\!\!\perp \mathbf{X}_j$ for $i \neq j$
  if $k > 1$ **then return** $\prod_{j=1}^{t}$ LearnSPN$(\mathbf{D}_{:,\mathbf{X}_j}, \mathbf{X}_j)$
  else
    Find subsets of data $\mathbf{x}_1, \dots, \mathbf{x}_k \subseteq \mathbf{D}$ st all assignments within $\mathbf{x}_i$ are all similar
    return $\sum_{i=1}^{k} \frac{|\mathbf{x}_i|}{|\mathbf{D}|} \cdot$ LearnSPN$(\mathbf{x}_i, \mathbf{X})$

3.1.1 LearnSPN

Recall the semantics of sum and product nodes in a smooth and decomposable probabilistic circuit. A sum is a mixture of distributions $p(\mathbf{X}) = \sum_{i=1}^{m} w_i \cdot p_i(\mathbf{X})$ whose children scopes are all the same. A product is a factorization $p(\mathbf{X}_1, \dots, \mathbf{X}_m) = \prod_{i=1}^{m} p(\mathbf{X}_i)$, implying that $\mathbf{X}_i \perp\!\!\!\perp \mathbf{X}_j$ for $i, j \in [m]$ and $i \neq j$. LearnSPN (Gens and P. Domingos, 2013) exploits these semantics in an intuitive and uncomplicated manner: sum children are defined by sub-PCs learned from similar (by some arbitrary metric) assignments, and product children are sub-PCs learned from data conditioned on the variables defined by their scope. In practice, this means that, for a dataset $\mathbf{D} \in \mathbb{R}^{n \times m}$, sums assign rows to their children, while product children are assigned columns. This procedures continues recursively until data are reduced to a $k \times 1$ matrix, in which case a univariate distribution acting as input node is learned from it. This recursive procedure is shown more formally in Algorithm 6.

Notably, (Gens and P. Domingos, 2013) purposely does not strictly specify which techniques should be used for assigning rows and columns, although they do provide empirical results on a particular form of LearnSPN where row assignments are computed through EM clustering and products by pairwise G-testing. Instead, they call the algorithm a *schema* that incorporates several actual learning algorithms whose concrete form depends on the choice of how to split data.

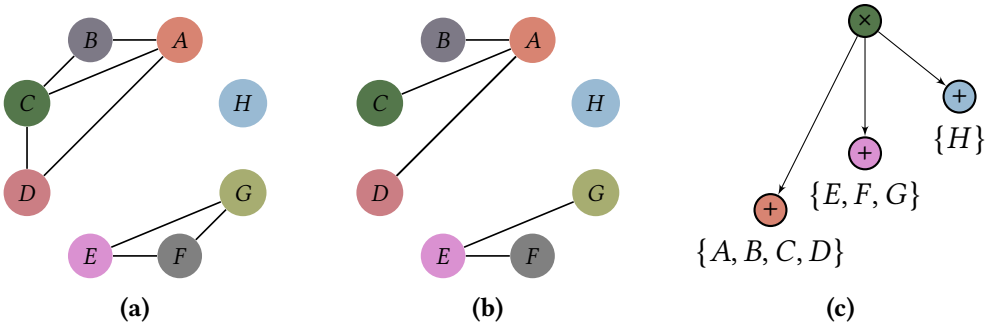


Figure 3.2: *The pairwise (in)dependence graph where each node is a variable. In (a) we show the full graph, computing independence tests for each pair of variables in $\mathcal{O}(m^2)$. However, it suffices to compute for only the connected components (b), saving up pairwise computation time for reachable nodes. The resulting product node and scope partitioning is shown in (c).*

Complexity

To be able to analyze the complexity of LearnSPN, we assume a common implementation where sums are learned from k-means clustering, and products through pairwise G-testing. We know learning sums is efficient: k-means takes $\mathcal{O}(n \cdot k \cdot m \cdot c)$ time, where k is the number of clusters and c the number of iterations to be run. Products, on the other hand, are much more costly. The naïve approach would be to compute whether $X_i \perp\!\!\!\perp X_j$ for every possible combination. This is clearly quadratic on the number of variables $\mathcal{O}\left(\binom{m}{2} = \frac{m!}{2(m-2)!}\right)$ assuming an $\mathcal{O}(1)$ oracle for independence testing. In reality, G-test takes $\mathcal{O}(n \cdot m)$ time, as we must compute a ratio of observed versus expected values for each cell in the contingency table. This brings the total runtime for products to a whopping $\mathcal{O}\left(n \cdot m^3\right)$, prohibitive to any reasonably large dataset. In terms of space, independence tests most commonly used require either a correlation (for continuous data) or contingency (for discrete data) matrix that takes up $\mathcal{O}(m^2)$ space, another barrier for scaling up to high dimensional data.

Alternatively, instead of computing the G-test for every possible combination of variables, (Gens and P. Domingos, 2013) constructs an independence graph $\mathcal{G}$ whose nodes are variables and edges indicate whether two variables are statistically dependent. Within this context, the variable partitions we attribute to product children are exactly the connected components of $\mathcal{G}$, meaning it suffices testing only some combinations. Even so, this heuristic is still quadratic worst case. Figure 3.2 shows $\mathcal{G}$, the spanning forest resulted from the connected component heuristic, and the equivalent product node from this decomposition.

Pros and cons

Pros. Perhaps the main factor for LearnSPN's popularity is how easily implementable, intuitive and modular it is. Even more remarkably, it is an empirically competitive PC learning algorithm despite its age, serving as a baseline for most subsequent works in PC literature. Lastly, the fact that each recursive call from LearnSPN is completely independent from each the other makes it an attractive candidate for CPU parallelization.

Algorithm 7 ExtendID

Input Data $\mathbf{D}$, whose columns are indexed by variables $\mathbf{X}$, and memoization function $\mathcal{M}$
Output A smooth and decomposable probabilistic circuit learned from $\mathbf{D}$

1: Find scope partitions $\mathbf{X}_1, \dots, \mathbf{X}_t \subseteq \mathbf{X}$ st
2: **if** $k > 1$ **then**
3: **for** each $j \in [t]$ **do**
4: $\mathsf{N}_j \leftarrow \textsc{LearnMarkov}(\mathbf{D}_{:,\mathbf{X}_j}, \mathbf{X}_j)$
5: Associate $\mathcal{M}(\mathsf{N}_j)$ with $\mathbf{D}_{:,\mathbf{X}_j}$ and $\mathbf{X}_j$
6: **return** $\prod_{j=1}^{t} \mathsf{N}_j$
7: **else**
8: Find subsets of data $\mathbf{x}_1, \dots, \mathbf{x}_k \subseteq \mathbf{D}$ st all assignments within $\mathbf{x}_i$ are all similar
9: **for** each $i \in [k]$ **do**
10: $\mathsf{N}_i \leftarrow \textsc{LearnMarkov}(\mathbf{x}_i, \mathbf{X})$
11: Associate $\mathcal{M}(\mathsf{N}_i)$ with $\mathbf{x}_i$ and $\mathbf{X}$
12: **return** $\sum_{i=1}^{k} \frac{|\mathbf{x}_i|}{|\mathbf{D}|} \cdot \mathsf{N}_i$

Cons. Debatably, one of the key weakness of LearnSPN is its tree-shaped computational graph, meaning that they are strictly less succint compared to non-tree DAG PCs (Martens and Medabalimi, 2014). In terms of runtime efficiency, the algorithm struggles on high dimensional data due to the complexity involved in computing costly statistical tests. Despite Algorithm 6 giving the impression that no hyperparameter tuning is needed for LearnSPN, in practice the modules for learning sums and products often take many parameters, most of which (if not all) are exactly the same for every recursive call. This can have a negative impact on the algorithm's performance, since the same parameters are repeatedly used even under completely different data.

3.1.2 ID-SPN

A subtle yet effective way of improving the performance of LearnSPN is to consider tractable probabilistic models over many variables as input nodes instead of univariate distributions. ID-SPN (Rooshenas and Lowd, 2014) does so by assuming that input nodes are Markov networks. Further, instead of blindly applying the recursion over subsequent sub-data, it attempts to compute some metric of quality from each node. The worst scored node is then replaced with a LearnSPN-like tree. This is repeated until no significant increase in likelihood is observed. Algorithm 8 shows the ID-SPN pipeline, where ExtendID is used in line 7 to grow the circuit in a divide-and-conquer fashion. The name ID-SPN comes from *direct* variable interactions, meaning the relationships modeled through the Markov networks as input nodes; and *indirect* interactions brought from the latent variable interpretation of sum nodes.

With respect to its implementation, ID-SPN is as modular as LearnSPN in the sense that the data partitioning is left as a subroutine. Indeed, even the choice of input distributions is customizable: although Rooshenas and Lowd recommend Markov networks, any tractable distribution will do. Despite this seemingly small change compared to the original LearnSPN algorithm, ID-SPN seems to perform better compared to its counterpart most

Algorithm 8 ID-SPN

Input Data $\mathbf{D}$, whose columns are indexed by variables $\mathbf{X}$
Output A smooth and decomposable probabilistic circuit learned from $\mathbf{D}$

Create a single-node PC: $\mathcal{C} \leftarrow$ LearnMarkov($\mathbf{D}, \mathbf{X}$)
Let $\mathcal{M}$ a memoization function associating a node with a dataset and scope
Call $\mathcal{C}'$ a copy of $\mathcal{C}$
while improving $\mathcal{C}$ yields better likelihood **do**
    Pick worse node N from $\mathcal{C}'$
    Extract sub-data $\mathbf{D}'$ and sub-scope $\mathbf{X}'$ from $\mathcal{M}(\mathsf{N})$
    Replace N with ExtendID($\mathbf{D}', \mathbf{X}', \mathcal{M}$)
    if $\mathcal{C}'$ has better likelihood than $\mathcal{C}$ **then** $\mathcal{C} \leftarrow \mathcal{C}$
return $\mathcal{C}$

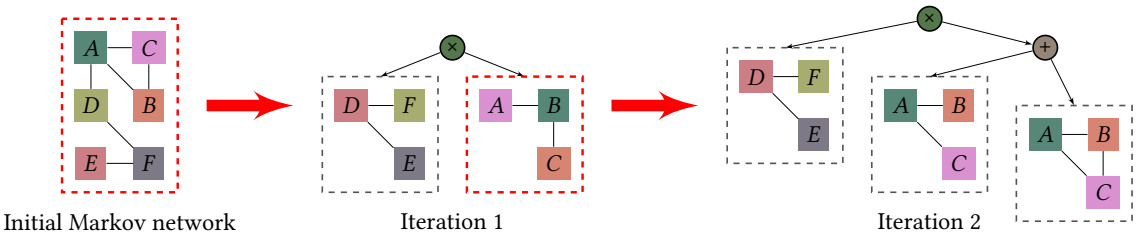


Figure 3.3: *Two iterations of ID-SPN, where the contents inside the dashed line are Markov networks. The red color indicates that a node has been chosen as the best candidate for an extension with ExtendID. Although here we only extend input nodes, inner nodes can in fact be extended as well.*

of the time (Rooshenas and Lowd, 2014; Jaini, Ghose, *et al.*, 2018), although at a cost to learning speed. Further, because of the enormous parameter space brought by having to learn Markov networks as inputs *and* perform the optimizations from sums and products, grid search hyperparameter tuning is infeasible. (Rooshenas and Lowd, 2014) recommend random search (Bergstra and Bengio, 2012) as an alternative.

Complexity

As ID-SPN is a special case of LearnSPN, the analysis for the sums and products subroutines holds. The only difference is on the runtime complexity for learning input nodes and the convergence rate for ID-SPN. Assuming input nodes are learned from the method suggested by Rooshenas and Lowd (2014), which involves learning a probabilistic circuit from a Markov network (Lowd and Rooshenas, 2013), then each "input" node takes time $\mathcal{O}(i \cdot c(k \cdot n + m))$, where i is the number of iterations to run, c is the size of the generated PC, and constant k is a bound on the number of candidate improvements to the circuit, which can grow exponentially for multi-valued variables. Importantly, opposite from LearnSPN where we only learn input nodes once per call *if* data is univariate, ID-SPN requires learning multiple multivariate inputs for *every* ExtendID call.

Pros and Cons

Pros. If we assume any multivariate distribution in place of Markov networks, PCs learned from ID-SPN are strictly more expressive than ones learned from LearnSPN, as

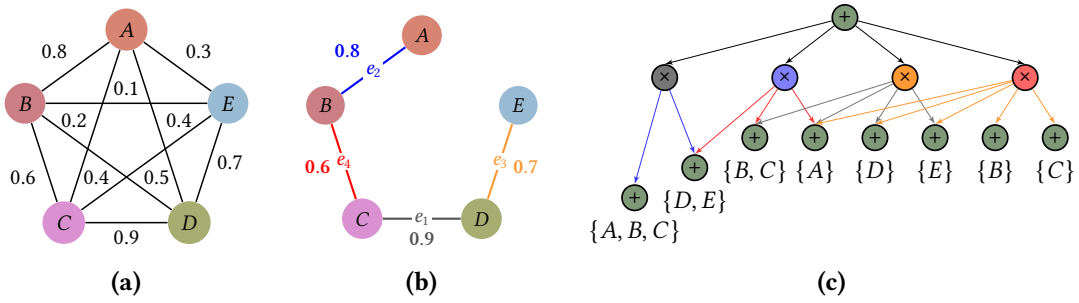


Figure 3.4: *The fully connected correlation graph (a) with weights as the pairwise correlation measurements for each pair of variables; the maximum spanning tree for determining decompositions (b); and the mixture of decompositions (c). Colors in (b) match their partitionings in (c).*

input nodes could potentially be replaced with LEARNSPN distributions. Additionally, the modularity inherited from LEARNSPN allows ID-SPN to adapt to data according to expert knowledge, bringing some flexibility to the algorithm.

Cons. Unfortunately, most of the disadvantages from LEARNSPN also apply to ID-SPN. Just like LEARNSPN, independence tests are more often than not a bottleneck for most executions with resonably large number of variables. However, ID-SPN relies on a likelihood improvement for the computational graph to be extended, which ends up curbing the easy parallelization aspect of LEARNSPN. Besides, the complexity involved in learning Markov networks (or any other complex multivariate distribution as input node) carries a heavy weight during learning. This, coupled with the fact that hyperparameter tuning in the huge parameter space of ID-SPN must be done by a random search method, can take a heavy price in terms of learning time.

3.1.3 PROMETHEUS

So far, we have only considered structure learning algorithms that produce tree-shaped circuits. Even though ID-SPN *might* produce non-tree graphs at the input nodes depending on the choice of families of multivariate distributions, it does not do so as a rule. We now turn our attention to a PC learner that *does* generate non-tree computational graphs in a divide-and-conquer manner.

Recall that in both LEARNSPN and ID-SPN the scope partitioning is done greedily; we define a graph encoding the pairwise (in)dependencies of variables and greedily search for connected components by comparing independence test results with some correlation threshold, adding an edge if the correlation is sufficiently high. The choice of this threshold is often arbitrary and subject to hyperparameter tuning during learning, which is especially worrying when dealing with high dimensional data. In this section we review PROMETHEUS (JAINI, GHOSE, *et al.*, 2018), a divide-and-conquer LEARNSPN-like PC learning algorithm with two main features that stand out compared to the last two methods we have seen so far: (1) it requires no hyperparameter tuning for variable partitionings, and (2) accepts a more scalable alternative to computing all pairwise correlations.

Let $\mathcal{G}$ the independence graph for scope $\mathbf{X} = \{X_1, X_2, \ldots, X_m\}$. Remember that $\mathcal{G}$'s vertices are $\mathbf{X}$ and each (undirected) edge $\overline{X_i X_j}$ coming from X_i to X_j means that $X_i \not\perp\!\!\!\perp X_j$.

Algorithm 9 PROMETHEUS

Input Data $\mathbf{D}$, whose columns are indexed by variables $\mathbf{X}$
Output A smooth and decomposable probabilistic circuit learned from $\mathbf{D}$

if $|\mathbf{X}|$ is sufficiently small **then return** an input node learned from $\mathbf{D}$
else
  Find subsets of data $\mathbf{x}_1, \ldots, \mathbf{x}_k \subseteq \mathbf{D}$ st all assignments within $\mathbf{x}_i$ are all similar
  Create a sum node S with initially no children and uniform weights
  for each $\mathbf{x}_i$ **do**
    $\mathcal{T} \leftarrow$ CORRELATIONMST$(\mathbf{x}_i, \mathbf{X})$
    for each weighted edge e_j in $\mathcal{T}$ in decreasing order **do**
      Remove edge e_i from $\mathcal{T}$
      Call $\mathrm{S}_1, \ldots, \mathrm{S}_t$ the scopes of each component in $\mathcal{T}$
      Create product node P_j and associate it with $\mathrm{S}_1, \ldots, \mathrm{S}_t$
      Associate P_j with dataset $\mathbf{x}_i$
      Add P_j as a child of S
  Let $\mathcal{H}$ a hash table (initially empty) associating scopes to sum nodes
  for each $\mathrm{P} \in \mathrm{Ch(S)}$ **do**
    for each scope S associated with P **do**
      if $\mathrm{S} \notin \mathcal{H}$ **then**
        Let $\mathbf{x}$ the dataset associated with P
        $\mathrm{N} \leftarrow$ PROMETHEUS$(\mathbf{x}_{:,\mathrm{S}}, \mathrm{S})$
        Add N as a child of P
        $\mathcal{H}_{\mathrm{S}} \leftarrow \mathrm{N}$
      else
        Add $\mathcal{H}_{\mathrm{S}}$ as a child of P
  return S

Previously, we constructed $\mathcal{G}$ by comparing the output of an independence test (such as the G-test) against a threshold (e.g. a sufficiently low p-value). Instead, suppose $\mathcal{G}$ is fully connected and that we attribute weights corresponding to a correlation metric of X_i against X_j for each edge (e.g. Pearson's correlation coefficient). The *maximum spanning tree* (MST) of $\mathcal{G}$, here denoted by $\mathcal{T}$, defines a graph where the removal of any edge in $\mathcal{T}$ partitions the component into two subcomponents. Let e_i the i-th lowest (weight) valued edge; PROMETHEUS obtains a set of decompositions by iteratively removing edges from e_1 to $e_{|\mathbf{X}|-1}$. In other words, the algorithm constructs a product node for each decomposition, assigning the scope of each child as the scope of each component at each edge removal. These products are then joined together by a parent sum node that acts as a mixture of decompositions. Figure 3.4 shows an example of $\mathcal{T}$, the subsequent decompositions, and the resulting mixture of decompositions.

Sum nodes are learned by clustering data into similar instances, just like in previous cases. Since the previously mentioned procedure involving products creates a mixture of decompositions (and thus a sum node), we can simply collapse the consecutive sum layers into a single sum node. Algorithm 9 shows the algorithm in its entirety. CORRELATIONMST computes the (fully connected) correlation graph, returning its MST. It is worth mentioning

that PROMETHEUS makes sure each recursive call shares subcircuits whenever scopes are the same (this is when the hash table $\mathcal{H}$ in Algorithm 9 comes into play). This avoids an exponential growth from the $k \cdot (|\mathbf{X}| - 1)$ potential recursive calls.

Complexity

Up to now, the computation of decompositions is done by a $\mathcal{O}(m^2)$ construction of a fully connected correlation graph. This gives PROMETHEUS no asymptotic advantage over neither LEARNSPN nor ID-SPN. To change this, JAINI, GHOSE, *et al.* propose a more scalable alternative: in place of constructing the entire correlation graph, sample $m \log m$ variables and construct a correlation graph where only $\log m$ edges are added for each of these sampled variables instead, bringing down complexity to $\mathcal{O}(m\,(\log m)^2)$.

The analysis of sum nodes is exactly the same as LEARNSPN if we assume the same clustering method. If PROMETHEUS is implemented with the same multivariate distributions as ID-SPN at the input nodes, the analysis for those also holds.

Pros and Cons

Pros. The notable achievements of PROMETHEUS are evidently the absence of parameters for computing scope partitionings, reducing the dimension of hyperparameters to tune; a scalable alternative to partitionings that runs in sub-quadratic time; and (more debatably) the fact that the algorithm produces non-tree shaped computational graphs. Further, since product nodes are learned through correlation metrics, PROMETHEUS is easily adaptable to continuous data. To some extent, PROMETHEUS also inherits the modularity of LEARNSPN, as the choice of how to cluster and what input nodes to use is open to the the user.

Cons. Although the construction of the correlation graph in PROMETHEUS is not done greedily (at least in the quadratic version), selecting the decompositions (i.e. partitioning the graph into maximal components) is; of course, this is not exactly a drawback but a compromise, as graph partitioning is a known NP-hard problem (FELDMANN and FOSCHINI, 2015). Because PROMETHEUS accounts for all decompositions yielded from components after the removal of each edge from the MST, the circuit can grow considerably, even if we reuse subcircuits at each recursive call. An alternative would be to globally reuse subcircuits (i.e. share $\mathcal{H}$ among different recursive calls) throughout learning, although this curbs expressivity somewhat, as these subcircuits are learned from possibly (completely) different data. Another option would be to bound the number of decompositions, or in other words remove only a bounded number of edges from the MST.

Remark 3.1: On variations of divide-and-conquer learning

Because of LEARNSPN's simplicity and modularity, there is a lot of room for improvement. This is reflected in the many works in literature on refining LEARNSPN to specific data, choosing the right parameters, producing non-tree shaped circuits, and choice of input nodes. In this remark segment, we briefly discuss other advances in divide-and-conquer PC learning.

As we have previously mentioned, one of the drawbacks of LEARNSPN is the

sheer volume of hyperparameters involved. Vergari, Mauro, *et al.* (2015) suggests simplifying clustering to only binary row splits, while Y. Liu and Luo (2019) proposes clustering methods that automatically decide the number of clusters from data. Together with Prometheus, the space of hyperparameters to tune is greatly reduced.

We again go back to the issue of reducing the cost of learning variable partitions. Apart from Prometheus, Di Mauro *et al.* (2017) also investigate more efficient decompositions, proposing two approximate sub-quadratic methods to producing variable splits: one by randomly sampling pairs of variables and running G-test, and the other by a linear time entropy criterion.

Vergari, Mauro, *et al.* (2015) proposes the use of Chow-Liu Trees as input nodes instead of univariate distributions, while Molina, Natarajan, *et al.* (2017) recommend Poisson distributions for modeling negative dependence. Bueff *et al.* (2018) combines LearnSPN with weighted model integration by learning polynomials as input nodes for continuous variables and counts for discrete data. Molina, Vergari, *et al.* (2018) adapts LearnSPN to hybrid domains by employing the randomized dependence coefficient for both clustering and variable partitioning, with pairwise polynomial approximations for input nodes.

Other contributions include adapting LearnSPN to relational data (Nath and P. Domingos, 2015), an empirical study comparing different techniques for clustering and partitioning in LearnSPN (Cory J. Butz, Oliveira, *et al.*, 2018), and LearnSPN post-processing strategies for deriving non-tree graphs (Rahman and Gogate, 2016).

3.2 Incremental Learning

Learning algorithms from the `DIV` class heavily rely on recursively constructing a probabilistic circuit in a top-down fashion. This facilitates learning, as we need only to greedily optimize at a local level. We now draw our attention to incremental algorithms that iteratively grow an initial circuit. These usually require a search over possible candidate nodes to be extended, and as such involve evaluating the entire circuit to determine best scores. In this section, we look at two examples of `INCR` class learning algorithms: LearnPSDD and Strudel.

3.2.1 LearnPSDD

As the name suggests, LearnPSDD (Liang, Bekker, *et al.*, 2017) learns a smooth, structure decomposable and deterministic probabilistic circuit (see Section 2.3.2), meaning its computational graph must respect a vtree. We therefore must address the issue of learning the vtree before we turn to the PC learning algorithm *per se*.

Recall that for a vtree $\mathcal{V}$, every inner node $v \in \mathcal{V}$ with $\mathbf{X} = \mathrm{Sc}(v^{\leftarrow})$ and $\mathbf{Y} = \mathrm{Sc}(v^{\rightarrow})$ determines that $\mathbf{X}$ and $\mathbf{Y}$ are independent, i.e. $p_{\mathcal{C}}(\mathbf{X}, \mathbf{Y}) = p_{\mathcal{C}}(\mathbf{X})p_{\mathcal{C}}(\mathbf{Y})$ for a PC $\mathcal{C}$. This means that a PC's vtree is pivotal in embedding the independencies of the circuit's distribution.

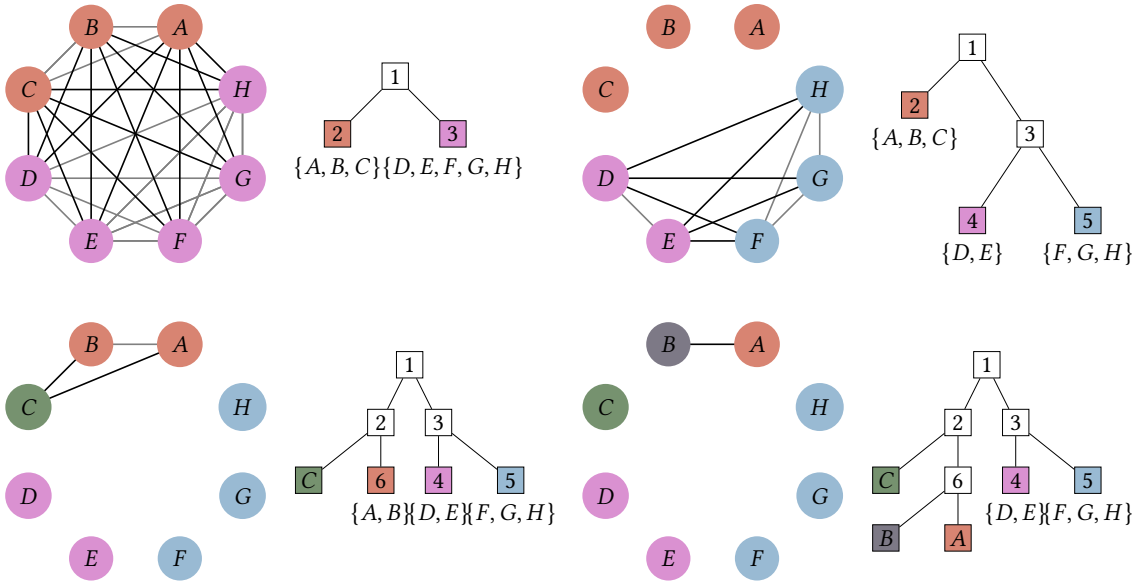


Figure 3.5: *Snapshots of four iterations from running the vtree top-down learning strategy with pairwise mutual information. Each iteration shows a variable partitioning, the cut-set that minimizes the average pairwise mutual information as black edges, and the subsequent (partial) vtree. The algorithm finishes when all partitions are singletons.*

With this in mind, Liang, Bekker, *et al.* (2017) propose two approaches to inducing vtrees from data, both of which use mutual information

$$\mathrm{MI}(\mathbf{X}, \mathbf{Y}) = \sum_{\mathbf{X}=\mathbf{x}} \sum_{\mathbf{Y}=\mathbf{y}} p(\mathbf{x}, \mathbf{y}) \log \frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x})p(\mathbf{y})}$$

for deciding independence. To avoid computing an exponential number of MI terms, an approximation based on the average pairwise MI is computed instead

$$\mathrm{pMI}(\mathbf{X}, \mathbf{Y}) = \frac{1}{|\mathbf{X}||\mathbf{Y}|} \cdot \sum_{X \in \mathbf{X}} \sum_{Y \in \mathbf{Y}} \mathrm{MI}(X, Y).$$

The first approach learns vtrees in a top-down fashion, starting with a full scope and recursively partitioning down to the unit set. The second learns bottom-up, starting with singletons and joining sets of variables up to full scope.

Top-down vtree learning. Let $\mathcal{G}$ a fully connected weighted graph where variables are nodes. For each edge $\overrightarrow{X\,Y}$, attribute its weight as $\mathrm{MI}(X, Y)$. Learning the vtree top-down amounts to partitioning $\mathcal{G}$ such that the cut-set that divides the two partitions $\mathbf{X}$ and $\mathbf{Y}$ is minimal with respect to pMI. Liang, Bekker, *et al.* (2017) further argue that balanced vtrees produce smaller PCs, and so they reduce learning to a balanced min-cut bipartition problem. Although this is known to be NP-complete (Garey and Johnson, 1990), optimized solvers are able to produce high quality bipartitions efficiently (Karypis and Kumar, 1998). In a nutshell, the vtree construction goes as follows: find a balanced min-cut bipartition $(\mathbf{X}, \mathbf{Y})$ in $\mathcal{G}$ minimizing the pMI of the edges; add a vtree inner node representing this bipartition and connect it to the two vtrees produced by the recursive calls over $\mathbf{X}$ and

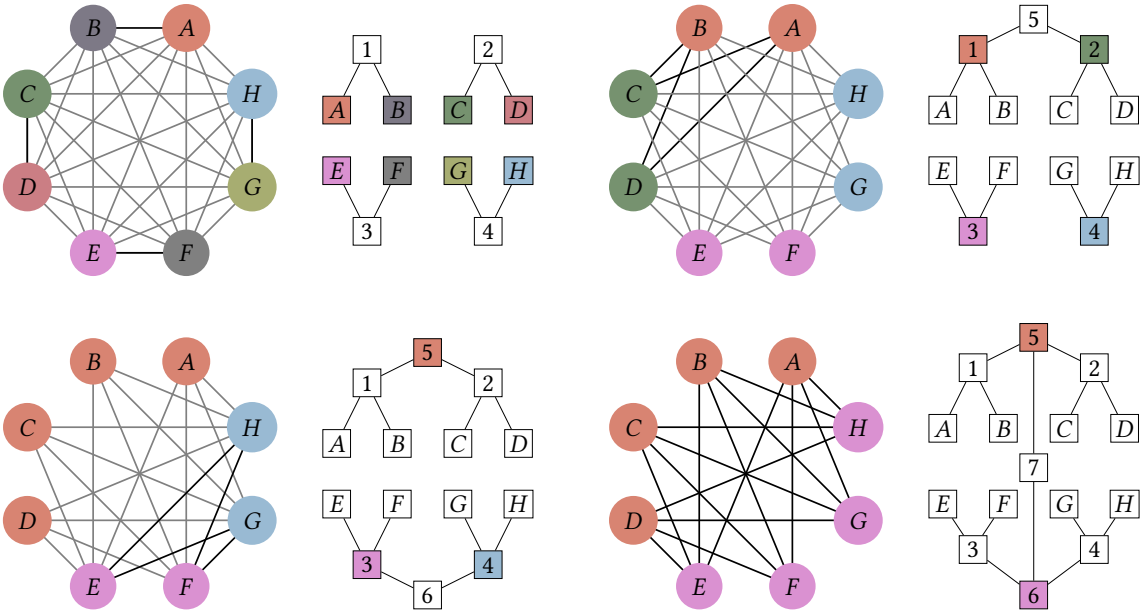


Figure 3.6: *Snapshots from running the vtree bottom-up learning strategy with pairwise mutual information. Snapshots show pairings of two vtrees, with edges between partitions joined into a single edge whose weight is the average pairwise mutual information of all collapsed edges. In black are edges that correspond to the matchings that maximize the average pairwise mutual information. The algorithm finishes when all vtrees have been joined together into a single tree.*

$\mathbf{Y}$; if $\mathbf{X} = \{X\}$ (resp. $|\mathbf{Y}| = \{Y\}$), produce a leaf node X (resp. Y). Figure 3.5 shows four iterations of this procedure.

Bottom-up vtree learning. Again, take $\mathcal{G}$ as the fully connected weighted graph from computing the pairwise mutual information of variables. Now consider that every node of $\mathcal{G}$ is a vtree whose only node is the variable itself. To learn a vtree bottom-up is to find pairings of vtrees such that the mutual information between them is high, meaning that the partitionings at higher levels are minimized (and so determine the "true" independence relationships between subsets of variables). To produce balanced vtrees, the algorithm attempts to join vtrees of same height whose pMI is maximal; this is equivalent to min-cost perfect matching, which can be solved, in our case, in $\mathcal{O}(m^4)$, where m is the number of variables (Edmonds, 1965; Kolmogorov, 2009). Figure 3.6 exemplifies the algorithm.

LearnPSDD is an incremental learning algorithm. This means that it takes an existing PC and incrementally grows the circuit by some criterion, preserving the structural constraints from the PC in the process. Once a vtree $\mathcal{V}$ has been learned from data, we use it to construct an initial circuit that respects $\mathcal{V}$. The choice of circuit initialization is dependent on our task. For example, within the context of PSDDs, we are mostly interested in starting out with a PC induced from an LC encoding a certain knowledge base (see Section 2.3); this is usually done in a case-by-case basis, where LCs are compiled for a particular task and then promoted to PCs (see Remark 3.2). However, if one does not require specifying the distribution's support, any PC will do.

How and *where* the circuit is grown – once we have acquired a vtree and an initial circuit – are the main topics of interest now. We first address the matter of *how*, i.e. how

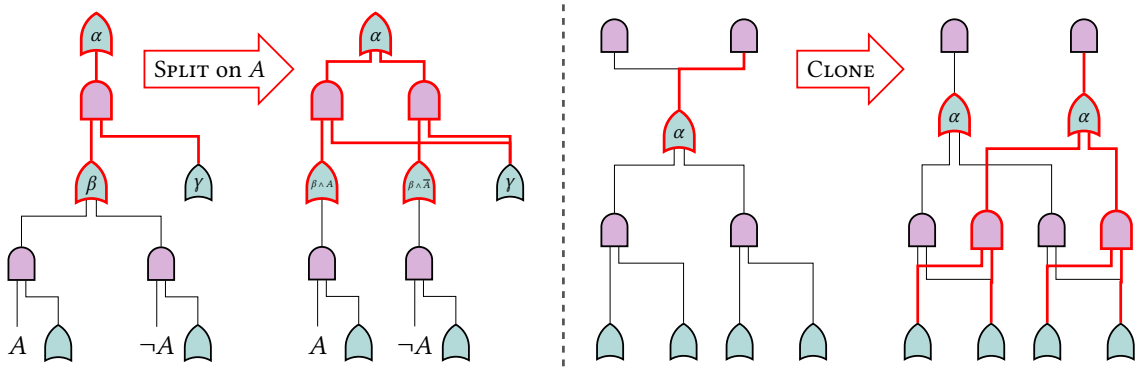


Figure 3.7: *Split (left) and Clone (right) operations for growing a circuit when $m = 1$. Nodes and edges highlighted in red show the modified structure. In both cases smoothness, (structure) decomposability and determinism are evidently preserved.*

can we increase a PC's expressivity such that we preserve a desired set of structural constraints; and later of *where*, i.e. which portions of the circuit are eligible for growth and how do we know they are good candidates.

Liang, Bekker, *et al.* propose two local transformations for growing a circuit $\mathcal{C}$: Split and Clone. The first acts by multiplying a sum node's product child P into $\mathrm{P}_1, \ldots, \mathrm{P}_k$ products such that $\pi_1, \ldots, \pi_k$ (primes of $\mathrm{P}_1, \ldots, \mathrm{P}_k$ respectively) are mutually exclusive. This is done by attributing all possible values of a variable in $\mathrm{Sc}(\mathrm{P})$, say A, to each prime, meaning that π_i will contain the assignment $A = i$ for every $i \in [k]$. This attribution is done by partially copying $\mathcal{C}_\mathrm{P}$ into k circuits $\mathcal{C}_\mathrm{P}^{(1)}, \ldots, \mathcal{C}_\mathrm{P}^{(k)}$ up to some depth m and then conditioning $\mathcal{C}_\mathrm{P}^{(i)}$ on $[\![A = i]\!]$. This is straightforward for the discrete case: at the appropriate vtree node (i.e. one that contains A as a leaf), replace the input node whose scope is A into an indicator node, setting it to the appropriate assignment of A. Although Liang, Bekker, *et al.* (2017) only considers the binary case, the transformation can be extended to the continuous if we consider k piecewise distributions whose support is over only a set interval. Naturally, input nodes must then have their support truncated to the appropriate i-th interval, which is no easy feat in the general case. The left side of Figure 3.7 shows Split for the binary case.

The other proposed transformation, Clone, does something similar for sum nodes. Pick a sum node S whose children are $\mathrm{C}_1, \ldots, \mathrm{C}_k$ and parents P_1 and P_2; double S and $\mathrm{C}_1, \ldots, \mathrm{C}_k$, producing clones S' and $\mathrm{C}'_1, \ldots, \mathrm{C}'_k$. Disconnect the edge coming from P_2 to S and instead connect it to S'. Connect all $\mathrm{C}'_1, \ldots, \mathrm{C}'_k$ to the same children as their original counterparts. This operation is visualized on the right side of Figure 3.7. One can further extend Clone to apply this operation cloning nodes up to some depth m and then joining the last remaining deepest nodes similar to what was described for $\mathrm{C}'_1, \ldots, \mathrm{C}'_k$.

It is easy to see that, in both cases, smoothness, structure decomposability and determinism are preserved. In fact, if the original circuit encodes a particular support (i.e. a knowledge base), the PC resulting from applying any of the two transformations must also encode the same support, since we have only made the underlying logic circuit more redundant. Probabilistically though, this "redudancy" only increases the parameterization space and as such increases the expressiveness of the PC. However, not all applications of

Algorithm 10 LearnPSDD

Input Data $\mathbf{D}$, vtree $\mathcal{V}$, initial PC $\mathcal{C}$, max depth m, scope $\mathbf{X}$
Output A smooth, structure decomposable and deterministic PC learned from $\mathbf{D}$

while there is score improvement or has not reached the iteration/time limit **do**
  $s_{\mathrm{S}} \leftarrow -\infty$
  Let $(\mathrm{S}^*, \mathrm{P}^*)$ the best Split candidate seen so far, initially empty
  for each candidate (S, P) of all possible Split candidates **do**
    $\mathcal{C}' \leftarrow \textsc{Split}(\mathcal{C}, \mathrm{S}, \mathrm{P}, \mathcal{V}, m)$
    $s' \leftarrow \mathrm{Score}(\mathbf{D}, \mathcal{C}, \mathcal{C}')$
    if $s' > s_{\mathrm{S}}$ **then** $s_{\mathrm{S}} \leftarrow s'$ and $\mathrm{S}^*, \mathrm{P}^* \leftarrow \mathrm{S}, \mathrm{P}$
  $s_{\mathrm{C}} \leftarrow -\infty$
  Let C^* the best Clone candidate seen so far, initially empty
  for each candidate C of all possible Clone candidates **do**
    $\mathcal{C}' \leftarrow \textsc{Clone}(\mathcal{C}, \mathrm{C}, \mathcal{V}, m)$
    $s' \leftarrow \mathrm{Score}(\mathbf{D}, \mathcal{C}, \mathcal{C}')$
    if $s' > s_{\mathrm{C}}$ **then** $s_{\mathrm{C}} \leftarrow s'$ and $\mathrm{C}^* \leftarrow \mathrm{C}$
  if $s_{\mathrm{S}} > s_{\mathrm{C}}$ **then** $\mathcal{C} \leftarrow \textsc{Split}(\mathcal{C}, \mathrm{S}^*, \mathrm{P}^*, \mathcal{V}, m)$
  else $\mathcal{C} \leftarrow \textsc{Clone}(\mathcal{C}, \mathrm{C}^*, \mathcal{V}, m)$
return $\mathcal{C}$

Split or Clone are equal in terms of performance. While it is true that the application of Split to any product node or Clone to any sum node strictly increases expressivity, it is more meaningful to choose candidates whose growth carries a bigger impact on the overall fit relative to the training data. LearnPSDD searches for reasonable candidates by computing

$$\mathrm{Score}(\mathbf{D}, \mathcal{C}, \mathcal{C}') = \frac{\log \mathcal{C}'(\mathbf{D}) - \log \mathcal{C}(\mathbf{D})}{|\mathcal{C}'| - |\mathcal{C}|},$$

where $\mathcal{C}$ and $\mathcal{C}'$ are, respectively, the PCs before and after the application of any of the two operations. In other words, the algorithm randomly evaluates applying Split and/or Clone and ultimately chooses the one candidate that maximizes the log-likelihood of training data penalized by the size of the resulting PC, iteratively growing the circuit until there is no more improvement or reaches an iteration step or time limit, as Algorithm 10 shows.

Complexity

Although learning the vtree top-down reduces to an NP-complete min-cut graph partitioning problem, there are approximate algorithms that provide high quality partitionings in $\mathcal{O}(|\mathbf{X}|^2)$ (Karypis and Kumar, 1998). Learning bottom-up is reduced to min-cost perfect matching, which can be done in $\mathcal{O}(|\mathbf{X}|^4)$ via the Edmonds Blossom algorithm (Edmonds, 1965; Kolmogorov, 2009).

Split runs, for a given variable X, in $\mathcal{O}(v \cdot |\mathcal{C}|)$ if unbounded by m, where v is $|\mathrm{Val}(X)|$, the number of possible assignments to X if X is discrete; or the number of intervals to fragment $\mathrm{Val}(X)$ if X is continuous. Clone's runtime is $\mathcal{O}(|\mathcal{C}|)$ when m is unbounded, as it

needs to produce an almost exact copy of the circuit. We say that a local transformation, such as Split or Clone, is *minimal* when the copy depth is $m = 0$. When Split and Clone are minimal and X is binary, then the transformation is done in constant time. In fact, any non-minimal transformation can be composed out of minimal transformations (Liang, Bekker, *et al.*, 2017).

Perhaps the most costly routine of LearnPSDD is its score function. Although log-likelihood is linear time computable on the number of edges of the circuit, $\mathcal{C}$ can grow substantially as transformations pile up. Each score evaluation requires four passes on the circuit: log-likelihoods and circuit sizes for both $\mathcal{C}$ and its updated circuit $\mathcal{C}'$. However, since transformations are local, log-likelihood and circuit sizes only change for the nodes affected in the transformation and their ancestors, allowing LearnPSDD to cache values. The overall complexity of LearnPSDD at each iteration is therefore $\mathcal{O}(|\mathcal{C}|^2)$ if we assume $m = 0$, with the first $|\mathcal{C}|$ coming from the search of all candidates in $\mathcal{C}$, and the second from the computation of Score. Each iteration further increases $|\mathcal{C}|$, slowing down the algorithm's runtime.

Pros and Cons

Pros. The fact that LearnPSDD preserves smoothness, structural decomposability, determinism *and* any logical semantic coming from its underlying LC is remarkable. On top of that, in theory and under minor modifications to Split and Clone, any PC is eligible as an initial circuit, even ones which do not respect any vtree. Besides, computing variable splits beforehand through a separate process of learning the vtree relieves the learning algorithm from having to compute costly statistical tests at each product node. Where LearnPSDD really shines (and perhaps more fittingly PSDDs in general) is when the support is explicitly defined through the initial circuit's LC; because the PC attributes non-zero probability only to events where the LC does not return false, the circuit wastes no mass on impossible events.

Cons. In practice, LearnPSDD is very slow even with caching; even worse, it may take several hours for only a minor (if any) improvement. (Liang, Bekker, *et al.*, 2017) suggests improving performance by producing ensembles of LearnPSDDs, although this negates determinism in the final model (as well as structure decomposability if different vtrees are used at each component), denying the access to tractably computing queries like divergences, MI and entropies, not to mention the time cost to learn all components. Another issue is with the choice of the initial circuit. As previously mentioned, any circuit will do, however the performance (and efficiency) of LearnPSDD is highly dependent on it. Within the context of PSDDs and encoding their support, LearnPSDD requires that a separate algorithm compiles an LC for a specific task without looking at data. Although there are many ways of doing so, they are often not task agnostic (see Remark 3.2). More importantly, because the process of learning the circuit (from data) is decoupled from the task of encoding logical constraints imposed by a knowledge base, all variables that do not appear in the logic formula are compiled into a trivial form (e.g. fully factorized circuit). Lastly, although decoupling the process of learning the vtree from learning the PC helps with scalability, the ability of identifying the proper vtree for the most expressive PC given data is certainly desirable, and one which might be hindered by this separated

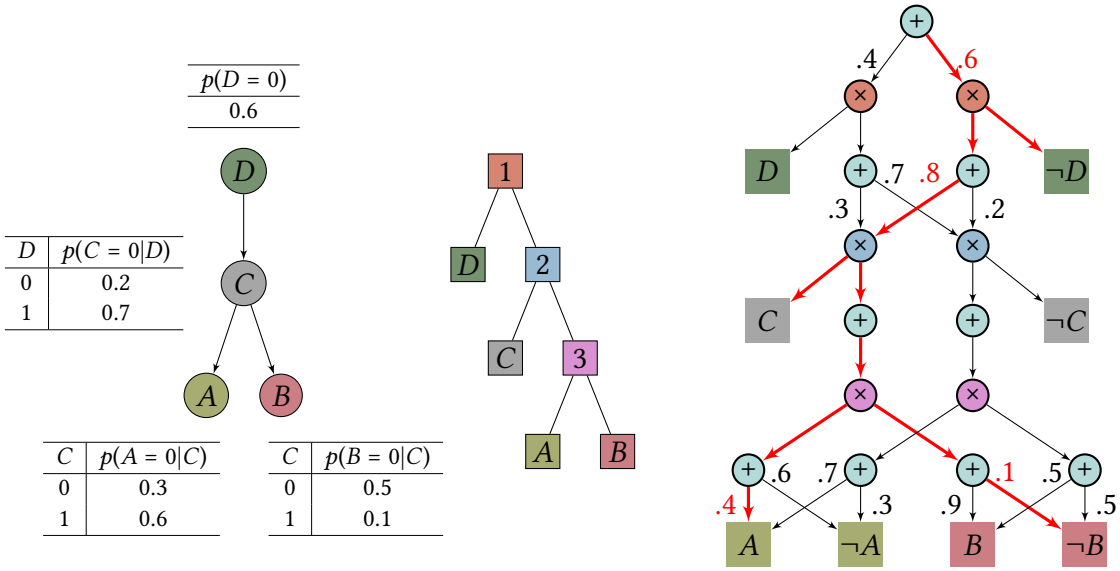


Figure 3.8: *A vtree (middle) and probabilistic circuit (right) compiled from a Chow-Liu Tree (left). Each conditional probability $p(Y|X)$ is encoded as a (deterministic) sum node where each of the two children sets Y to 0 or 1. Colors in the CLT indicate the variables in the PC, while vtree inner node colors match with product nodes that respect them. Edges in red indicate the induced subcircuit activated on assignment $\{A = 1, B = 0, C = 1, D = 0\}$.*

process.

3.2.2 STRUDEL

DANG, VERGARI, *et al.* (2020) build upon the work of LEARNPSDD and propose STRUDEL, which mainly improves LEARNPSDD on two fronts: (1) by providing a simple algorithm for generating an initial circuit and vtree from data, and (2) proposing a heuristic for efficiently searching for good transformation candidates.

We first address how to construct the initial circuit from data. DANG, VERGARI, *et al.* suggests doing so by compiling both a vtree and linear sized PC (in the number of variables) from a Chow-Liu Tree (CLT, CHOW and C. LIU, 1968). Let $\mathcal{T}$ a CLT over variables $\mathbf{X} = \{X_1, \ldots, X_m\}$. A vtree $\mathcal{V}$ is extracted from $\mathcal{T}$ by traversing $\mathcal{T}$ top-down. For each node $X_i \in \mathcal{T}$, if X_i is a leaf node in $\mathcal{T}$, then create a vtree leaf node of X_i; otherwise create an inner vtree node v, attach a vtree leaf node of X_i as $v^{\leftarrow}$ and assign $v^{\rightarrow}$ as a vtree built over all the vtrees coming from the children of X_i. The construction of $v^{\leftarrow}$ depends on how balanced one wishes the vtree to be: if we want a more right-leaning vtree, it suffices to construct a right-linear vtree connecting all vtrees from each child $X_j \in \mathrm{Ch}(X_i)$. Likewise, a balanced vtree is built by balancing the vtree connecting the recursive vtree calls from each X_j. Note that this does not necessarily mean that $v^{\rightarrow}$ is completely right-linear or balanced, only that it is somewhat close to it, as the rest of the structure depends on the recursive calls of each CLT node.

STRUDEL compiles an initial circuit by looking at the vtree bottom-up and caching subcircuits. Let v a vtree node and $Y \in \mathcal{T}$ a CLT node with conditional probability $p(Y|X)$, where X is the parent of Y. If v is a leaf node in $\mathcal{V}$ and v's variable is also a leaf

node in $\mathcal{T}$, two sum nodes S_0 and S_1 over literal nodes $\neg Y$ and Y are created, each with weights $w_{S_0,\neg Y} = p(Y = 0|X = 0)$, $w_{S_0,Y} = p(Y = 1|X = 0)$ and $w_{S_1,\neg Y} = p(Y = 0|X = 1)$, $w_{S_1,Y} = p(Y = 0|X = 1)$. The two sum nodes connecting B and $\neg B$ in the PC shown on the right of Figure 3.8 show this exact case. The left sum node encodes $p(B|C = 1)$ and the right one $p(B|C = 0)$. These circuits are then cached by associating them with v. When Y is not a leaf node in $\mathcal{T}$ but v is, we simply return literal nodes. If v is an inner node, we must define a scope partition, splitting $\mathbf{X} = \text{Sc}(v^{\leftarrow})$ and $\mathbf{Y} = \text{Sc}(v^{\rightarrow})$ into product nodes $P_1, \dots, P_k$, one for each value cached value in v. Each prime is set to the cached circuits from $v^{\leftarrow}$ and each sub the cached circuits from $v^{\rightarrow}$. Finally, if two variables $X \in \mathbf{X}$ and $Y \in \mathbf{Y}$ are such that their parents are the same variable, say Z, then X and Y are independent when Z is given (because of a divergent connection in $\mathcal{T}$) and thus cannot be merged together into a single sum because of the context-specific independence set by Z (Boutilier *et al.*, 1996). This is visualized in the ⊗ nodes; in this situation, A and B are siblings coming from C, and so $A \perp\!\!\!\perp B|C$ (redundant sum nodes are added for standardization). When the prior situation is not true, then not only X is the only variable in $\mathbf{X}$, but X must also be the parent of Y and so we must model $p(\mathbf{Y}|X)$. This is the case for ⊗, where C is the parent of B and so we have to be join the two by sum nodes attributing the conditional probabilities $p(A, B|C = 0)$ for the right-most ⊗ and $p(A, B|C = 1)$ for the left-most sibling. This procedure is shown more formally in Algorithm 11.

Now that we have an initial PC constructed from InitialStrudel, we are ready to discuss Strudel's second contribution. To do so, we must first understand the notion of *circuit flows* introduced in Dang, Vergari, *et al.* (2020). In short, the circuit flow of a deterministic probabilistic circuit $\mathcal{C}$ with respect to a variable assignment $\mathbf{x}$ is the induced tree (see Definition 2.1.2) whose edges are all non-zero when $\mathcal{C}$ is evaluated under $\mathbf{x}$. Such an induced tree is unique in deterministic PCs because every sum node admits only one non-zero valued child for $\mathbf{x}$ (or any assignment for that matter). Note how circuit flows are more specific in the sense they are intrinsically linked to an assignment, while induced subcircuits specify a deterministic subcircuit within its supercircuit.

The circuit flow of deterministic PCs helps us understand how to efficiently compute inference in circuits of that nature. As we briefly mentioned before, for any assignment $\mathbf{x}$ in a smooth, decomposable and deterministic PC $\mathcal{C}$, there exists a unique circuit flow $\mathcal{F}$ that encodes the log-likelihood computation

$$\mathcal{C}(\mathbf{x}) = \mathcal{F}_{\mathcal{C}}(\mathbf{x}) = \prod_{(S,C)\in \text{Edges}(\mathcal{F}_{\mathcal{C}})} w_{S,C} \prod_{L\in \text{Inputs}(\mathcal{F}_{\mathcal{C}})} p_L(\mathbf{x}),$$

where Inputs$(\cdot)$ returns the set of input nodes of a circuit. When inputs are all binary, then one might encode $\mathcal{F}_{\mathcal{C}}$ as a mapping $f_{\mathcal{C}} : \mathcal{X} \longrightarrow \{0, 1\}^{|\mathcal{W}_{\mathcal{C}}|}$, here $\mathcal{W}_{\mathcal{C}}$ denoting the set of all parameters (i.e. sum node weights) of $\mathcal{C}$, which "activates" edge $w \in \mathcal{W}_{\mathcal{C}}$ under assignment $\mathbf{x}$. With this, the above operation under log-space is reduced to a vector multiplication

$$\log \mathcal{C}(\mathbf{x}) = f_{\mathcal{C}}(\mathbf{x})^{\intercal} \cdot \log(\mathcal{W}_{\mathcal{C}}).$$

Importantly, by aggregating circuit flows through counting the number of activations of each parameter $w_{S,C}$ in the entire training dataset $\mathbf{D}$, we get a sense of the number of samples $w_{S,C}$ impacts over $\mathbf{D}$, and thus a sense of how meaningful is that edge on the

Algorithm 11 InitialStrudel

Input Data $\mathbf{D}$, whose columns are indexed by variables $\mathbf{X}$
Output A smooth, structure decomposable and deterministic initial PC and vtree

$\mathcal{T} \leftarrow$ LearnCLT($\mathbf{D}, \mathbf{X}$)
$\mathcal{V} \leftarrow$ CompileVtree($\mathcal{T}$)
Let $\mathcal{M}$ a hash table for caching circuits, initially empty
for each vtree node $v \in \mathcal{V}$ in reverse topological order **do**
  if v is a leaf node **then**
    Let $X \in \mathcal{T}$ the variable represented by v, and Y its parent
    if X is a leaf node in $\mathcal{T}$ **then**
      $\mathsf{S}_j \leftarrow \sum_{i \in \mathrm{Val}(X)} p(X = i | Y = j) \cdot [\![X = i]\!]$ for each $j \in \mathrm{Val}(Y)$
      $\mathcal{M}(v) \leftarrow \mathcal{M}(v) \cup \{\mathsf{S}_j \,|\forall j \in \mathrm{Val}(Y)\}$
    else
      $\mathcal{M}(v) \leftarrow \mathcal{M}(v) \cup \{[\![X = i]\!] | i \in \mathrm{Val}(X)\}$
  else
    Attribute $\mathbf{X} \leftarrow \mathrm{Sc}(v^{\leftarrow})$ and $\mathbf{Y} \leftarrow \mathrm{Sc}(v^{\rightarrow})$
    Let $X \in \mathbf{X}$ and $Y \in \mathbf{Y}$
    Attribute $\mathbf{N}^{\leftarrow} \leftarrow \mathcal{M}(v^{\leftarrow})$ and $\mathbf{N}^{\rightarrow} \leftarrow \mathcal{M}(v^{\rightarrow})$
    $k \leftarrow |\,\mathrm{Val}(X)|$
    Construct product nodes $\mathbf{P} = \{\mathbf{N}_i^{\leftarrow} \times \mathbf{N}_i^{\rightarrow} \,|\forall i \in [k]\}$
    if $\mathrm{Pa}(X) = \mathrm{Pa}(Y)$ **then**
      Create sum nodes S_i each with only a single child $\mathsf{P}_i \in \mathbf{P}$, for each $i \in [k]$
      $\mathcal{M}(v) \leftarrow \mathcal{M}(v) \cup \{\mathsf{S}_1, \ldots, \mathsf{S}_k\}$
    else
      $\mathsf{S}_j \leftarrow \sum_{i \in \mathrm{Val}(X)} p(\mathbf{Y} | X = j) \cdot [\![X = i]\!]$, for each $j \in \mathrm{Val}(Y)$
      $\mathcal{M}(v) \leftarrow \mathcal{M}(v) \cup \{\mathsf{S}_j \,|\forall j \in \mathrm{Val}(Y)\}$
return $\mathcal{M}(v_r)$, where v_r is $\mathcal{V}$'s root node

fitness of data. As we shall see briefly, this aggregated circuit flow shall then be used as a score for a greedy search over the space of candidates for local transformations.

To overcome the scalability limitations of LearnPSDD, Strudel proposes using only Split to reduce the search space, looking at performing the search greedily instead of exhaustively and exploiting the efficiency of aggregate circuit flows as a fast heuristic in place of computing the whole likelihood. Searching is done by finding the edge to Split whose aggregate circuit flow is maximal

$$\mathrm{Score}_{\mathsf{eFlow}}(w_{\mathsf{S},\mathsf{C}} | \mathcal{C}, \mathbf{D}) = \sum_{\mathbf{x} \in \mathbf{D}} f_{\mathcal{C}}(\mathbf{x})\,[w_{\mathsf{S},\mathsf{C}}]\,,$$

while the choice of which variable to condition Split on is done by selecting the variable X that shares the most dependencies (and thus the higher pairwise mutual information) with other variables within the scope of that edge, estimated from the aggregate flows

$$\mathrm{Score}_{\mathsf{vMI}}(X, w_{\mathsf{S},\mathsf{C}} | \mathcal{C}, \mathbf{D}) = \sum_{\substack{Y \in \mathrm{Sc}(\mathsf{S}) \\ Y \neq X}} \mathrm{MI}(X, Y).$$

Algorithm 12 STRUDEL

Input Data $\mathbf{D}$, max depth m, scope $\mathbf{X}$
Output A smooth, structure decomposable and deterministic PC learned from $\mathbf{D}$

1: $\mathcal{C}, \mathcal{V} \leftarrow$ INITIALSTRUDEL($\mathbf{D}, \mathbf{X}$)
2: **while** there is score improvement of has not reached the iteration/time limit **do**
3: Compute the aggregate flow over all edges
4: $w^*_{\mathrm{S,C}} \leftarrow \arg\max_{w \in \mathcal{W}_\mathcal{C}} \mathrm{Score}_{\mathrm{eFlow}}(w | \mathcal{C}, \mathbf{D})$
5: $X^* \leftarrow \arg\max_{X \in \mathrm{Sc(S)}} \mathrm{Score}_{\mathrm{vMI}}(X, w^*_{\mathrm{S,C}} | \mathcal{C}, \mathbf{D})$
6: $\mathcal{C} \leftarrow$ SPLIT($\mathcal{C}, \mathrm{S}, \mathrm{C}, \mathcal{V}, m$)
7: **return** $\mathcal{C}$

The entire algorithm for STRUDEL is showcased in Algorithm 12.

Complexity

Learning the Chow-Liu Tree is done in $\mathcal{O}(|\mathbf{X}|^2 \cdot |\mathbf{D}|)$ through Chow-Liu's algorithm (CHOW and C. LIU, 1968), while the vtree is compiled in time linear to the size of the CLT, i.e. $\mathcal{O}(|\mathbf{X}|)$ since the Bayesian network is a tree. Consequentially, INITIALSTRUDEL runs in $\mathcal{O}(|\mathbf{X}| \cdot |\,\mathrm{Val}(X)|)$, or linear on $|\mathbf{X}|$ if we assume binary variables as originally intended. The bulk of the computation falls under STRUDEL, which runs in $\mathcal{O}\left(|\mathbf{X}|^2 \cdot |\mathbf{D}| + i(|\mathcal{C}| \cdot |\mathbf{D}| + |\mathbf{X}|^2)\right)$ assuming a bounded max depth m and binary variables. Term $|\mathbf{X}|^2 \cdot |\mathbf{D}|$ corresponds to learning the CLT, $|\mathcal{C}| \cdot |\mathbf{D}|$ to the computation of the aggregate circuit flows, $|\mathbf{X}|^2$ to the computation of $\mathrm{Score}_{\mathrm{vMI}}$ which involves the pairwise mutual informations of $\mathbf{X}$, and i the number of iterations of STRUDEL.

Pros and Cons

Pros. Arguably, the most valuable contribution of STRUDEL is its improvement on LEARNPSDD's scalability. Compared to LEARNPSDD, STRUDEL can take orders of magnitude less time per iteration, which in practice means a higher number of transformations accomplished in the same range of time. In addition, the nature of circuit flows allows for easy vectorization and thus CPU or GPU parallelization. In terms of data fitness, DANG, VERGARI, *et al.* (2020) empirically shows that initial circuits constructed from STRUDELINITIAL greatly improve performance compared to fully factorized initial PCs from LEARNPSDD. Similar to LEARNPSDD, one can learn an ensemble of STRUDELS to further boost performance at the cost of losing determinism. Opposite to LEARNPSDD however, DANG, VERGARI, *et al.* employ structure-sharing components so that the act of learning the circuit's structure is done once, greatly reducing learning time. Parameters are then learned through closed form EM (see Remark 3.3) and bagging.

Cons. Although STRUDEL's greedy heuristic search strategy translates into possibly more accurate PCs, it also produces more sizable circuits when compared to the exhaustive search of LEARNPSDD. Indeed, DANG, VERGARI, *et al.* (2020)'s empirical evaluation shows STRUDEL PCs up to 12 times bigger than LEARNPSDD's with the two somewhat tied in terms of fitness. This is especially worrying given that STRUDEL's complexity grows with its circuit size. In fact, experiments show a sharp increase in seconds per iterations for

the two INCR algorithms, with both reaching multiple digits for each iteration even in smaller sized datasets; though LearnPSDD much sharper and sooner comparatively (Dang, Vergari, *et al.*, 2020).

Remark 3.2: On the choice of initial circuits

We only briefly mentioned in Section 3.2.1 how we might want to start out with an initial PC conveying a specific support and then run an INCR class algorithm to further boost its probabilistic expressiveness without changing the underlying knowledge base. We devote this remark segment to discussing several works in literature that construct a so-called *canonical* (i.e. minimal with respect to their size without sacrificing its logical semantics) logic circuit, becoming perfect candidates to be used as an initial circuit in INCR learners.

Just like in probabilistic reasoning, the field of knowledge compilation and symbolic reasoning is often interested in finding succinct representations capable of tractably computing queries, a subject which we briefly touched in Section 2.3.1. For this reason, smooth, structure decomposable and deterministic logic circuits, who usually go by the name of Sentential Decision Diagrams (SDDs, Darwiche, 2011) have proven to be a useful tool in several applications (Vlasselaer, Renkens, *et al.*, 2014; Vlasselaer, Broeck, *et al.*, 2015; Lomuscio and Paquet, 2015; Herrmann and Barros, 2013). Fortunately, both LearnPSDD and Strudel preserve all the necessary structural constraints for both logical *and* probabilistic queries in (P)SDDs. With this in mind, we highlight compilation of SDDs in this short remark.

For most cases, SDDs can be compiled directly from CNFs and DNFs. (A. Choi and Darwiche, 2013) constructs SDDs bottom-up by first compiling C/DNF clauses and then combining smaller SDDs by either conjoining or disjoining them. In contrast, (Oztok and Darwiche, 2015) presents a faster compilation process which recursively breaks down C/DNFs by decomposing the formula into components according to a vtree, and then combines them into an SDD.

Although CNFs and DNFs are the most common form of encoding propositional knowledge bases, they struggle under specific logical constraints such as cardinality constraints (Nishino *et al.*, 2016; Sinz, 2005). Interesting alternatives include BDDs (see Example 2.6) which are also widely used in formal methods and program verification, and for which efficient compilation from cardinality constraints are available (Eén and Sörensson, 2006). Because BDDs are special case SDDs whose vtrees are always right-linear (Darwiche, 2011; Bova, 2016), their reduced representations (Bryant, 1986) are natural initial circuit candidates (see Section 4.1.1).

We now cover some of the existing literature on producing task specific (P)SDDs. A. Choi, Tavabi, *et al.* (2016) analyzes the feasibility of compiling LCs (and subsequently producing a PC by parameterizing disjunction edges) from tic-tac-toe game traces, and route planning within a city. Both involve exhaustively disjoining all permutations of valid conjoined configurations and compiling the resulting DNF through previously cited SDD compilers. A. Choi, Shen, *et al.* (2017) further studies route planning by compiling them into SDDs, but analyze the feasibility of

(P)SDDs in route planning in larger scale maps. A. Choi, Broeck, *et al.* (2015) explore (P)SDDs in preference learning and rankings, providing an algorithm for compiling an SDD from total or partial rankings. Similarly, Shen *et al.* (2017) investigates (P)SDDs in probabilistic cardinality constraint tasks, also known as subset selection or n-choose-k models.

3.3 Random Learning

We now explore random approaches to constructing probabilistic circuits, which we classify as `RAND` class learning algorithms. Essentially, `RAND` class circuits are constructed either by a completely random procedure (Section 3.3.1), or guided by data (Section 3.3.2). We first look at RAT-SPN (Peharz, Vergari, *et al.*, 2020), a connectionist PC structure learning algorithm for randomly generating tensorized smooth and decomposable probabilistic circuits. We then address XPC (Mauro *et al.*, 2021), a flexible algorithm capable of learning smooth and decomposable PCs as well as structure decomposable and/or deterministic circuits through simple modifications to their method.

3.3.1 RAT-SPN

A key ingredient to RAT-SPN (Peharz, Vergari, *et al.*, 2020) is the concept of *region graphs*. First introduced in PC literature in Dennis and Ventura (2012), region graphs are tensorized templates for PC construction. Informally, a region graph is composed out of *region nodes* and *partition nodes*; the former a set of sum or input nodes, and the latter of products. Regions can be thought of sets of computational units explaining the same interactions among variables (Dennis and Ventura, 2012), for instance semantically similar pixel regions in an image; while partitions define independencies between these regions. Edges coming out of region (resp. partition) nodes must necessarily connect to a partition (resp. region) node.

Definition 3.3.1 (Region graph)**.** *A* region graph *is a rooted connected DAG whose nodes are either* regions *or* partitions*. Children of regions are partitions, and children of partitions are regions. The root is always a region node.*

Region graphs simplify the process of constructing PCs by ensuring that they are *at the least* smooth and decomposable. Call $\mathcal{G}$ a region graph; $\mathcal{G}$ is easily translated to a PC by applying the procedure described in Algorithm 13. Every region is compiled into a set of sums or inputs, fully connecting children; every partition into a set of products, producing a distinct permutation of children. Evidently, the resulting PC is exponential on s and l, as products must ensure that they encode different permutations. To deal with this blow-up, this number is often restricted to only two children per partition.

RAT-SPN works by randomly generating a region graph in a top-down divide-and-conquer approach similar to LearnSPN, except that the learned structure eventually produces non-tree shaped circuits and the procedure is done *completely* random (see Algorithm 14). In fact, Peharz, Vergari, *et al.* (2020) argue that the parameterization of the circuit by means of sum weights is as important as its structure, looking at probabilistic

Algorithm 13 CompileRegionGraph

Input A region graph $\mathcal{G}$, parameters s for sums and l for inputs
Output A smooth and decomposable probabilistic circuit

Let $\mathcal{M}$ a mapping of region nodes to PC nodes
for each node N in $\mathcal{G}$ except the root in reverse topological order **do**
    if N is a region **then**
        if N is a leaf node in $\mathcal{G}$ **then**
            Construct $\mathbf{L} = \{\mathsf{L}_1, \dots, \mathsf{L}_l\}$ input nodes over variables Sc(N)
            Associate N with $\mathbf{L}$
        else
            Construct $\mathbf{S} = \{\mathsf{S}_1, \dots, \mathsf{S}_s\}$ sum nodes
            for each partition node $\mathsf{P} \in \mathrm{Ch}(\mathsf{N})$ **do**
                Every sum in $\mathbf{S}$ connects with every product in $\mathcal{M}(\mathsf{P})$
    else if N is a partition **then**
        Let $\mathrm{Ch}(\mathsf{N}) = \{\mathsf{R}_1, \dots, \mathsf{R}_k\}$ regions and $q = \prod_{i=1}^{k} |\mathcal{M}(\mathsf{R}_i)|$
        Construct $\mathbf{P} = \{\mathsf{P}_1, \dots, \mathsf{P}_q\}$ product nodes
        for every product $\mathsf{P} \in \mathbf{P}$ **do**
            Connect P with a distinct combination of sums in $\mathcal{M}(\mathsf{R}_1), \dots, \mathcal{M}(\mathsf{R}_j)$
Construct a root node R
Connect R to all products in every child of $\mathcal{G}$'s root
return R

circuits as a specific subclass of neural networks. Indeed, they show that this connectionist approach heavily inspired by traditional deep learning produces very competitive PCs. However, to do so requires extensive optimization of the circuit's weights, which unsurprisingly is where RAT-SPN shines: because of the tensorized nature of region graphs, the resulting PC is able to exploit the advantages of known deep learning frameworks, making the most of efficient stochastic gradient descent optimizers and GPU parallelization.

To ensure that the compiled PC is smooth and decomposable, the region graph must also be so. We extend the definition of scope function to region graphs. As long as leaf region nodes are assigned the correct scope, the PC is by construction smooth (every region is fully connected to their children) and decomposable (every partition splits variables into two regions). Function CreateLayer in Algorithm 14 does exactly that, making sure each partition decomposes into two distinct variable splits down to leaf region nodes. How deep the region graph (and consequentially the resulting PC) goes depends on a parameter d, which corresponds to half the true depth, as each CreateLayer call produces a partition and their children. After the region graph is randomly buily, a PC is then constructed through CompileRegionGraph, passing the random region graph and number of nodes per region as parameters. The function ultimately produces a dense probabilistic circuit from the region graph blueprint, as Figure 3.9 exemplifies.

Once the PC structure is successfully generated, Peharz, Vergari, *et al.* (2020) suggest Expectation-Maximization (EM, Dempster *et al.*, 1977; Peharz, Gens, Pernkopf, *et al.*, 2016; H. Zhao, Poupart, *et al.*, 2016) for optimizing the circuit parameters (i.e. sum weights and input node distributions). Although parameter learning of PCs is not the focus of this

Algorithm 14 RAT-SPN

Input Data $\mathbf{D}$, variables $\mathbf{X}$, max depth d, r # subcircuits, s # sums, and l # inputs
Output A smooth and decomposable probabilistic circuit

function CreateLayer(R, d, $\mathbf{X}$)
    Assign $\mathbf{X}$ as Sc(R)
    Sample a variable split $(\mathbf{Y}, \mathbf{Z})$ from $\mathbf{X}$
    Create a partition P and add it as a child of R
    if d>1 **then**
        if $|\mathbf{Y}| > 1$ **then**
            Create a region R_1
            CreateLayer(R_1, $d-1$, $\mathbf{Y}$)
        if $|\mathbf{Z}| > 1$ **then**
            Create a region R_2
            CreateLayer(R_2, $d-1$, $\mathbf{Z}$)
Start with a root region node R
for each $i \in [r]$ **do**
    CreateLayer(R, d, $\mathbf{X}$)
$\mathcal{C} \leftarrow$ CompileRegionGraph(R, s, l)
return $\mathcal{C}$

dissertation, we briefly touch the subject in Remark 3.3.

Worthy of note is a discriminative version of RAT-SPN where instead of a single root sum node, k roots are learned, each connecting to every CreateLayer subcircuit. Each i-th root describes the conditional probability $p(\mathbf{X}|Y=i)$, where Y is the query variable and $\mathbf{X}$ evidence. Classification follows directly from Bayes Rule $p(Y|\mathbf{X}) = \frac{p(\mathbf{X}|Y)p(Y)}{\sum_{i=1}^{k} p(\mathbf{X}|Y=i)p(Y=i)}$, where $p(Y)$ is either estimated from the training data or assumed to be fixed. Accordingly, a discriminative objective function is proposed involving cross-entropy and log-likelihood for hybrid generative-discriminative optimization (Bouchard and Triggs, 2004) instead of running EM.

Complexity

Although the procedure described in Algorithm 14 is $\mathcal{O}(r \cdot d(s+l))$ if $d < |\mathbf{X}|$ and $\mathcal{O}\left(r \cdot \log_2 |\mathbf{X}|(s+l)\right)$ otherwise, making the algorithm extremely fast, it does not paint the whole picture. The main bulk of the complexity when learning RAT-SPN comes from parameter learning. Peharz, Vergari, *et al.* (2020) calculate the number of sum weights to be

$$|\mathcal{W}_C| = \begin{cases} r \cdot k \cdot l^2 & \text{if } d = 1, \\ r \cdot \left(k \cdot s^2 + (2^{d-1} - 2)s^3 + 2^{d-1} \cdot s \cdot l^2\right) & \text{if } d > 1; \end{cases}$$

if we assume that the number of children of partitions is at most two. This means that learning only the non-input parameters of RAT-SPN takes time $\mathcal{O}\left(\left(r \cdot 2^d \cdot \left(s^3 + s \cdot l^2\right) + r \cdot k \cdot s^2\right) \cdot |\mathbf{D}|\right)$. However, given that most structure learning algorithms covered in this dissertation also require parameter learning, one might argue that the true cost of structure learning in RAT-SPN is indeed subquadratic.

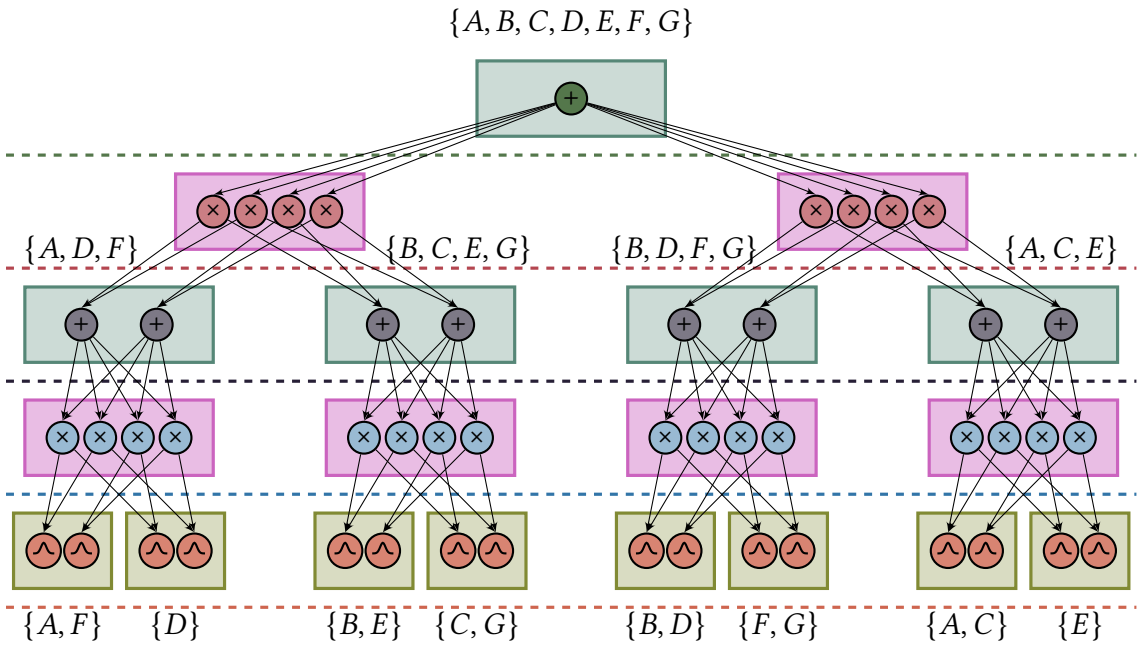


Figure 3.9: *A RAT-SPN generated from parameters $d = 3$, $r = 2$, $s = 2$ and $l = 2$. Nodes within a* ▭ *belong to inner region nodes,* ▭ *to partitions and* ▭ *to leaf regions; dashed lines (and node colors) indicate different PC layers. Scope of region nodes are shown in curly braces.*

Pros and Cons

Pros. As expected from `RAND` algorithms, the random, data-blind nature of RAT-SPN makes for a very fast structure learning algorithm. More importantly, because the structure is expected to have somewhat uniform layers with a fixed number of computational units in each, the computations from parameter optimization can easily be brought to the GPU. This not only helps with scalability in terms of speed, but also brings all the advantages of deep learning frameworks to the table via well-studied stochastic gradient descent optimizers and diagnostic tools.

Cons. Clearly, RAT-SPN is *completely* random with its structure generation. Particularly, variable splits are done randomly, disregarding the independencies encoded by data, meaning that certain factorizations may be assumed to be true when they would otherwise not be. Although RAT-SPNs are certainly competitive against other learning algorithms for PCs, they only produce smooth and decomposable circuits, denying the access to more complex queries.

Remark 3.3: On parameter learning of probabilistic circuits

Literature in probabilistic circuits often divides learning into two (often distinct) tasks: structure learning and parameter learning. Although in this dissertation we almost exclusively cover *structure* learning algorithms, it is worth also going through (even if superficially) some of the works on parameter optimization in PCs, as most structure learning algorithms assume this as a post-processing procedure.

Expectation-Maximization (EM, Dempster *et al.*, 1977) is perhaps the most common maximum likelihood estimation (MLE) optimization procedure for probabilistic circuits. Poon and P. Domingos (2011), Peharz, Tschiatschek, *et al.* (2015) and H. Zhao, Poupart, *et al.* (2016) derived EM for generative learning in PCs, while Rashwan, Poupart, *et al.* (2018) formulated a discriminative EM version for PCs through Extended Baum-Welch (Gopalakrishnan *et al.*, 1991).

Notably, when a circuit is smooth, decomposable and deterministic, MLE can be easily computed through closed-form by counting (Kisa *et al.*, 2014; Peharz, Gens, and P. Domingos, 2014). Indeed, this is an attractive feature that extends to discriminative PCs (Liang and Van den Broeck, 2019).

Following other more traditional deep learning models, PCs learned with stochastic gradient descent (SGD) have also appeared in literature, especially under convolutional and tensorial extensions (Sharir, Tamari, *et al.*, 2018; Peharz, Vergari, *et al.*, 2020; Peharz, Lang, *et al.*, 2020; Gens and P. Domingos, 2012).

Bayesian approaches have also received some attention by the PC community. Jaini, Rashwan, *et al.* (2016) and Rashwan, H. Zhao, *et al.* (2016) developed online Bayesian moment matching algorithms to learn from streaming data; H. Zhao, Adel, *et al.* (2016) showed a variational optimization procedure that leverages inference tractability in PCs to efficiently compute the ELBO; Trapp *et al.* (2019) propose learning both structure and parameters by Gibbs sampling from a generative model on a (restricted) space of PCs; finally Vergari, Molina, *et al.* (2019) propose PCs for automatic Bayesian density analysis.

3.3.2 XPC

While RAT-SPN produces a data-blind PC architecture and then relies on parameter optimization to learn from data, the algorithm that we shall see next does the exact opposite: XPC (Mauro *et al.*, 2021) randomly samples a structure from data and requires no parameter learning. To do this, it restricts the circuit sampling space to a particular class of PCs whose primes are logical restrictions and inputs are CLTs. By assigning a fixed number $k + 1$ of (product) children per sum node and assuming that the k first primes are (random) conjunctions of literals of a fixed length t, with the last $k + 1$ prime their negation, the resulting PC is naturally deterministic, as CLTs are themselves deterministic. In more practical terms, both the conjunctions of literals as well as the $(k + 1)$-th prime derived from the negation of the first k conjunctions are translated into products of (degenerate) Bernoullis. Determinism can be relaxed by applying any form of regularization, for instance Laplace smoothing, both on CLTs and on the products of Bernoullis.

Following the footsteps of RAT-SPN, they generate a tree-shaped random region graph and produce a PC from it. Despite both employing region graphs, the graph in Mauro *et al.* (2021) is only used as an artifice for formalizing the structure construction: their process for reconstructing a PC from a region graph boils down to replacing an inner region with a single sum, a leaf region with a single input and a partition with a single product. Although one *could* generate a non-tree shaped PC by setting $s > 1$ and $l > 1$ (i.e.

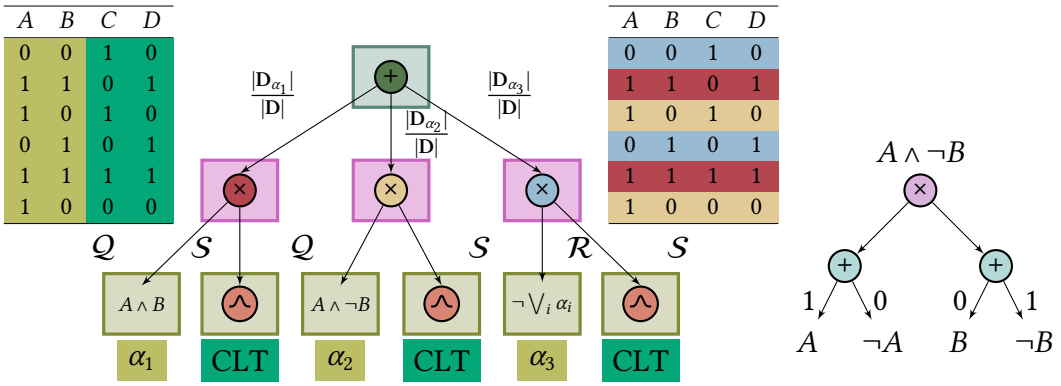


Figure 3.10: *The first iteration of XPC, where $t = 2$ variables are selected, A and B; $k = 2$ conjunctions of literals are sampled, $\alpha_1 = A \wedge B$, $\alpha_2 = A \wedge \neg B$ and $\alpha_3 = \neg(\alpha_1 \vee \alpha_2)$; with primes set to a product of Bernoullis corresponding to each α_i and subs to CLTs. Leaf region nodes $\mathcal{S}$ are candidates for expansion. Sums, products and CLT input nodes are the resulting probabilistic circuit from the sampled region graph. Conjunctions of literals are expanded into product of Bernoullis whose weights are inferred from data, as the circuit on right shows; if no smoothing is applied, the circuit is deterministic.*

number of sums and inputs per inner and leaf region respectively), the resulting circuit could be reduced to a tree, since both sums (and inputs) coming from the same region would be syntatically the same[1].

A critical step to efficiently ensuring consistency with the logical restrictions is to assign only consistent subsets of data to subcircuits. Just like in `DIV` class algorithms, partition (i.e. product) nodes in the region graph define column splits over data and regions (i.e. sums and inputs) correspond to row splits. The algorithm then associates a node with a portion of data according to its scope and logical constraint. More specifically, when the i-th prime defines a conjunction of literals α_i, only assignments $\mathbf{x}$ whose application $\alpha_i(\mathbf{x})$ are true are transferred down, effectively splitting data row-wise. To ensure that the resulting circuit is also decomposable, only $\text{Sc}(\alpha_i)$ variables are passed to primes, with the remaining variables going to the subs. This way, sum weights can be estimated as the subdata size ratios just like in LearnSPN, as Figure 3.10 shows. Each subdata $\mathbf{D}_{\alpha_i}$ corresponds to joining all assignments consistent with α_i, as shown through matching colors on the table on the right. Data is divided by rows according to the satisfiability of each prime α_i and by column according to the scope of each prime.

At each iteration of Algorithm 16, sub leaf region nodes, denoted here as $\mathcal{S}$ regions, are randomly selected for further expansion. Algorithm 15 takes a candidate region R and samples k conjunctions $\alpha_1, \ldots, \alpha_k$ of length t that appear at least δ times in the subdata associated with R. If no such constraint has been found, R is discarded as a candidate for expansion. Otherwise, another layer of partitions and regions similar to Figure 3.10 is constructed, making sure that data splits obey both scope and constraints α_i. Once no more candidates are available or a limit on the number of expansions has been reached, the region graph is translated into a probabilistic circuit by replacing leaf region nodes of

[1] Whether this "expanded" circuit could have its performance improved if one were to run, say EM, to exploit this increase in capacity is an interesting question that unfortunately was left unexplored in Mauro *et al.* (2021).

Algorithm 15 ExpandXPC

Input Region R, data $\mathbf{D}$, variables $\mathbf{X}$, min. # of assignments per partition δ, # of conjunctions of literals k, length of conjunctions t

1: Let $\mathbf{A}$ a set of logical constraints initially empty
2: Copy all data from $\mathbf{D}$ to S
3: Sample a subset Y of size t from $\mathbf{X}$
4: **while** $|\mathbf{A}| < k$ **do**
5: Sample a conjunction of literals α over Y distinct from any in $\mathbf{A}$
6: $\mathbf{Q} \leftarrow \{\mathbf{x} \mid \forall \mathbf{x} \in \mathrm{S} \wedge \alpha(\mathbf{x}) = 1\}$
7: **if** $|\mathbf{Q}| \geq \delta$ **and** $|\mathrm{S} \setminus \mathbf{Q}| \geq \delta$ **then**
8: Append α to $\mathbf{A}$
9: $\mathrm{S} \leftarrow \mathbf{D} \setminus \mathbf{Q}$
10: Create a partition node P as a child of R
11: Create a region R'_p of type $\mathcal{Q}$ and assign it as a prime of P
12: Assign scope Y and data $\mathbf{Q}$ to R'_p
13: Create a region R'_s of type $\mathcal{S}$ and assign it as a sub of P
14: Assign scope $\mathbf{X} \setminus \mathrm{Y}$ and data $\mathrm{S} \setminus \mathbf{Q}$ to R'_s
15: **if** no constraint is suitable **then** unset R as a candidate and **return**
16: **else**
17: Create a partition node P as a child of R
18: Create a region R'_p of type $\mathcal{R}$ and assign it as a prime of P
19: Assign scope Y and data S to R'_p
20: Create a region R'_s of type $\mathcal{S}$ and assign it as a sub of P
21: Assign scope $\mathbf{X} \setminus \mathrm{Y}$ to R'_s

type $\mathcal{Q}$ into products of Bernoullis, type $\mathcal{S}$'s into CLTs and inner regions as sums whose weights are the proportions of (row-wise) split data; partitions are replaced with product nodes.

Determinism is not the only constraint that can be enforced. In fact, since every product is by construction 2-standardized, the circuit is structure decomposable if not only the scopes of $\mathcal{Q}$ regions follow a vtree, but the CLTs in $\mathcal{S}$ regions do as well. This forces the sampling done in line 3 to instead deterministically assign Y the scope of $\mathrm{Sc}(v^{\leftarrow})$, where v is the vtree node associated with the product splitting $\mathbf{X}$.

Complexity

To simplify, we assume that all k distinct logical constraints pass the condition of containing at least δ samples in the dataset. With this, the complexity of ExpandXPC is $\mathcal{O}(t + k \cdot |\mathbf{D}|)$, where the first term comes from sampling a subset of size t from $\mathbf{X}$ and the second from selecting all assignments in $\mathbf{D}$ that agree with the constraint α. Sampling conjunctions of literals can be done in constant time by representing α as a bit vector where a 1 indicates a positive literal and 0 a negative literal; sampling a number in $\left[0, 2^{|\mathrm{Y}|-1}\right]$ (here assumed to be done in $\mathcal{O}(1)$) is equivalent to producing α.

The analysis for XPC relies on either the number of maximum iterations or available

Algorithm 16 XPC

Input Dataset $\mathbf{D}$, variables $\mathbf{X}$, min. # of assignments per partition δ, # of conjunctions of literals k, length of conjunctions t

Output A smooth, decomposable and deterministic probabilistic circuit

Start with a region graph $\mathcal{G}$ with a single region node as root
while there are candidate region nodes of type $\mathcal{S}$ **do**
    Select a random region R of type $\mathcal{S}$
    Let $\mathbf{Q}$ the subdata associated with R
    ExpandXPC(R, $\mathbf{Q}$, Sc(R), δ, k, t)
for each node $\mathsf{N} \in \mathcal{G}$ in reverse topological order **do**
    Let $\mathbf{D}_{\mathsf{N}}$ the data associated with N
    if N is a leaf region node of type $\mathcal{Q}$ **then**
        Replace N with a product of Bernoullis according to $\mathbf{D}$
    else if N is a leaf region node of type $\mathcal{S}$ **then**
        Replace N with a CLT learned from $\mathbf{D}$
    else if N is a region node **then**
        Replace N with a sum node whose weights are $w_{\mathsf{N},\mathsf{C}} = \frac{\mathbf{D}_{\mathsf{C}}}{\mathbf{D}_{\mathsf{N}}}$ for each $\mathsf{C} \in \mathrm{Ch}(\mathsf{N})$
    else
        Replace N with a product node
return $\mathcal{G}$'s root sum node

candidates. At every call to ExpandXPC, we create at least $3(k+1)$ new PC nodes, of which $k+1$ of them are $\mathcal{S}$ regions. Assuming that we let the algorithm run a fixed number of iterations i, we get a total runtime of $\mathcal{O}\left(i \cdot (t + k \cdot |\mathbf{D}|)\right)$. for the main loop in XPC. We then need to compile the PC and learn CLTs for every $\mathcal{S}$ leaf. Because we ran for i iterations, we should have $i \cdot k$ CLTs to learn, which is done in $\mathcal{O}(|\mathbf{X}|^2 \cdot \mathbf{D})$, bringing the total runtime to $\mathcal{O}\left(i \cdot (t + k \cdot |\mathbf{D}|) + i \cdot k \cdot |\mathbf{X}|^2 \cdot |\mathbf{D}|\right)$. Note, however, that this is a rough upper bound on the true complexity, as both scope and data shrink considerably at each depth.

Pros and Cons

Pros. XPC is flexible in the sense that it can produce both deterministic and structure decomposable circuits with little change to the algorithm. More importantly, because it essentially divides data in a `DIV` approach, the most costly operation, i.e. learning CLTs at the leaves, is done extremely fast, since the optimization is done only on a fraction of the data and scope. As an example, learning XPCs from binary datasets of hundreds of variables and tens of thousands of instances takes a matter of seconds, while most competitors usually take hours for learning from the same data. In terms of performance, although single circuit XPCs rarely beat state-of-the-art competitors, Mauro *et al.* (2021) showed that by merely aggregating sampled circuits into a simple mixture boosts performance considerably, reaching competitive results.

Cons. When it comes to circuit size, although a single XPC generated circuit has comparable size to other state-of-the-art structure learning competitors, for these to be competitive requires ensembles of a few dozens of components, meaning that in its final form, these

can be tens of times the size of other structure learners. Moreover, because of the number of parameters involved in sampling these PCs (δ, k, t, number of components per ensemble, and whether to produce deterministic and/or structure decomposable PCs), a grid-search over parameters is necessary to produce optimal results. Although this is generally faster than other structure learning algorithms, the sheer size of all generated circuits from every hyperparameter combination can easily overwhelm memory space.

4

Scalable Learning of Probabilistic Circuits

Considering the many benefits and drawbacks of the current state-of-the-art learning algorithms addressed in Chapter 3, and emphasizing the need for scalability and accessibility, we now present the main contributions of this dissertation, proposing two novel structure learning algorithms for probabilistic circuits. We approach the problem of learning scalable PCs from two distinct points of view. In Section 4.1, we are interested in PCs whose support encodes a given logical constraint as certain knowledge; we show how both the probabilistic issue of data fitness, as well as the logical question of whether the circuit successfully compiles a knowledge base can be accomplished by aggregating PC samples into ensembles of models. In Section 4.2, we look at PCs solely from the perspective of data fitness; we exploit the connection between PCs and generative random forests (Correia *et al.*, 2020; Ho, 1995) and revisit a well-known technique based on random projections for constructing random trees (Freund *et al.*, 2008; Dasgupta and Freund, 2008), presenting a simple and fast yet effective way of learning PCs.

The contents of Section 4.1 come from our contributions in R. L. Geh and Denis Deratani Mauá (2021b), while Section 4.2 comes, in part, from R. L. Geh and Denis Deratani Mauá (2021a).

4.1 A Logical Perspective

Remark 3.2 briefly mentioned the question of compiling logical constraints into smooth, structure decomposable and deterministic logic circuits (i.e. (P)SDDs Darwiche, 2011; Kisa *et al.*, 2014). Indeed, although there are many existing approaches to learning circuits from logical formulae, most are only useful for specific tasks (A. Choi, Tavabi, *et al.*, 2016; A. Choi, Broeck, *et al.*, 2015; Shen *et al.*, 2017; A. Choi, Shen, *et al.*, 2017). Although there are more generalistic ways of producing circuits, namely from CNFs and DNFs (Oztok and Darwiche, 2015; A. Choi and Darwiche, 2013); logic formulae which incorporate more complex relationships such as cardinality constraints either have no tractable representation (Nishino *et al.*, 2016) or require the addition of latent variables (Sinz, 2005). More importantly, because variables which do not play a role in the logical formulae are completely discarded in the compilation process, translating these *logic* circuits into *probabilistic* circuits involves naïve assumptions on the discarded variables, such as fully

factorizing them.

Surprisingly, to our knowledge there have been next to no work on learning the structure of PCs from scratch by looking at both logical formulae *and* data. Even worse, the couple that do are restricted to very preliminary work: Mattei, Soares, *et al.* (2019) came up with a `DIV` prototype for a top-down approach to sampling a special class of PSDDs whose primes are conjunctions of literals in a similar manner to XPCs, proposing a Bayesian information criterion to searching the sample space, yet no practical algorithm was fully formulated; R. Geh, D. Mauá, and Antonucci (2020) expanded on Mattei, Soares, *et al.*'s work by formalizing an algorithm and introducing a BDD to guide sampling, however the generated circuits suffered from an exponential blow-up in size.

In this section, we propose a solution inspired by R. Geh, D. Mauá, and Antonucci (2020) and Mattei, Soares, *et al.* (2019), yet without the previously mentioned problems that come with them. In summary, we propose a sampling procedure to efficiently generating PSDDs whose primes are always conjunctions of literals; to overcome the exponential blow-up, these PSDDs only partially encode their prior logical restrictions. To diversify sampling, local transformations similar in spirit to `INCR` algorithms are used. Of worth, we found that not only is this process incredibly fast even under intricate logical formulae, but by combining samples into an ensemble we achieve competitive results against the state-of-the-art.

Before we address our contributions, we should first fix some notation on the issue of propositional logic. We treat propositional variables as 0/1-valued random variables and use them interchangeably. Given a Boolean formula, 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, i.e. 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 overload the scope function once again for logical formulae: $\mathrm{Sc}(f)$ denotes the set of variables that appear in f.

Because we are only interested in smooth, structure decomposable and deterministic PCs whose support is defined by a logical formula, we shall adopt the usual notation of PSDDs, which we present next.

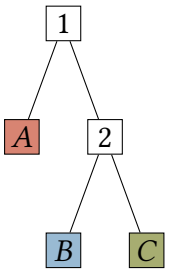
Definition 4.1.1 (Partition)**.** *Let $\phi(\mathbf{x}, \mathbf{y})$ be a Boolean function over disjoint sets of variables $\mathbf{X}$ and $\mathbf{Y}$, and $\mathcal{D} = \{(p_i, s_i)\}_{i=1}^{k}$ be a set of tuples where p_i (the prime) and s_i (the sub) are formulae over $\mathbf{X}$ and $\mathbf{Y}$ respectively, satisfying $p_i \wedge p_j \equiv \bot$ for each $i \neq j$ and $\bigvee_{i=1}^{k} p_i \equiv \top$. We say that $\mathcal{D}$ is an $(\mathbf{X}, \mathbf{Y})$-partition of ϕ if and only if $\phi \equiv \bigvee_{i=1}^{k} (p_i \wedge s_i)$.*

An (exact) partition[1] is no more than a smooth, structure decomposable and deterministic circuit rooted at a sum (or disjunction) node whose children are products (or conjunctions); the primes of these products must necessarily be mutual exclusive (formally, $p_i \wedge p_j \equiv \bot$) and exhaustive (formally, $\bigvee_{i=1}^{k} p_i \equiv \top$). Semantically, a partition states that a logical formula decomposes into k exact conjunctions of pairs of prime and sub. The box in Figure 4.1 shows a partition whose primes are $p_1 = A$ and $p_2 = \neg A$, and subs are

[1] The naming *partition* is unfortunate. The nomenclature in probabilistic circuits is full of many other partitions, either using the term to conjure meaning from set theory when dealing with data splits (see Section 3.1), partition nodes in region graphs (see Section 3.3) or in PSDD literature in this section. Here (and only here), partitions will mean stricly the latter.

A	B	C	$p(\mathbf{x})$
0	0	0	0.1
0	1	0	0.1
1	0	0	0.2
1	0	1	0.6

$\phi(A, B, C) = (A \rightarrow \neg B) \wedge (C \rightarrow A)$



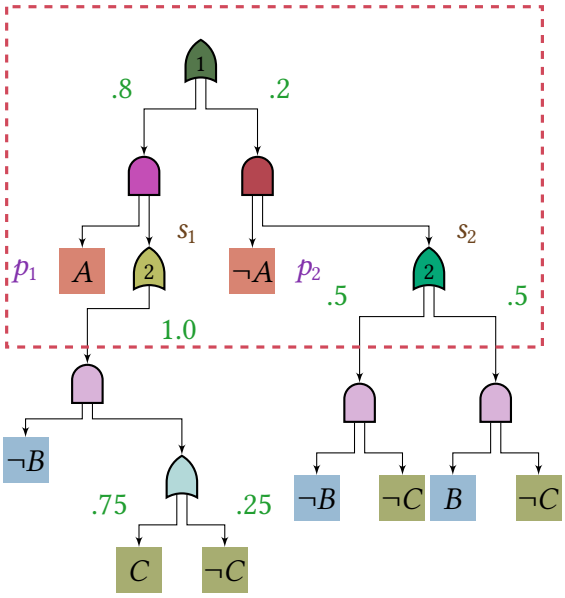


Figure 4.1: *A PSDD encoding the logical constraint $\phi(A, B, C) = (A \rightarrow \neg B) \wedge (C \rightarrow A)$, following the distribution set by the probability table on the top left corner and whose structure is defined by the vtree pictured on the bottom left corner.*

$s_1 = \neg B$ (represented as a PC rooted at ②) and $s_2 = \neg C$ (represented as the PC rooted at ②). Recall that the conjunction between a prime and sub is called an *element*, here shown as ▮ and ▮.

4.1.1 SamplePSDD

We now describe how to efficiently learn PSDDs by sampling and averaging. The procedure takes inspiration from DIV algorithms in the sense that we construct a PSDD structure top-down by recursively decomposing a logical formula (instead of data). At the same time, we employ local transformations similar to INCR approaches on a partially constructed circuit to diversify samples. All this procedure is done randomly in a similar fashion to XPCs, where we restrict primes to be random conjunctions of literals and sample variables according to a previously learned or randomly sampled vtree. To better understand how this is done, we must first consider a naïve approach.

Let ϕ a logical formula acting as our knowledge base, and assume that a vtree $\mathcal{V}$ is given beforehand. To compile a PSDD from ϕ, we must decompose it down to a disjunction of prime and sub conjunctions. This is a non-trivial problem, as primes must not only be mutual exclusive (to ensure determinism) but exhaustive (to make sure the circuit is coherent with ϕ in all possible assignments). If we assume primes to be conjunctions of literals, then to adhere to Definition 4.1.1 there must be an exponential number of elements $2^{|\mathrm{Sc}(v^{\leftarrow})|}$, where v is the vtree node that corresponds to the partition. Subs, however, are easy to retrieve as they correspond to the restriction of ϕ under the assignment induced by the prime. Figure 4.2 shows a partition whose primes are conjunctions over A and B. This problem is the same as the one faced by R. Geh, D. Mauá, and Antonucci (2020): under the assumption of conjunctions of literals as primes, ϕ can only be faithfully represented

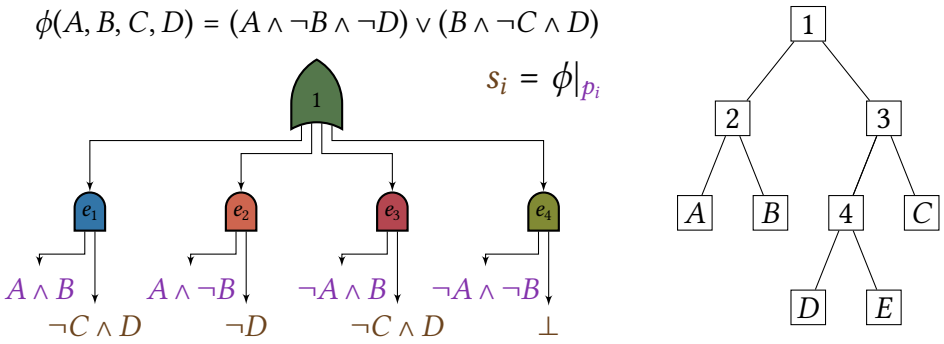


Figure 4.2: *A(n exact) partition of ϕ where we assume that primes are conjunctions of literals. Primes must be exhaustive, mutually exclusive, and have to follow the vtree's scope, here* $\text{Sc}(1^{\leftarrow}) = \{A, B\}$. *The subs are then the restriction of ϕ under the assignment induced by the primes.*

as a PSDD if the circuit is exponential.

To overcome this exponential blow-up, we might restrict the number of primes at each partition. Unfortunately, if we bound this number to a constant, say k, and randomly sample primes from the space of all possible conjunctions of literals, then we face yet another problem: the scope of subs might contain variables not in their corresponding vtree node. Take the top circuit in Figure 4.3 as an example. Note that the scope for primes is defined by $\text{Sc}(1^{\leftarrow}) = \{A, B, C\}$, with $\text{Sc}(1^{\rightarrow}) = \{D, E\}$ for subs; so sampled primes $p_1 = A \wedge B$, $p_2 = A \wedge \neg B$ and $p_3 = \neg A$ must come from $\text{Sc}(1^{\leftarrow})$. However, because $s_1 = \phi|p_1 = \neg C \wedge D$ and $s_3 = \phi|p_3 = B \wedge \neg C \wedge D$, meaning that $\text{Sc}(s_1) \not\subseteq \text{Sc}(1^{\rightarrow})$ and $\text{Sc}(s_3) \not\subseteq \text{Sc}(1^{\rightarrow})$, subs violate the factorization imposed by the vtree $\mathcal{V}$, making the circuit non-structure decomposable (albeit decomposable). Here, we point out that the scope of the formula needs to be a subset of the scope of its corresponding vtree for the PC to be structure decomposable, and not necessarily the set itself, as variables that do not appear in the formula yet are part of the vtree's scope play a *probabilistic* role in the PSDD.

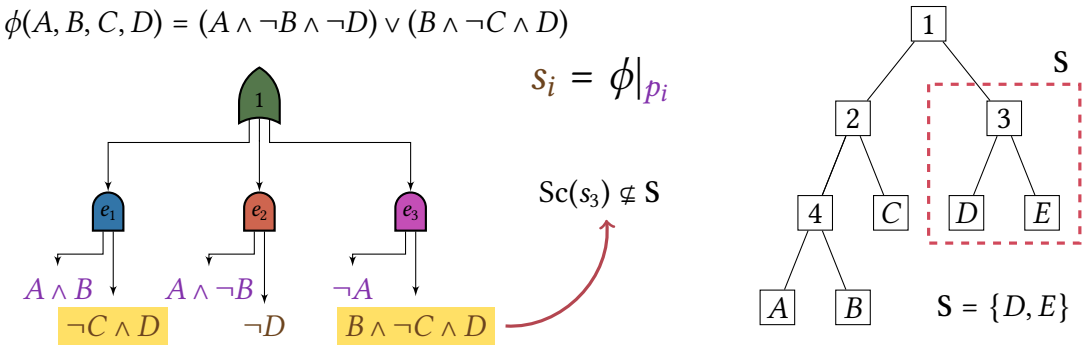
For these circuits to both preserve structure decomposability *and* have tractable representation, we need to resort to a weaker definition of a partition that relaxes the logical constraints.

Definition 4.1.2 (Partial partition). *Let $\phi(\mathbf{x}, \mathbf{y})$ be a Boolean function over disjoint sets of variables $\mathbf{X}$ and $\mathbf{Y}$, and $\mathcal{D} = \{(p_i, s_i)\}_{i=1}^{k}$ be a set of tuples where p_i (the prime) and and s_i (the sub) are formulae over $\mathbf{X}$ and $\mathbf{Y}$ respectively, satisfying $p_i \wedge p_j \equiv \bot$ for each $i \neq j$ and $\bigvee_{i=1}^{k} p_i \equiv \top$. We say that $\mathcal{D}$ is a partial partition of ϕ if*

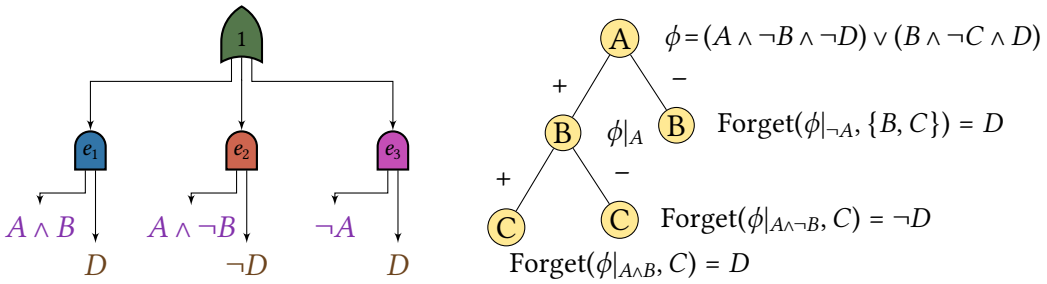
$$\left\langle \bigvee_{i=1}^{k} (p_i \wedge s_i) \right\rangle \geq \phi,$$

where the inequality is taken coordinate-wise.

Definition 4.1.2 essentially states that the disjunction over elements has to only encode a relaxation of the original formula ϕ. This is somewhat similar to what Gatterbauer and Suciu (2014) propose in probabilistic databases, where they relax a formula in such a way that the approximate probabilities provide an upper bound independent of the actual



(a) *Partially constructed PSDD with vtree infracting subs*



(b) *Partial partition where subs are relaxed*

Figure 4.3: *An example of an invalid partition* ***(a)*** *due to subs disrespecting the vtree's right branch, here shown as the box with scope* S. *To fix this infraction, variables who do not belong to* S *are* forgotten, *as* ***(b)*** *shows.*

probabilities.

Looking back to the issue of bounding the number of elements per partition, a solution to the problem of tractability and structure decomposability comes by employing *partial* partitions instead of *exact* partitions. Let S a sum node, and call s_i one of its sub and v the vtree node for S; denote by $\mathbf{F} = \mathrm{Sc}(s_i) \setminus \mathrm{Sc}(v^{\rightarrow})$, that is, the variables in s_i which should *not* have been in the sub. We already know that S cannot be turned into an exact partition unless it has an exponential number of elements, and so we look to *partial* partitions. The *forget* operation takes a formula ψ and marginalizes variable X: $\mathrm{Forget}(\psi, X) = \psi|_X \vee \psi|_{\neg X}$; by construction $\mathrm{Forget}(\psi, X) \geq \psi$. By forgetting all variables in $\mathbf{F}$, we secure structure decomposability and produce a relaxation of the original formula. To do this efficiently, we make use of a BDD for representing formulae, as reduced BDDs are canonical and permit polynomial time restricting and forgetting.

In more practical terms, the overall process of sampling a PSDD starts with a logical formula ϕ, a vtree $\mathcal{V}$ and scope $\mathbf{X}$. We recursively construct partial partitions by first sampling a fixed number of k primes and evaluating subs with restrictions and Forgets. Elements whose subs are $\bot$ are removed, as their probability is always zero. For each prime and sub, we recursively call the same procedure on their formulae. Just like in most `DIV` class algorithms, if $|\mathbf{X}| = 1$, then we either return a literal node consistent with ϕ, or a Bernoulli distribution input node over $\mathbf{X}$'s only variable. Another special case arises when $\phi \equiv \top$, in which case any smooth, structure decomposable and deterministic PC

Algorithm 17 SamplePartialPartition

Input BDD ϕ, vtree node v, number of primes k
Output A set of pairs of primes and subs

Define **E** as an empty collection of pairs
Sample an ordering $X_1, \ldots, X_m$ of $\text{Sc}(v^{\leftarrow}) \cap \text{Sc}(\phi)$
Let **Q** be a queue initially containing $(\phi, 1, \{\})$
$j \leftarrow 1$ ▷ Counter of sampled elements
while $|\mathbf{E} < k|$ **do**
    Pop top item (ψ, i, p) from **Q**
    if $j \geq k$ **or** $i > m$ **or** $\psi \equiv \top$ **then**
        Add $(p, \text{Forget}(\phi|_p, \text{Sc}(v^{\leftarrow})))$ to **E**
        continue
    $\alpha \leftarrow \psi|_{X_i}, \beta \leftarrow \psi|_{\neg X_i}$
    if $\alpha \equiv \beta$ **then** enqueue $(\psi, i+1, p)$ into **Q**
    else
        if $\alpha \not\equiv \bot$ **then** enqueue $(\alpha, i+1, p \wedge X_i)$ into **Q**
        if $\beta \not\equiv \bot$ **then** enqueue $(\beta, i+1, p \wedge \neg X_i)$ into **Q**
        $j \leftarrow j + 1$
return E

will do. This PC can either be learned purely from data or generated from a template. Alternatively, we might even choose to continue sampling partitions as before, except in this case all partial partitions are also exact partitions. Algorithm 18 shows the entire recursive procedure of SamplePSDD.

The sampling process of generating primes and their subs is shown in Algorithm 17 and goes as follows. To produce primes (and subs), we must look at the space of all possible variable assignments coming from $\text{Sc}(v^{\leftarrow})$, where v is the relevant vtree node. If we fix a variable ordering to $\text{Sc}(v^{\leftarrow})$, say an m-uple $\mathbf{O} = \{X_1, \ldots, X_m\}$, then we might structure this space as a binary decision tree whose nodes are labeled as a variable and every edge denotes positive or negative literals over that variable. The path coming from a node to a leaf in this decision tree represents all chosen literals in a prime. An example of such a tree is shown as the right tree in Figure 4.3b. We efficiently generate k primes by starting from the root node labeled as variable X_1 and repeatedly expanding a leaf labeled X_i with two children X_{i+1} until the number of leaves is between $k-1$ and k (expanding further would mean violating the bound on the number of primes). Every time we expand a leaf, we must generate the restrictions $\psi|_{X_i}$ and $\psi|_{\neg X_i}$, where ψ is the formula up to that path, and associate them with the left and right children respectively. If $\psi|_{X_i} \equiv \psi|_{\neg X_i}$, or in other words the assignment of X_i does not change ψ's semantics, then we relabel the node as X_{i+1} and re-expand it with children X_{i+2}, effectively ignoring X_{i+1}. When this process terminates, we have at most k conjunctive primes represented by all the paths coming from the root down to the leaves, each of these with an associated formula equivalent to restricting ϕ to all assignments $\phi|_{\mathbf{x}}$. Now, to obtain valid subs as previously mentioned, we apply the Forget operation to each sub over the scope of $\text{Sc}(v^{\leftarrow})$, removing any variables from the wrong side of the vtree.

Algorithm 18 SamplePSDD

Input BDD ϕ, vtree node v, number of primes k
Output A sampled PSDD structure

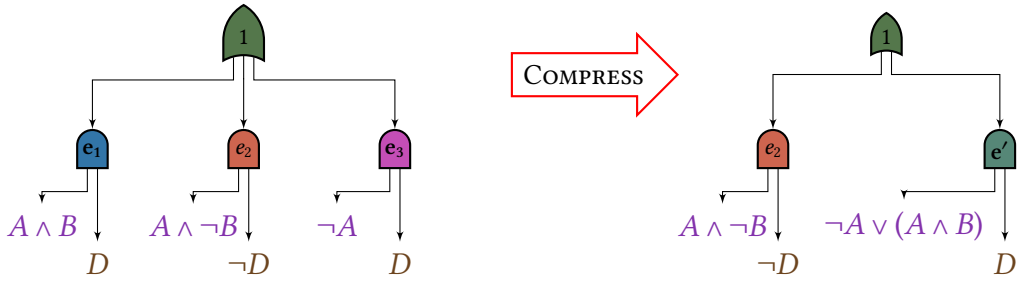
if $|\text{Sc}(v)| = 1$ **then**
  if ϕ is a literal **then return** ϕ as a literal node
  else return a Bernoulli distribution input node over variable $\text{Sc}(v)$
else if $\phi \equiv \top$ **then**
  return any smooth, structure decomposable and deterministic PC over $\text{Sc}(v)$
E $\leftarrow$ SamplePartialPartition$(\phi, \text{Sc}(v^{\leftarrow}), k)$
Create a sum node S
Randomly compress elements in **E** with equal subs
Randomly merge elements in **E** with equal subs
for each element $(p, s) \in$ **E** **do**
  $l \leftarrow$ SampleExactPSDD$(p, v^{\leftarrow}, k)$
  $r \leftarrow$ SamplePSDD$(s, v^{\rightarrow}, k)$
  Add a product node with children l and r as a child of S
return S

Once primes and subs are generated, SamplePSDD randomly applies local transformations to add variety to sampled circuits and reduce their size. Here we introduce two *shrinking* local transformations, directly opposed to INCR's *growing* local transformations. We borrow the concept of *compression*, used to minimize a logic circuit down to a canonical representation (Darwiche, 2011), and use it to join multiple elements into a single one during learning. Let $e_1, \ldots, e_q$ elements whose subs $s_1, \ldots, s_q$ are all equivalent to s, or more formally $s \equiv s_i \equiv s_j$, $i \neq j$; in this case, the disjunction over these elements factorizes over s

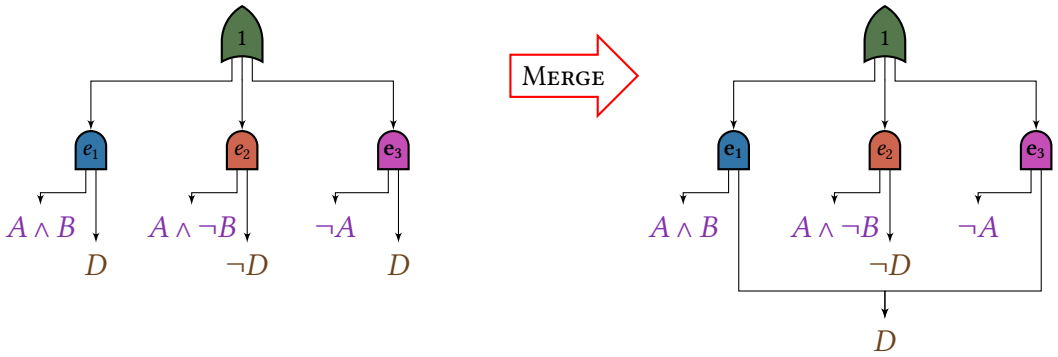
$$\bigvee_{i=1}^{q}(p_i \wedge s_i) = \bigvee_{i=1}^{q}(p_i \wedge s) = s \wedge \left(\bigvee_{i=1}^{q} p_i\right).$$

Figure 4.4a shows a compression of elements e_1 and e_3 whose subs are both D. The resulting compressed element e' is equivalent to the disjunction of the primes with no change to the sub. Compression is the exact inverse of Split, seen in Section 3.2 (cf. Figure 3.7). Apart from compression, we propose *merging* two equivalent subs into the same circuit as shown in Figure 4.4b. Merging is a common (previously nameless) operation in PC literature and is the inverse of Clone (cf. Figure 3.7). In both cases, shrinking local transformations preserve smoothness, structure decomposability, determinism and the circuit's formula, although they change the PSDD's underlying distribution by reducing the number of parameters.

To ensure that elements are mutual exclusive (and by consequence the partition is deterministic), we need to disallow relaxations in recursive calls to primes. For instance, if we had not imposed this restriction, a possible relaxation of e_1's prime $A \wedge B$ into, say B, in Figure 4.3b might contradict prime mutual exclusivity, as B conflicts with e_3's prime $\neg B$ (because $B \wedge \neg A \not\equiv \bot$). This is trivially solved by making sure that every partition in subcircuits rooted at primes is exact (here denoted by the function SampleExactPartition). If we bound the number of primes to a constant k, these exact subcircuits will never



(a) *Compressing elements e_1 and e_3 into e'*



(b) *Merging subs s_1 and s_3 into a single sub*

Figure 4.4: *Examples of compression **(a)** and merging **(b)** as local transformations for reducing the size of PSDDs. Both act on elements whose subs are logically equivalent.*

suffer from an exponential blow-up, as all subsequent (exact) partitions contain primes with at most $\lceil \log_2(k) \rceil$ variables and thus at most $2^{\lceil \log_2(k) \rceil}$ elements are constructed at each call.

4.1.2 Experiments

Just like in STRUDEL and LEARNPSDD, to boost the performance of our approach we resort to mixtures of PSDDs. We separately sample t models in parallel with SAMPLEPSDD, learn their parameters through closed-form smoothed MLE (KISA *et al.*, 2014) and then learn only mixture weights in five different approaches: (1) likelihood weighting (LLW), where each component's weight is proportional to its train likelihood; (2) uniform weights, (3) Expectation-Maximization, (4) stacking (SMYTH and WOLPERT, 1998), and (5) Bayesian Model Combination (BMC, MONTEITH *et al.*, 2011).

We compare our results against STRUDEL, mixtures of 10 STRUDELS, LEARNPSDD and LEARNSPN. We used existing implementations coming from the Juice probabilistic circuits library (DANG, KHOSRAVI, *et al.*, 2021) for the first two, while LEARNPSDD and SAMPLEPSDD were implemented into the library. For LEARNSPN, we used the PySPN library[2] whose implementation uses k-means for learning sums and G-test for products. We look at four different datasets that contain some kind of structure to them, modeling them as logical formulae. We observe the impact of this prior knowledge by learning PCs both under low data regimes and lots of data. For STRUDEL, as proposed in DANG, VERGARI, *et al.* (2020),

[2] https://gitlab.com/pgm-usp/pyspn

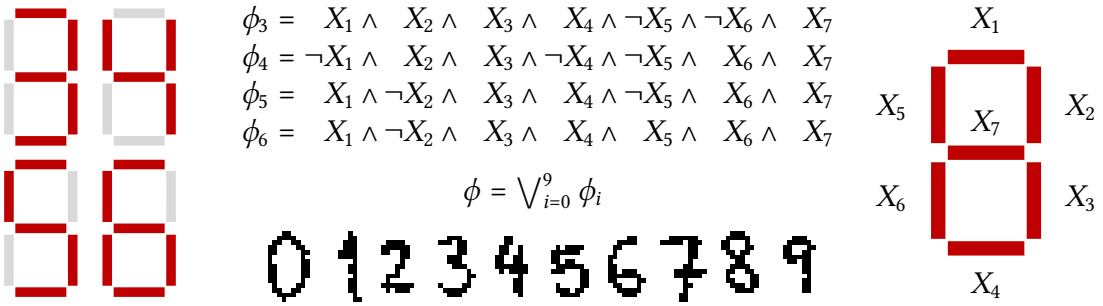


Figure 4.5: *Seven-segment LED digits for 3, 4, 5 and 6 (left), the logical constraints for each of these digit ϕ_i (top middle) and the resulting formula derived from listing all valid configurations ϕ (middle), each latent variable X_i corresponding to a segment's supposed state, and samples of pixel variants* `led-pixels` *for each digit (bottom middle).*

we used an initial PC compiled from a CLT learned purely from data (see Section 3.2.2). Initial circuits for LearnPSDD were compiled into canonical logic circuits from either a CNF or DNF when the logical restrictions permitted a tractable representation in such forms; when this was not the case, a BDD was compiled into a circuit instead. For the resulting initial circuit to contain variables not present in the formula, a product node whose children were the compiled PC and a fully factorized circuit over absent variables was created and set as root.

All experiments were run on an Intel i7-8700K 3.70 GHz machine with 12 cores and 64GB. We limited LearnPSDD and Strudel both to 100 iterations, although runs with 1000 iterations can be found in the supplementary material of Annex B.1. For all experiments with SamplePSDD, when $\phi \equiv \top$ (line 5 of Algorithm 18) we produced a fully factorized circuit. In the remaining part of this section, we first address the performance of our proposed approach compared to the state-of-the-art and then provide an empirical analysis on the impact of vtrees and parameter choice for ensembles of SamplePSDD

LED Display

A seven-segment LED display consists of LED light segments which are separately turned on or off in order to represent a digit. Figure 4.5 shows some digits represented by a seven-segment display. Each digit is associated with a local constraint on the values of each segment. We adapt the approach by Mattei, Antonucci, *et al.* (2020b) and generate a `led` dataset of faulty observations of the segments as follows. Each segment is represented by a pair of variables (X_i, Y_i), where Y_i is the observable state of segment i (i.e. whether the segment is on or off) and X_i is the latent state of i. We randomly sampled a PSDD over variables X_i and Y_i whose support are the valid configurations of segments X_i representing the digits, and use that model to generate a dataset of 5,000 training instances and 10,000 test instances.

A more complex alternative configuration for the LED setting, `led-pixels`, is the interpretation of digits as images and segments as pixel regions. The segment constraints remain unchanged, but now pixels act as the latent variables. Figure 4.5 (bottom) shows ten samples for each the ten digits; each instance from the dataset is a 10×15 black-and-white image. In this pixelized version, we do not explicitly describe, in the form of

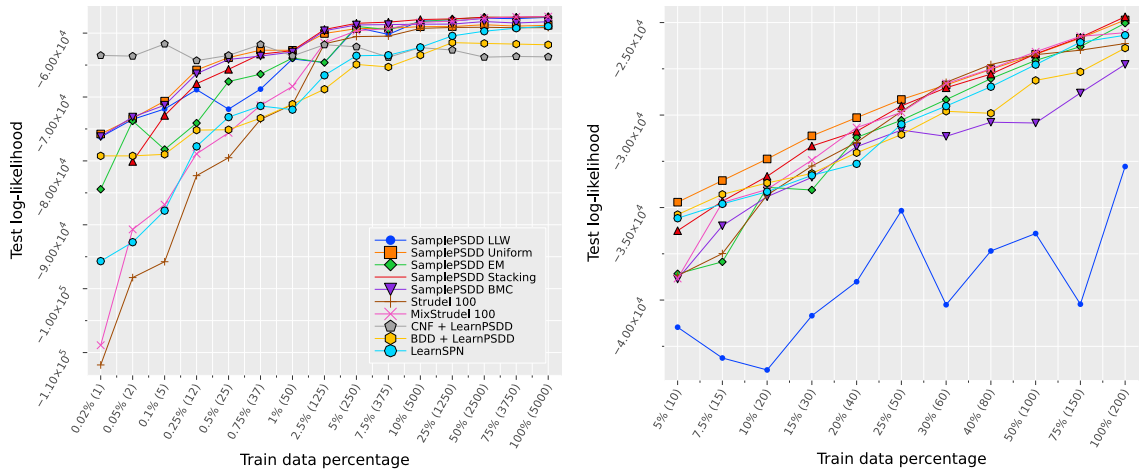


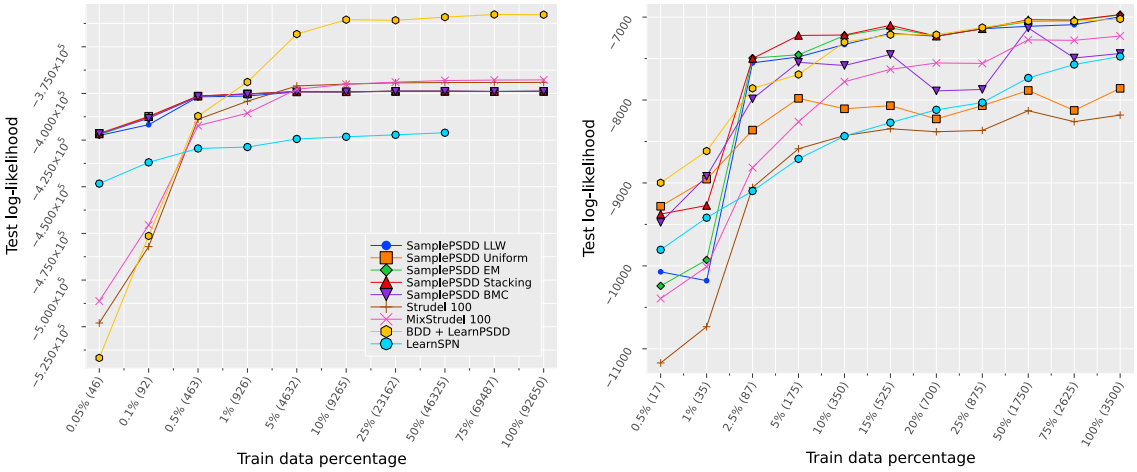
Figure 4.6: *Log-likelihoods for the unpixelized* `led` ***(a)*** *and pixelized* `led-pixels` ***(b)*** *datasets.*

logical constraints, a one-to-one mapping of pixel regions as segments; instead, we visually identify key points where pixels most often activated given a segment's value. Let $\mathbf{R}_s$ be pixel variables which are most oftn set to 1 when a segment s is on. We build a constraint for each segment: $\psi(s) = s \longrightarrow \bigvee_{r \in \mathbf{R}_s} r$. We futher recognize which pixels are always off given a valid digit segment configuraton: $\phi(\mathbf{s}) = \left(\bigwedge_{p\,:\,p=0|\mathbf{s}} \neg p\right) \wedge \left(\bigwedge_{s \in \mathbf{s}} s\right)$. The full logic formula encoding all constraints is the conjunction of every possible ϕ and ψ.

Figure 4.6 shows how our approach fairs against competitors using different percentages of available training data on the unpixelized and pixelized versions of the dataset. The labels on the x-axis indicate percentage and number of training instances. We sampled $t = 100$ circuits for both settings, with $k = 32$ and $k = 8$ for `led` and `led-pixels` respectively. Note how the use of logical constraints greatly improves performance even under extremely scarce data (with 1 or 2 datapoints). Most of the SamplePSDD approaches obtain the best performance with the full dataset, and ranks among the best when data size is small.

Cardinality Constraints

The DOTA dataset contains the result of 102,944 online matches of the Dota 2 videogame, made available at the UCI Repository. In this game, each team is composed of 5 players players, with each one controlling a single character out of a pool of 113. Each character can be controlled by at most one single player in a match. We represent the domain by 2 groups of 113 Boolean variables $C_1^{(i)}$ and $C_2^{(i)}$, denoting whether the i-th character was selected by the first or second team, respectively. We then encode 113-choose-5 cardinality constraints on the selection of each team (i.e. $\sum_{i=1}^{1} 13 C_j^{(i)} = 5$ for $j \in \{1, 2\}$). Unfortunately, adding the constraint that no character can be selected by both teams $\neg(C_1^{(i)} \wedge C_2^{(i)})$ made the BDD representation of the formula intractable, and so was ignored. Since the CNF representation of cardinality constraints is intractable, we used a PSDD compiled from a BDD to generate an initial circuit for LearnPSDD (as BDDs can efficiently encode such restrictions (Eén and Sörensson, 2006)). We set the number of components for



(a) **(b)**

Figure 4.7: *Log-likelihoods for the* `dota` ***(a)*** *and* 10*-choose-*5 `sushi` ***(b)*** *datasets.*

SamplePSDD to $t = 30$ and bound the number of sampled elements to $k = 3$.

The plot in Figure 4.7a shows the test log-likelihood of the tested approaches. Despite accurately encoding logical constraints, LearnPSDD initially obtains worse performance when compared to SampledPSDD, but quickly picks up, outperforming other models by a large margin. SamplePSDD ranks first for small data regimes, and is comparable to Strudel (and mixtures of) for large training datasets. LearnSPN encountered problems scaling to more than 50,000 instances due to intensive memory usage in both clustering and pairwise independence testing.

We also compared methods on the `sushi` dataset (Kamishima, 2003), using the setting proposed in Shen *et al.* (2017). The data contains a collection of 5,000 rankings of 10 different types of sushi. For each ranking, we create 10 Boolean variables denoting whether an item was ranked among the top 5, and ignore their relative position. The logical constraints represent the selection of 5 out of 10 items. We split the dataset into 3,500 instances for training and 1,500 for the test set and evaluated the log-likelihood on both tasks. The plot in Figure 4.7b shows the log-likelihood for this data. For this dataset, we set $t = 30$ and $k = 3$ for ensembles of SamplePSDD. LearPSDD obtains superior performance accross some of the low sample sizes, but our approaches were able to quickly pick up and tie with LearnPSDD when using the LLW, stacking and EM strategies.

Preference Learning

We also evaluated performance on the original task of ranking items on the `sushi` dataset. We adopt the same encoding and methodology as (A. Choi, Broeck, *et al.*, 2015), where each ranking is encoded by a set of Boolean variables X_{ij} indicating whether the i-th item was ranked in the j-th position. We use same parameters for ensembles of SamplePSDD as the previous dataset and set $t = 30$ and $k = 3$. The test log-likelihood performance of each different method is shown in Figure 4.8a. The results are qualitatively similar to the previous experiments: SamplePSDD performed better than pure data approaches under low data yet achieved competitive results when given the full data. In this

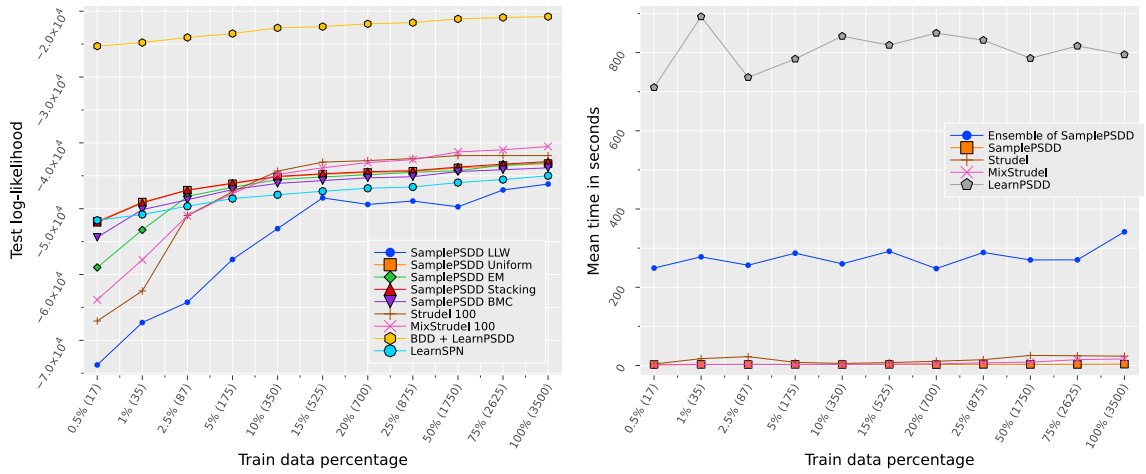


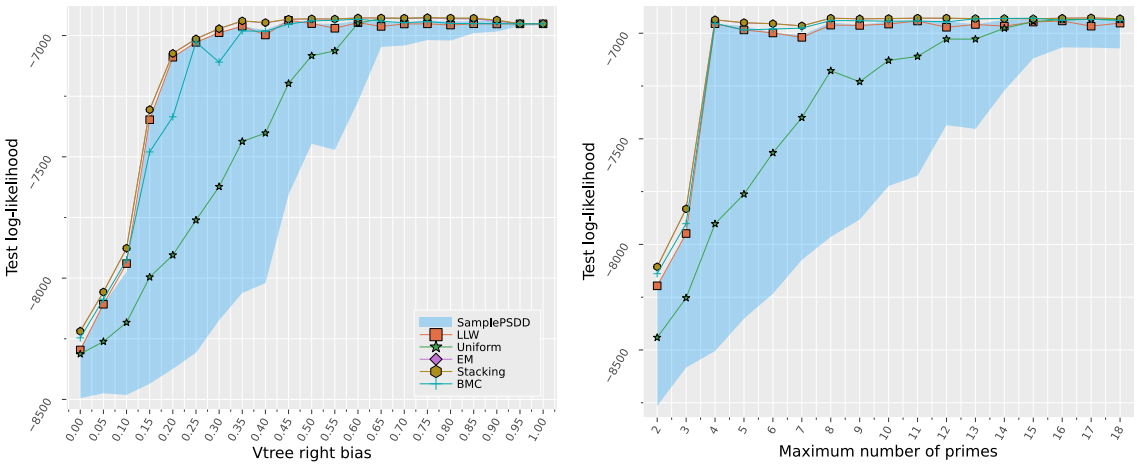
Figure 4.8: *Log-likelihood for the* `sushi` *ranking* ***(a)*** *dataset and curves for mean average time (in seconds) of learning a single* LearnPSDD *circuit, one* Strudel *circuit (CLT initialized), a mixture of 10 shared-structure* Strudel *components, a single* SamplePSDD *PC and an ensemble of 100* SamplePSDD *circuits.*

case, however, we found that LearnPSDD ranked first by a large margin compared to others.

Scalability, Complexity and Learning Time

The major advantage of SamplePSDD compared to other PSDD learning algorithms comes from its ability to learn from both data and a logical formula ϕ even when ϕ defines an intricate Boolean formula over many variables. Interestingly, how capable SamplePSDD is of learning from ϕ comes not only from the algorithm itself, but how ϕ is represented. In fact, any data structure with tractable restriction and reduction (to a canonical form) can be used in place of the BDD shown in Algorithm 18. We do not require forgetting to be tractable due to an implementational "trick" in SamplePSDD that allows a fast implementation to ignore variables not in the scope of the vtree. More details can be found in the supplemental material of Annex B.1. Consequently, how scalable our proposed algorithm is depends on the representational power of the tool used for manipulating logical formulae. This is shown more concretely when we learn from the constraints set by the `dota` dataset: had we tried to manipulate formulae with a CNF, the intractability of cardinality constraints would unfortunately impede any progress.

We no provide an analysis on the complexity of SamplePSDD. We start with the SamplePartialPartition subroutine. If we choose a BDD for manipulating formulae, then restrictions are done in $\mathcal{O}(c \log c)$, where c is the size of the BDD's graph. At every iteration of the main loop in line 5 of Algorithm 17, a leaf of the binary decision tree is split into two, increasing the number of leaves (and therefore primes) by one. This is repeated until k leaves of the decision tree have been expanded, bringing SamplePartialPartition's complexity to $\mathcal{O}(k \cdot c \log c)$. Every call of SamplePSDD (apart from base cases) produces a new partition and randomly compress and merge elements. Compression requires applying a disjunction over two primes, both of which are conjunctions of literals,



(a) **(b)**

Figure 4.9: *Impact of the structure of vtree (left) and number of bounded primes (right) on the test log-likelihood for the* 10*-choose-*5 `sushi` *dataset.*

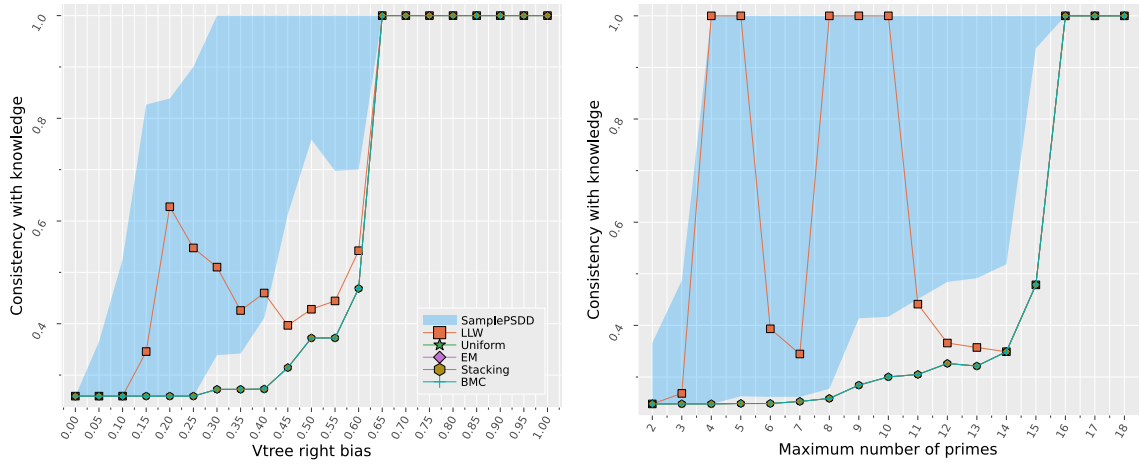
represented in BDDs as a graph of size linear to the number of terms. Because primes can have at most $\lceil \log_2(k) \rceil$, the disjunction of two such conjunctions is done in $\mathcal{O}(\log_2^2 k)$. Merging (or compressing) n elements essentially subtracts the number of recursive calls for each merge (or compression) by $n - 1$. Therefore, every SamplePSDD recursive call is $\mathcal{O}\left(k \cdot c \log c + \log_2^2 k\right)$.

We empirically evaluate the time it takes to learn a single circuit from each of LearnPSDD, Strudel and SamplePSDD. We also measure running times for learning 10 structure-sharing circuits as components of a mixture of Strudels and 100 (structurally) distinct PCs sampled from SamplePSDD, each with parameters learned from closed-form MLE. Figure 4.8b shows the time it takes to run each of these settings on the `sushi` ranking dataset. On average, Strudel took approximately 15 seconds, LearnPSDD 13 minutes and 25 seconds, and SamplePSDD about 2.76 seconds for learning a single PSDD.

Performance and Sampling Bias

The approximation quality of SamplePSDD is highly dependent on both the vtree and maximum number of primes. In this section, we compare the impact of both in terms of performance and circuit complexity. We assess performance by the log-likelihoods in the test set, as well as consistency with the original logical constraints. The latter is measured by randomly sampling 5,000 (possibly invalid) instances and evaluating whether the circuit correctly decides their value. A set of the top 100 sampled PSDDs (in terms of log-likelihood in the train set) are selected out of 500 circuits learned on the 10-choose-5 `sushi` dataset to compose the ensemble. Circuit complexity is estimated in terms of both time taken to sample all 500 circuits and graph size (i.e. number of nodes) of each individually generated PSDD.

It is quite clear that the structure of the vtree is tightly linked to the structure of a PSDD, especially given the graphical constraints imposed by SamplePSDD and the fact that subs need to obey a vtree's scope (and thus its structure). For instance, (near) right vtrees keep

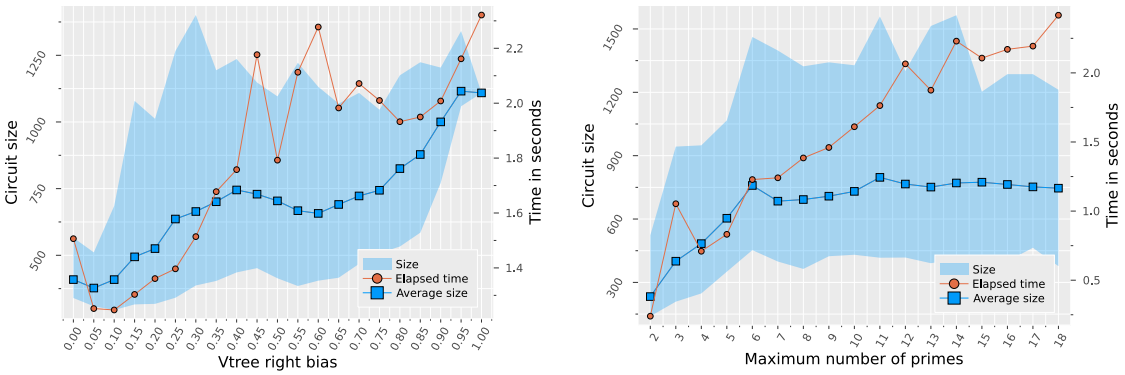


(a) (b)

Figure 4.10: *Impact of the structure of vtree (left) and number of bounded primes (right) on the consistency of sampled PSDDs with the original logical constraints for the* 10*-choose-*5 `sushi` *dataset.*

the number of primes fixed and require no approximation, while (near) left vtrees discard a large number of primes. In order to evaluate the effect of the type of vtree on the quality of sampled structures, we compared the performance of SamplePSDD as we vary the bias towards generation of right-leaning vtrees. Given a parameter p, we grow a vtree in a top-down manner where at each node we independently assign each variable to the right child with probability p. Small values of p produce left-leaning vtrees, while vtrees are more likely to lean to the right when $p > 0.5$. Left leaning vtrees produce especially small networks compared to other vtrees, as more variables are left unmentioned because of relaxations coming from the need for a bounded number of primes. To produce decently sized circuits, we increase the number of sampled primes k when p is low and decrease k when p is high.

Figure 4.9 shows the log-likelihood, Figure 4.10 shows consistency and Figure 4.11 shows circuit complexity when varying the bound on the number of primes (left) and the type of vtrees used for guiding the PSDD construction (right). The blue shaded area represents the interval of values (worse to best ranked) for individual circuits. To verify consistency, we evaluate the PSDDs in terms of satisfiability of a given example. An ensemble returned a configuration as satisfiable if any of its models attributed some nonzero probability to it; and unsatisfiable if all models gave zero probability. This evaluation gives a lower bound to consistency, which means all models eventually unanimously agreed on satisfiability when vtree right bias ≥ 0.65. Alternatively, since SamplePSDD is a relaxation of the original formula, an upper bound on consistency could be achieved by evaluating whether any model within the ensemble gave a zero probability to the example; this upper bound curve on consistency would be equivalent to the top side of the shaded area. Interestingly, we note that the likelihood weighting strategy (LLW) dominates over others on consistency. This is because LLW often degenerates to a few models, giving zero probability to lower scoring PSDDs, which means only a small subset of circuits decide on satisfiability, and thus a more relaxed model is less likely to disagree with the consensus. On the other hand, this does not translate to better data fitness on the general case, as we



(a) (b)

Figure 4.11: *Impact of the structure of vtree (left) and number of bounded primes (right) on circuit size (in number of nodes) and learning time (in seconds) for the* 10*-choose-*5 `sushi` *dataset.*

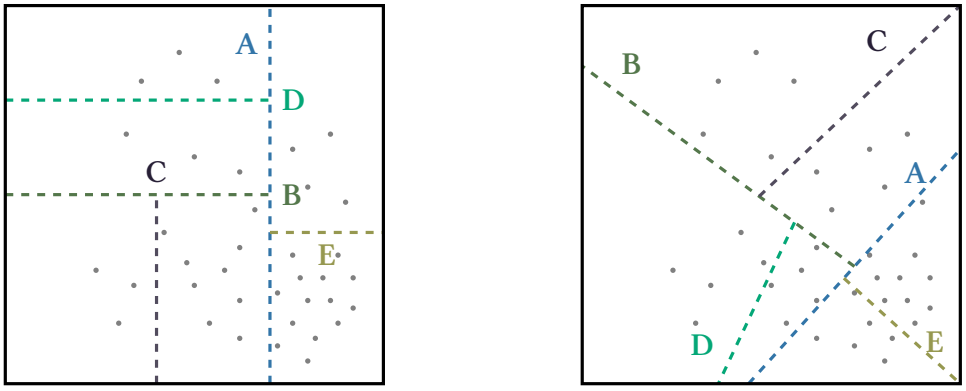
clearly see in Figures 4.6 to 4.8.

4.2 A Data Perspective

We now turn our attention to scalably learning a PC purely from data. Throughout this section, we introduce and motivate a novel approach to learning smooth and structure decomposable circuits by randomly partitioning the data space in a `DIV` class fashion. We show that our method produces competitive PCs at a fraction of the time. Before we go through with our proposal in detail, we must first lay the groundwork and motivate the decisions behind our structure learning algorithm. We begin by re-emphasizing the connection between probabilistic circuits and density estimation trees briefly discussed in Example 2.9. We follow by revisiting *random projections* (Freund *et al.*, 2008; Dasgupta and Freund, 2008), a well-known technique for hierarchically partitioning data through oblique hyperplanes. Next, we present in detail a very fast structure learning algorithm for quickly generating smooth and structure decomposable circuits. Despite their simplicity, we empirically show their competitive performance compared to state-of-the-art.

Recently, Correia *et al.* (2020) showed that (ensembles of) decision trees (DTs) learned for prediction tasks can be easily extended into full probabilistic models represented as probabilistic circuits. Besides equipping decision forests with more principles approaches to handling missing data and diagnosing outliers, this bridge between decision trees and PCs suggests an interesting alternative to learning the latter using the efficient inductive algorithms available for the former (Correia *et al.*, 2020; Ram and Gray, 2011; Khosravi, Vergari, *et al.*, 2020). Despite this, most works addressing such a connection have focused on the discriminative side of DTs, with much of the effort put onto classification rather than generative tasks such as density estimation. Here, we explore the generative side of DTs, often referred as density estimation trees (DETs, Ram and Gray, 2011; Hang and Wen, 2019; Smyth, Gray, *et al.*, 1995), within the framework of PCs, taking inspiration from known algorithms for building DTs and DETs, and transplanting them to PCs.

As shortly discussed in Example 2.9, a DET can be represented as a smooth and deterministic PC with only sums and input nodes, the latter's supports restricted to the



(a) *Axis-aligned projections* **(b)** *Random projections*

Figure 4.12: *Two partitionings induced by k-d trees:* ***(a)*** *shows axis-aligned splits and* ***(b)*** *random projection splits. Gray dots are datapoints, dashed lines are (hyper)planes.*

data cells induced by the partitioning data hyperplanes. The resulting density of this DET PC is given by

$$p_C(\mathbf{x}) = \sum_{\mathsf{L} \in \text{Inputs}(C)} w_{\mathsf{L}} \cdot \mathsf{L}(\mathbf{x}) \cdot [\![\mathbf{x} \in \mathsf{L}]\!],$$

where $[\![\mathbf{x} \in \mathsf{L}]\!]$ is an indicator function that returns 1 if $\mathbf{x}$ is within L's cell and 0 otherwise. The above formula comes from collapsing a circuit with only sum layers, where each sum corresponds to a latent variable representing a partitioning of the data, into a single-layer shallow PC. These latent variables usually consist of partitioning data through hyperplanes, dividing data into two parts, each represented as the subcircuit rooted at each child of the sum node.

A k-d tree is a subclass of decision trees which hierarchically partitions data into more or less equally sized parts, usually by splitting the data according to the value of a single variable at a time (Bentley, 1975; Hang and Wen, 2019; Ho, 1995), essentially producing axis-aligned hyperplanes. Dasgupta and Freund (2008) noted that such an approach cannot ensure that the resulting partitioning of the input space approximates the intrinsic dimensionality of data (roughly understood as a manifold of low dimension). In contrast, they provide a simple strategy for space partitioning that consists in recursively partitioning the space according to a random separating hyperplane. This approximates a random projection of the data and has the following theoretical guarantee (Dasgupta and Freund, 2008):

> If the data has intrinsic dimension d, then with constant probability the part of the data at level d or higher of the tree has average diameter less than half of the data.

Accordingly, the depth of the tree needs only to grow proportionally to the intrinsic dimension and not to the number of variables. In addition to that and to other theoretical insurances (Dhesi and Kar, 2010), the recursive partitioning scheme proposed is extremely fast, taking linearithmic time in the dataset size (number of instances and variables). Freund *et al.* (2008) further empirically show that employing random projections boosts performance significantly compared to regular axis-aligned projections.

Algorithm 19 SplitSID

Input Dataset $\mathbf{D} \subset \mathbb{R}^m$

Output A partition $\mathbf{S}_1, \mathbf{S}_2$ of $\mathbf{D}$

Let n be the number of examples in $\mathbf{D}$
Sample a random unit direction $\mathbf{w}$
Sort $\mathbf{a} = \mathbf{w} \cdot \mathbf{x}$ for $\mathbf{x} \in \mathbf{D}$ s.t. $a_1 \leq a_2 \leq \cdots \leq a_n$
for each $i \in [n-1]$ **do**
    $\mu_1 = \frac{1}{i} \sum_{j=1}^{i} a_i, \quad \mu_2 = \frac{1}{n-i} \sum_{j=i+1}^{n} a_i$
    $c_i = \sum_{j=1}^{i} (a_j - \mu_1)^2 + \sum_{j+1}^{n} (a_j - \mu_2)^2$
Find i that minimizes c_i and set $\theta = (a_i + a_{i+1})/2$
$\mathbf{S}_1 \longleftarrow \{\mathbf{x} \in \mathbf{D} : \mathbf{w} \cdot \mathbf{x} \leq \theta\}$
return $(\mathbf{S}_1, \mathbf{D} \setminus \mathbf{S}_1)$

Algorithm 20 SplitMax

Input Dataset $\mathbf{D} \subset \mathbb{R}^m$ and constant r

Output A partition $(\mathbf{S}_1, \mathbf{S}_2)$ of $\mathbf{D}$

Sample a random unit direction $\mathbf{w}$
Pick any $\mathbf{x} \in \mathbf{D}$ and let $\mathbf{y}$ be $\mathbf{x}$'s farthest point in $\mathbf{D}$
Sample δ uniformly in $[-c, c]$, where $c = r \cdot \text{dist}(\mathbf{x}, \mathbf{y}) / \sqrt{m}$
$\mathbf{S}_1 \longleftarrow \{\mathbf{x} \in \mathbf{D} : \mathbf{w} \cdot \mathbf{x} \leq \text{median}(\{\mathbf{z} \cdot \mathbf{w} : \mathbf{z} \in \mathbf{D}\}) + \delta\}$
return $(\mathbf{S}_1, \mathbf{D} \setminus \mathbf{S}_1)$

4.2.1 Random Projections

Let $\mathbf{D}$ a dataset with $\mathbf{X}$ variables. A function $f : \mathcal{X} \longrightarrow \{0, 1\}$ describes a hyperplane over variables in $\mathbf{X}$ and is here called a *rule*. A rule partitions data by assigning observations to either one, $\mathbf{S}_1 = \{\mathbf{x} \in \mathbf{D} : f(\mathbf{x}) = 0\}$, or the other, $\mathbf{S}_2 = \{\mathbf{x} \in \mathbf{D} : f(\mathbf{x} = 1\}$, of two data partitions. In k-d trees, this partitioning proceeds recursively until $|\mathbf{D}|$ is sufficiently small. When employing axis-aligned partitions, f typically selects the variable with the largest variance (or some other measure of spread) in $\mathbf{D}$ and separates instance according to the median value of that variable. The process is similar to the induction of decision trees, except that in this case the rules discriminate against a target variable (Breiman, 2001).

The statistical properties of estimates obtained from the instances at the leaves of a k-d tree depend on the rate at which the diameter of the partitions are reduced once we move down the tree. For a space of dimension m, a k-d tree induced by the process described might require m levels to halve the diameter of the original data (Dasgupta and Freund, 2008). This is true even for datasets of low intrinsic dimension. The latter is variously defined, and different definitions lead to different theoretical properties. A common surrogate metric is the *doubling dimension* of the dataset $\mathbf{D} \subset \mathbb{R}^m$, given by the smallest integer d such that the intersection of $\mathbf{D}$ and any ball of radius r centered at $\mathbf{x} \in \mathbf{D}$ can be covered by at most 2^d balls of radius $\frac{r}{2}$ (Dhesi and Kar, 2010).

Random Projection Trees (RPTrees) are a special type of k-d trees that split along a random direction of the space. Two such splitting rules are given by Algorithms 19

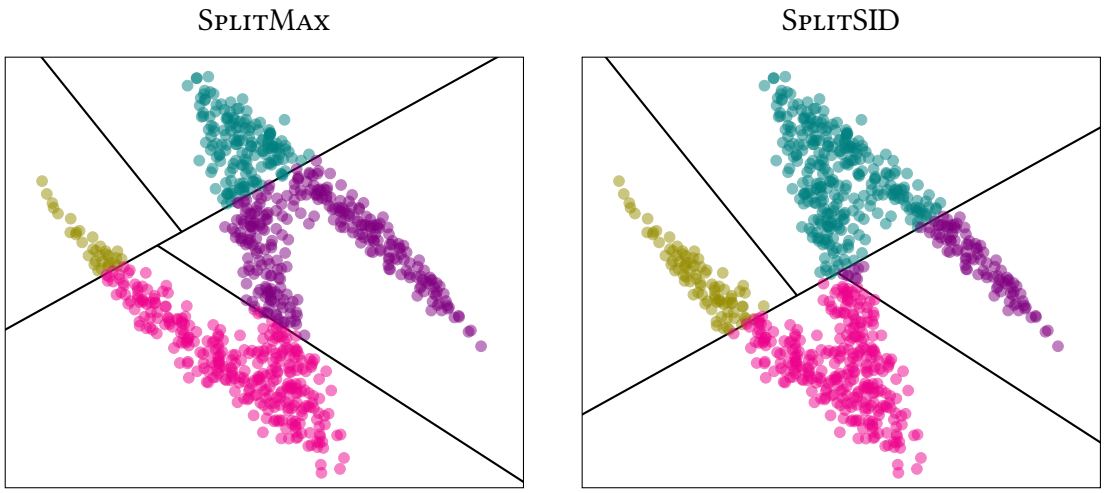


Figure 4.13: *Example of space partitioning by RPTrees grown using different split rules but the same random directions.*

and 20, where in the latter dist($\mathbf{x}, \mathbf{y}$) refers to the Euclidean distance. The intuition behind either rule is to generate a random hyperplane (unit direction) and then find a threshold projection value that roughly divides dataset $\mathbf{D}$ into two approximately equally sized subsets. Algorithm 19 attempts at finding such a threshold by minimizing the average squared interpoint distance (SID), while Algorithm 20 uses a random noise proportional to the average diameter of $\mathbf{D}$. As discussed by Dasgupta and Freund (2008) and by Freund *et al.* (2008), either optimizing or randomizing the threshold leads to better separation of data than simply selecting the median point. Figure 4.12 shows the difference between axis-aligned and random projections, while Figure 4.13 shows an example of space partitioning induced by 2-level RPTrees using each of the rules with the same direction vectors w. Note that the rules produce quite different splits despite using the same random directions.

Unlike standard k-d trees, RPTrees ensure that, for a data with doubling dimension d, at most d levels are necessary to half the diameter of the data, irrespective of its dimension. This leads to improved statistical properties that are connected to that notion of low intrinsic dimensionality (Dasgupta and Freund, 2008; Dhesi and Kar, 2010).

4.2.2 LearnRP

4.2.3 Experiments

A

Appendices

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

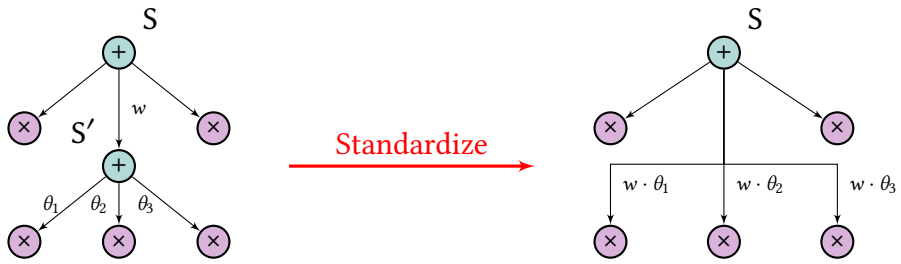
procedure until there are no more consecutive sum nodes. This results in a PC of the form

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

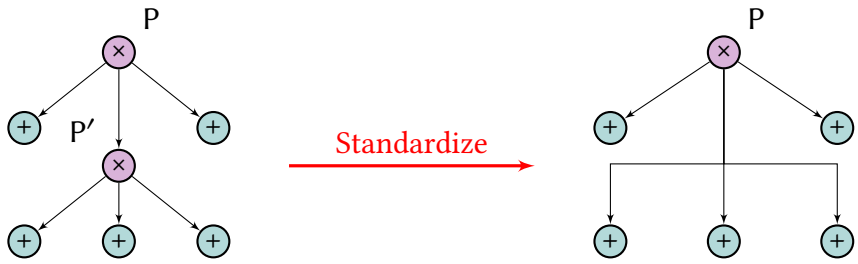
where $\mathrm{N} \in \mathbf{N}$. The number of children of the resulting root sum node will be exponential on the number of edges of its children. □

Theorem A.1.2 (Standardization). *Any probabilistic circuit $\mathcal{C}$ can be reduced to a circuit where every sum node contains only products or inputs and every product node contains only sums or inputs.*

Proof. If $\mathcal{C}$ is already standard we are done. Otherwise, there exists either (i) a sum node S with a sum S′ as child; or (ii) a product node P with a product P′ as child. We first address (i): let w be the weight of edge $\overrightarrow{\mathrm{S\,S'}}$ and θ_i the weights from all edges coming out from S′.



Connect S with every child of S′, assigning as weight $w \cdot \theta_i$ for each child i. Delete S′ and all edges coming out from it. The resulting circuit is computationally equivalent but now without a consecutive pair of sums. This transformation is visualized by the figure above. We do a similar procedure in (ii), but now instead remove P′ and connect all children of P′ to P, as we show below.



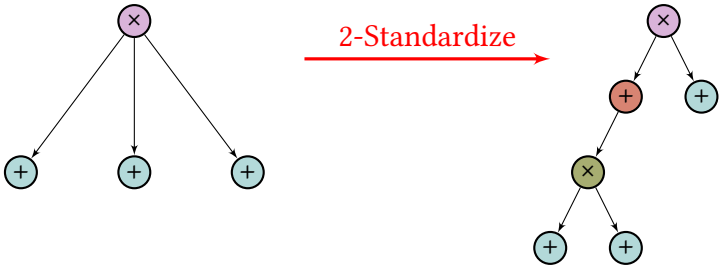
□

Theorem A.1.3 (2-Standardization). *Any probabilistic circuit $\mathcal{C}$ can be transformed into a circuit where every sum node contains only products or inputs and every product node contains only* two *sums or inputs.*

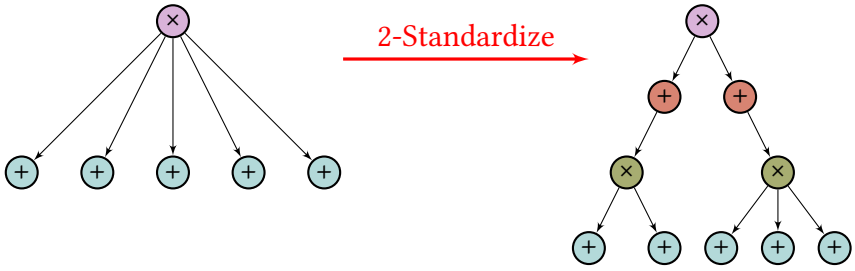
Proof. For sums, apply the same standardization procedure as theorem A.1.2. Let P a product and call $n = |\mathrm{Ch(P)}|$. If $n = 1$ and Ch(P) is a product, then remove P and connect

all previous parents of P with its child. If $n = 1$ and Ch(P) is not a product, remove P and apply the standardization procedure for sums on all of Pa(P).

For $n > 2$, we simply need to split into 2-products recursively. We prove this by induction. The base case is when $n = 2$, which is already done, or $n = 3$, in which case we need apply the transformation below.



Where ⊕ and ⊗ are newly introduced nodes. When $n > 3$, we create two products P_1 and P_2, each connected with a sum and product, and with $\lfloor \frac{n}{2} \rfloor$ and $\lceil \frac{n}{2} \rceil$ potential children. By the induction hypothesis, we can recursively binarize the subsequent grandchildren products.



As an example, we have $n = 5$ in the figure above. We introduce the sums ⊕ and products ⊗ and then recursively apply the transformation again on the ⊗s.

When Ch(P) are product nodes we do the same procedure as before, but with the added post-process addition of a sum node connecting ⊗ to every Ch(P). □

Theorem 2.2.1 (Poon and P. Domingos, 2011; Y. Choi, Vergari, and Van den Broeck, 2020; Vergari, Y. Choi, *et al.*, 2021)**.** *Let $\mathcal{C}$ a* smooth *and* decomposable *PC. Any one of EVI, MAR or CON can be computed in linear time (in the number of edges of $\mathcal{C}$).*

Proof. For a sum node S, we have the following marginalization query

$$\begin{aligned}\int \mathrm{S}(\mathbf{x}, \mathbf{y})\, d\mathbf{y} &= \int \sum_{\mathrm{C} \in \mathrm{Ch}(\mathrm{S})} w_{\mathrm{S},\mathrm{C}}\, \mathrm{C}(\mathbf{x}, \mathbf{y})\, d\mathbf{y} \\ &= \sum_{\mathrm{C} \in \mathrm{Ch}(\mathrm{S})} w_{\Sigma,\mathrm{C}} \int \mathrm{C}(\mathbf{x}, \mathbf{y})\, d\mathbf{y}.\end{aligned}$$

Analogously, for a product node

$$\int \mathrm{P}(\mathbf{x}, \mathbf{y})\, d\mathbf{y} = \int \prod_{\mathrm{C} \in \mathrm{Ch}(\mathrm{P})} \mathrm{C}(\mathbf{x}, \mathbf{y})\, d\mathbf{y} = \prod_{\mathrm{C} \in \mathrm{Ch}(\mathrm{P})} \int \mathrm{C}(\mathbf{x}, \mathbf{y})\, d\mathbf{y}.$$

This ensures that marginals are pushed down to children. This can be done recursively until C is an input node L_p, in which case we marginalize $\mathbf{y}$ according to p, which by definition should be tractable and here we assume can be done in $\mathcal{O}(1)$. We have proved the case for MAR. For EVI, we simply assign $\mathbf{y} = \emptyset$ with input nodes acting as probability density functions. Conditionals can easily be computed by an EVI or MAR followed by a second pass marginalizing the conditional variables $p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{x},\mathbf{y})}{p(\mathbf{y})}$ which are both done in linear time as we have seen here. □

Theorem 2.2.2 (Peharz, Gens, Pernkopf, *et al.*, 2016)**.** *Let $\mathcal{C}$ a smooth, decomposable and* deterministic *PC. MAP is computable in linear time (in the number of edges of $\mathcal{C}$).*

Proof. For a sum node S, we want to compute the following query

$$\max_{\mathbf{y}} \mathrm{S}(\mathbf{y}|\mathbf{x}) = \frac{1}{\mathrm{S}(\mathbf{x})} \max_{\mathbf{y}} \mathrm{S}(\mathbf{y}, \mathbf{x}) = \frac{1}{\mathrm{S}(\mathbf{x})} \max_{\mathbf{y}} \sum_{\mathrm{C} \in \mathrm{Ch}(\mathrm{S})} w_{\mathrm{S,C}}\, \mathrm{C}(\mathbf{y}, \mathbf{x}),$$

yet notice that for any assignment of $\mathbf{x}$ and $\mathbf{y}$ only one $\mathrm{C} \in \mathrm{Ch}(\mathrm{S})$ must have a nonnegative value by the definition of determinism, so we may replace the summation with a maximization over the children, giving

$$\max_{\mathbf{y}} \mathrm{S}(\mathbf{y}|\mathbf{x}) = \frac{1}{\mathrm{S}(\mathbf{x})} \max_{\mathbf{y}} \max_{\mathrm{C} \in \mathrm{Ch}(\mathrm{S})} w_{\mathrm{S,C}}\, \mathrm{C}(\mathbf{y}, \mathbf{x}) = \frac{1}{\mathrm{S}(\mathbf{x})} \max_{\mathrm{C} \in \mathrm{Ch}(\mathrm{S})} \max_{\mathbf{y}} w_{\mathrm{S,C}}\, \mathrm{C}(\mathbf{y}, \mathbf{x}).$$

For a product node P, we compute

$$\max_{\mathbf{y}} \mathrm{P}(\mathbf{y}|\mathbf{x}) = \frac{1}{\mathrm{P}(\mathbf{x})} \max_{\mathbf{y}} \mathrm{P}(\mathbf{y}, \mathbf{x}) = \frac{1}{\mathrm{P}(\mathbf{x})} \max_{\mathbf{y}} \prod_{\mathrm{C} \in \mathrm{Ch}(\mathrm{P})} \mathrm{C}(\mathbf{y}, \mathbf{x}) = \frac{1}{\mathrm{P}(\mathbf{x})} \prod_{\mathrm{C} \in \mathrm{Ch}(\mathrm{P})} \max_{\mathbf{y}} \mathrm{C}(\mathbf{y}, \mathbf{x}).$$

This is equivalent to an inductive top-down pass where we maximize instead of sum until we reach all input nodes, in which case we simply maximize the supposedly tractable functions. Once these are computed, we unroll the induction, maximizing over all values. □

Theorem 2.3.1 (Y. Choi, Vergari, and Broeck, 2020)**.** *If $\mathcal{C}$ is a smooth and structure decomposable probabilistic circuit with vtree $\mathcal{V}$, and $\mathcal{L}$ a structure decomposable logic circuit also respecting $\mathcal{V}$, then $\mathbb{E}_{\mathcal{C}}[\mathcal{L}]$ is polynomial time computable (in the number of edges).*

Proof. For completeness, we show the proof of this claim as stated in Y. Choi, Vergari, and Broeck, 2020. We assume, without loss of generality, that the layers of both $\mathcal{C}$ and $\mathcal{L}$ are compatible, i.e. they both have the same number of layers and if the i-th layer of $\mathcal{C}$ is made out of sums (resp. products), then the i-th layer of $\mathcal{L}$ is made out of disjunctions

(resp. conjunctions). The expectation $\mathbb{E}_{\mathcal{C}}[\mathcal{L}]$ has the following form when the root of $\mathcal{C}$ is a product

$$\begin{aligned}\mathbb{E}_{\mathcal{C}}[\mathcal{L}] &= \int \mathcal{C}(\mathbf{x})\mathcal{L}(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int \left(\mathcal{C}_p(\mathbf{x})\mathcal{C}_s(\mathbf{x})\right)\left(\mathcal{L}_p(\mathbf{x})\mathcal{L}_s(\mathbf{x})\right)\mathrm{d}\mathbf{x} \\ &= \int \left(\mathcal{C}_p(\mathbf{x})\mathcal{L}_p(\mathbf{x})\right)\left(\mathcal{C}_s(\mathbf{x})\mathcal{L}_s(\mathbf{x})\right)\mathrm{d}\mathbf{x} = \int \left(\mathcal{C}_p(\mathbf{x})\mathcal{L}_p(\mathbf{x})\right)\mathrm{d}\mathbf{x} \int \left(\mathcal{C}_s(\mathbf{x})\mathcal{L}_s(\mathbf{x})\right)\mathrm{d}\mathbf{x} \\ &= \mathbb{E}_{\mathcal{C}_p}\left[\mathcal{L}_p\right] \cdot \mathbb{E}_{\mathcal{C}_s}\left[\mathcal{L}_s\right],\end{aligned}$$

where the subscript p and s indicate the prime and sub of a node. When the root is a sum

$$\begin{aligned}\mathbb{E}_{\mathcal{C}}[\mathcal{L}] &= \int \mathcal{C}(\mathbf{x})\mathcal{L}(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int \left(\sum_{\mathrm{C}'\in\mathrm{Ch}(\mathcal{C})} w_{\mathcal{C},\mathrm{C}'}\,\mathrm{C}'(\mathbf{x})\right)\left(\sum_{\mathrm{C}''\in\mathrm{Ch}(\mathcal{L})} \mathrm{C}''(\mathbf{x})\right)\mathrm{d}\mathbf{x} \\ &= \int \sum_{\mathrm{C}'\in\mathrm{Ch}(\mathcal{C})}\sum_{\mathrm{C}''\in\mathrm{Ch}(\mathcal{L})} w_{\mathcal{C},\mathrm{C}'} \cdot \mathrm{C}'(\mathbf{x}) \cdot \mathrm{C}''(\mathbf{x})\,\mathrm{d}\mathbf{x} = \sum_{\mathrm{C}'\in\mathrm{Ch}(\mathcal{C})}\sum_{\mathrm{C}''\in\mathrm{Ch}(\mathcal{L})} w_{\mathcal{C},\mathrm{C}'} \int \mathrm{C}'(\mathbf{x})\,\mathrm{C}''(\mathbf{x})\,\mathrm{d}\mathbf{x} \\ &= \sum_{\mathrm{C}'\in\mathrm{Ch}(\mathcal{C})}\sum_{\mathrm{C}''\in\mathrm{Ch}(\mathcal{L})} w_{\mathcal{C},\mathrm{C}'} \cdot \mathbb{E}_{\mathrm{C}'}\left[\mathrm{C}''\right].\end{aligned}$$

Therefore, if expectation is tractable for input nodes, then expectation is tractable for the whole circuit. □

B

Annexes

B.1 Learning PSDDs Under Logic Constraints by Sampling and Averaging

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B.2 Fast And Accurate Learning of PCs by Random Projections

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