

### Mobile Robot Self-Driving Through Image Classification Using Discriminative Learning of Sum-Product Networks

**Undergraduate Thesis** 

Student: Renato Lui Geh

Advisor: Prof. Denis Deratani Mauá

# INSTITUTE OF MATHEMATICS AND STATISTICS UNIVERSITY OF SÃO PAULO

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### **Abstract**

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Driving has proven to be a very difficult task for machines to emulate, not only due to the inherent complexity of the problem but also because of the need for accurate real-time predictions. Nonetheless, recent advances in computer vision and machine learning have shown promising results in the real-world. Mobile robots are low-cost miniature computers with limited processing power and memory. The problem of self-driving can be similarly applied to the mobile robot domain as a down-scaled version of the same task, with an additional hardware constraint. Sum-product networks are probabilistic graphical models capable of representing tractable probability distributions containing a great number of variables. Exact inference is asymptotically linear to the number of edges in the network's graph, and its deep architecture is capable of representing a wide range of distributions. In this work, we attempt to model autonomous driving by using sum-product networks on a small mobile robot. We model this task as an imitation learning problem through image classification. We present accuracy results on an artificial self-driving dataset for different sum-product network learning algorithms, providing a comparative study not only for different network architectures, but also discriminative and generative models. Finally, we provide a real-world mobile robot implementation on a miniature computer.

**Keywords:** sum-product networks, probabilistic graphical models, machine learning, robotics

### **Abbreviations**

DAG	Directed	acvelie	graph
DI10	Diffettu	acyciic	graph

- EM Expectation-maximization
- GD Gradient descent
- IV Indicator variable
- MAP Maximum a posteriori probability
- MPE Most probable explanation
- MPN Max-product network
- PGM Probabilistic graphical model
  - RV Random variable
- SGD Stochastic gradient descent
- SPN Sum-product network
- SPT Sum-product tree

# Symbols and notations

- $\mu$  Gaussian distribution mean
- $\sigma$  Gaussian distribution standard deviation
- X Sample space of random variables
- Z Partition function
- $\phi$  Factor (potential)
- [X = x] Indicator function for random variable valuation X = x

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# **Chapter 1**

### Introduction

In this chapter we first describe the motivations and objectives of this thesis. Next, we describe the structure of this document.

#### 1.1 Motivation and objectives

Self-driving is a challenging computer vision task, mainly due to its inherent complexity and the necessity for real-time decision making. Although there have been many promising results the past few years on autonomous driving, the task still relies on the underlying problem of following a pathway through visual cues (usually road markings). A possible approach to this task is through imitation learning by means of image classification. That is, the agent tasked with driving should be able to reliably mimic human behavior by correctly classifying whether to turn, stop or go straight given an image captured in front of the car.

Mobile robots are low cost machines capable of movement. These robots are usually small, and because of their size and cost often don't have the same performance capabilities as a desktop computer. However, these domain traits make mobile robot self-driving a very similar analogue to real-world autonomous cars. Processing power and memory constraints play a big role in this case, and translate well to embedded systems present in a self-driving car.

Sum-product networks (SPNs) are probabilistic graphical models that are able to represent a wide range of tractable probability distributions of many variables. SPNs have shown impressive results in several domains, and particularly that of image classification. Their deep architecture seems to capture features and contexts well, and since inference is computed in time linear to the network's edges, SPNs are promising models for fast inference in self-driving.

In this work, we attempt to model self-driving of mobile robots through image classification. For the task of classification our objective is to use sum-product networks learned discriminatively, though we also give results for generative SPNs, comparing not only generative and discriminative learning, but also different SPN architectures.

#### 1.2 Thesis structure

This thesis is structured as follows. In chapter 2, we first provide background on sum-product networks, where we formally define an SPN, present key properties on their structure, explain how to compute exact inference and find an approximation of the maximum a posteriori probability (MAP).

In chapter 3, we show how to compute the partial derivatives with respect to a sub-SPN and to its weights, leading on how to perform gradient descent and then on learning the weights of the network through gradient descent both generatively and discriminatively.

chapter 4 is dedicated to algorithms for learning the structure of an SPN. We explain the two structural learning algorithms that were used in the experiments.

For ??, we first show how we model self-driving as an image classification problem. We then specify the architecture of the robot used in the experiments, giving specifications on the hardware and software used. Furthermore, we describe some concepts of control we use for navigation.

In ??, we provide classification results on many image classification datasets from various domains with different learning algorithms. We then describe the self-driving dataset used for training, and give in-dataset accuracies as well as real-world empirical results on the mobile robot itself.

Finally, in ?? we give our conclusions and provide some discussion of the results.

There is an additional section of this thesis in which we give a brief subjective insight on the work done for this thesis. We also list subjects we deemed important for the work done in this thesis.

Furthermore, ?? contains all proofs done in this thesis.

## **Chapter 2**

### **Sum-product networks**

In this chapter we provide some background concepts needed for defining a sumproduct network. Once this is covered, we formally define an SPN, list some interesting properties on their structure, and describe how to perform exact inference (i.e. extract the probability of evidence of some valuation) and how to find an approximation of the maximum a posteriori probability.

We leave all proofs in ??.

#### 2.1 Background

The objective of probabilistic modelling is to compactly represent a probability distribution, be able to find a good approximation to the real function and be able to efficiently compute both the marginals and modes. Probabilistic graphical models (PGMs) attempt to solve this through the use of graphs, representing distributions as a normalized product of factors (Pearl, 1988).

$$P(X = x) = \frac{1}{Z} \prod_{k} \phi_k(x_{\{k\}})$$

Where  $x \in \mathcal{X}$  is a d-dimensional vector valuation of RVs X on sample space  $\mathcal{X}$ , and factor (also called a potential)  $\phi_k$  is a function mapping instantiations of X to a non-negative number. Z is the partition function  $Z = \sum_{x \in \mathcal{X}} \prod_k \phi_k(x_{\{k\}})$  that sums out all variables and normalizes the term above it to the [0,1] range.

A downside of this representation is that inference is exponential on the worst case, which makes learning also exponential, as it uses inference as a subroutine. To get around this problem, Darwiche proposed in Darwiche, 2003 the notion of *network polynomial*.

A network polynomial is a function over the probabilities of each instantiation. Let  $\Phi(x)$  be a probability distribution. The network polynomial of  $\Phi(x)$  is the function  $f = \sum_{x \in \mathcal{X}} \Phi(x) \Pi(x)$ , where  $\Pi(x)$  is the product of the IVs of each variable on instantiation x,

where each indicator variable [Y = y] has a value of zero if  $Y \neq y$  in x and a value of one otherwise (i.e. if Y = y in x or  $Y \notin x$ ).

As an example, take the bayesian network  $\mathcal{N}=A\to B$  with binary variables. Let  $\lambda_a$ ,  $\lambda_{\overline{a}}$ ,  $\lambda_b$  and  $\lambda_{\overline{b}}$  be the indicator variables for when A=1, A=0, B=1 and B=0 respectively. The network polynomial of  $\mathcal{N}$  is the expression

$$f_{\mathcal{N}} = P(a)P(b|a)\lambda_a\lambda_b + P(a)P(\overline{b}|a)\lambda_a\lambda_{\overline{b}} + P(\overline{a})P(b|\overline{a})\lambda_a\lambda_{\overline{b}} + P(\overline{a})P(\overline{b}|\overline{a})\lambda_{\overline{a}}\lambda_{\overline{b}}.$$

The main advantage of this representation is to avoid recomputing terms. For instance, take an instantiation of  $x = \{A = 0\}$ . Then, the network polynomial will be as follows.

$$f_{\mathcal{N}}(x) = P(a)P(b|a) \cdot 0 \cdot 1 + P(a)P(\overline{b}|a) \cdot 0 \cdot 1 + P(\overline{a})P(b|\overline{a}) \cdot 1 \cdot 1 + P(\overline{a})P(\overline{b}|\overline{a}) \cdot 1 \cdot 1 =$$

$$= P(\overline{a})P(b|\overline{a}) + P(\overline{a})P(\overline{b}|\overline{a})$$

Which means we can avoid computing values from the two first terms. We can also compute the network polynomial of some unnormalized probability distribution as long as we divide by the partition function, defined as the network polynomial with all indicators set to one. Although the network polynomial has exponential size in terms of variables, computing the probability of evidence is linear in its size. By representing the network polynomial as an arithmetic circuit of sums and products, one can prove that the cost of inference is indeed polynomial.

#### 2.2 Definitions and properties

Sum-product networks borrow many concepts from network polynomials and arithmetic circuits. There are many definitions of SPNs and in this thesis we present two. The first definition is given by the seminal article Poon and Domingos, 2011, and can be seen as a more low-level approach to defining the network. The second, based on Gens and Domingos, 2013, is a stronger definition, but one which we will use more throughout this thesis, as it lends itself better to continous data.

Let  $X = \{X_1, X_2, \dots, X_n\}$  be the set of all variables. We shall call this set the root scope. Let G be a graph G. The sets of vertices and edges of G will be denoted by V(G) and E(G). We will call Ch(n) and Pa(n) the sets of children and parents of node  $n \in V(G)$ .

**Definition 2.1** (Sum-product network; Poon and Domingos, 2011). A sum-product network (SPN) over variables  $X_1, X_2, \ldots, X_n$  is a DAG whose leaves are indicator variables  $[X_1 = x_1^1], [X_2 = x_2^1], \ldots, [X_n = x_n^1], \ldots, [X_1 = x_1^d], [X_2 = x_2^d], \ldots, [X_n = x_n^d]$ . Its internal nodes are weighted sums or products. Each edge coming out from a sum node n to another node j has a non-negative weight associated with it. We denote such weight by  $w_{n,j}$ . The value of a sum node n is  $v_n = \sum_{j \in Ch(n)} w_{n,j}v_j$ , where  $v_j$  is the value of node j. The value of a product node n is  $v_n = \prod_{j \in Ch(n)} v_j$ . The value of a leaf node is the value of the indicator variable. The value of the SPN is the value of its root node.

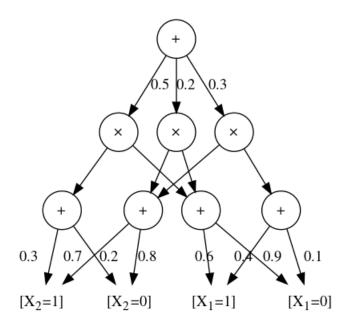


Figure 2.1: An example of an SPN.

Throughout this thesis, we denote by S(X = x) the value of an SPN S given evidence x. A sub-SPN  $S_n$  of S is the subgraph of S rooted at n. A node in an SPN is itself an SPN. When all indicator variables are set to one, the value of S is denoted by S(\*). The scope of an SPN S, denoted by Sc(S), is the union set of all scopes of its children. A leaf's scope is the scope of its IV.

**Definition 2.2** (Validity). An SPN is valid iff, for all evidence E = e,  $S(E = e) = \Phi_S(E = e)$ , where  $\Phi_S$  is an unnormalized probability distribution.

**Definition 2.3** (Completeness). An SPN is complete iff all children of the same sum node have the same scope.

**Definition 2.4** (Consistency). An SPN is consistent iff no variable appears with a value v in one child of a product node and valued u, with  $u \neq v$ , in another.

Validity in an SPN means that the network correctly and efficiently computes the probability of evidence of the distribution it represents. In this document we only work with valid SPNs, as we wish to always compute exact inference. However, non-valid SPNs are an interesting field of research for approximate inference in SPNs.

A sufficient condition for validity is completeness and consistency. Yet whilst this condition is sufficient, it is not necessary, as the converse (i.e. an incomplete and inconsistent valid SPN) can hold.

**Theorem 2.1** (Poon and Domingos, 2011). An SPN is valid if it is complete and consistent.

When an SPN S is valid, then S(\*) is the partition function, and we can extract the probability of evidence from an SPN by computing P(X = x) = S(x)/S(\*). If for every sum node all of their weights are non-negative and sum to one, then the partition function is S(\*) = 1, and the SPN is the distribution itself.

**Corollary 2.1** (Validity recursion; Poon and Domingos, 2011). *If an SPN S is valid, then* 

all sub-SPN of S is valid.

**Definition 2.5** (Decomposability). An SPN is decomposable iff no variable appears in more than one child of a product node.

In other words, an SPN is decomposable if and only if, for every product node, every child node has disjoint scopes with relation to all their other siblings. It is easy to see that decomposability implies in consistency, as there can be no inconsistency between product children since scopes are disjoint. Therefore, a complete and decomposable SPN is valid. Indeed it is much easier to produce decomposable SPNs then only consistent ones, and although this condition may seem too strong and restrictive, Peharz et al., 2015 showed that a consistent SPN is representable by a polynomially larger decomposable SPN.

So far, SPNs are restricted to the discrete domain, as we rely on IVs to define possible valuations to variables. We can generalize SPNs to the continuous by assuming an infinite number of IVs and thus replacing sum nodes whose children are IVs with integral nodes. A leaf node then becomes an integral node with infinite IVs as children. Particularly, it represents an unnormalized univariate probability distribution, such as a Gaussian. The value of this integral node n becomes the fdp  $p_n(x)$ . This extension brings us to a second definition of SPNs.

**Definition 2.6** (Sum-product networks; GENS and DOMINGOS, 2013). A sum-product network is defined recursively as follows.

- 1. A tractable univariate probability distribution is an SPN.
- 2. A product of SPNs with disjoint scopes is an SPN.
- 3. A weighted sum of SPNs with the same scope is an SPN, provided all weights are positive.
- 4. Nothing else is an SPN.

This second definition limits our scope to only complete and decomposable SPNs. Note that an IV is also an SPN, as we can assume that an indicator variable is a degenerate tractable univariate distribution, taking a value of one if it agrees with the given evidence and zero otherwise.

#### 2.3 Inference

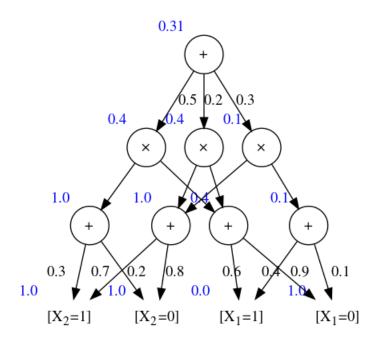
Throughout this thesis we assume that all sum nodes are normalized and sum to one, meaning the partition function is S(\*) = 1 and the SPN's value is the probability itself.

Let  $X = \{X_1 = x_1, X_2 = x_2, \dots, X_k = x_k\}$  be a valuation and S be an SPN. We say that X is a complete valuation if Sc(X) = Sc(S). That is, X contains a valuation for all variables in S. An incomplete valuation has some variable assignment missing.

Computing the probability of evidence is done through a bottom-up backwards pass through the SPN. To find the value of an SPN, we must know the value of the root node, which depends on all nodes below it. This is done through a topological traversal of the graph.

Finding the value of a leaf node depends on the valuation given. Let n be a leaf node, and  $Sc(n) = \{X_j\}$ . Let X be some valuation. Assuming the univariate probability distribution of n has fpd  $p_n(x)$ , then if X has a valuation  $X_j = x_j$ , the value of node n will be  $S_n(X) = p_n(x_j)$ . If X has no valuation for variable  $X_j$ , then  $S_n(X)$  is the distribution's mode. Note that this holds for indicator variables, as if X has a valuation for  $X_j = x_j$  and the IV matches with  $x_j$ , then  $p_n(x_j) = 1$ . In case it does not,  $p_n(x_j) = 0$ . For the incomplete case, the mode of an indicator variable is one, which holds the equivalence.

Once we compute leaf nodes, we can compute each internal node's values by following the topological order until we reach the root. For sum nodes, we compute the weighted sum  $S_n(X) = \sum_{j \in Ch(n)} w_{n,j} S_j(X)$ , and for products  $S_n(X) = \prod_{j \in Ch(n)} S_j(X)$ .



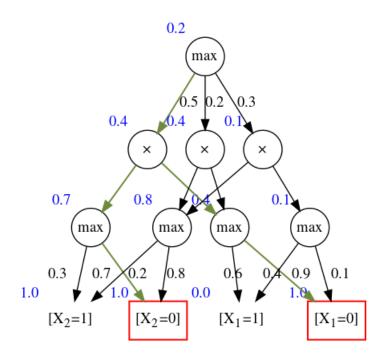
**Figure 2.2:** Computing the probability of evidence on a sample SPN.

Figure 2.2 shows the value of the SPN in Figure 2.1 given a valuation  $X = \{X_1 = 0\}$ . Values in blue are the values of each sub-SPN. Finding the probability of evidence P(X = x) is fast, as computing the value of an SPN is linear to the number of edges of the graph.

Additionally, we might want to find the probability that maximizes a certain valuation, i.e. the maximum a posteriori probability (MAP). To compute the approximate value of the MAP of some valuation X, we first transform the SPN into a max-product network (MPN) by replacing all sums with max nodes. The value of a max node is the maximum value of its weighted children. More formally, the value of an MPN's max node n is given by  $M_n(X) = \max_{j \in Ch(n)} w_{n,j} M_j(X)$ . Other nodes behave identically to an SPN. The computed value of an MPN is an approximation of  $\max_y P(X = x, Y = y)$ , where X is incomplete and Y is the set of variables that are missing. This is called the max-product algorithm.

In SPNs, computing the exact MAP was shown to be NP-hard (Peharz et al., 2015; Conaty et al., 2017; Mei et al., 2018), and better approximation algorithms were proposed as an alternative to the max-product algorithm described here. However, in this thesis,

when we talk about computing the (approximate) MAP, we are referring to the usual max-product algorithm.



**Figure 2.3:** *Computing the approximate MAP of an SPN through its MPN.* 

Once the MPN values are computed, we can find the most probable explanation (MPE) of the distribution given an evidence. This is done through a top-down forward pass, where we take a maximum sub-circuit path of the MPN by always taking the max path at a max node and taking all paths on a product node. The MPE are the maximum sub-circuit leaves' instantiations.

Figure 2.3 shows the MPN of the SPN shown in Figure 2.1 given  $X = \{X_1 = 0\}$ , where the numbers in blue represent the MPN values at each node, green arrows indicate the sub-circuit of maximum value and red boxes indicate the most probable valuations given evidence. The resulting MPE  $\arg\max_{y\in\mathcal{Y}}P(X=\{X_1=0\},Y=y)$  is the valuation  $\{X_1=0,X_2=0\}$ .

Therefore, computing the probability of evidence, which is also called *soft* inference, of an SPN is done through a single bottom-up pass. Similarly, computing the MAP probability, refered to as *hard* inference, is done through a bottom-up pass on the SPN's MPN. On the other hand, finding the MPE valuations requires a bottom-up pass to first compute the MAP, and then a top-down search to find the most probable instantiations.

We provide next pseudocode for computing both soft and hard inference. We assume as input only valid, (weight) normalized SPNs. However, one could easily extend the included algorithms for unnormalized networks.

16:

#### Algorithm 1 SoftInference: Computes the probability of evidence in SPNs

**Input** A valid SPN *S* with normalized weights and a valuation *X* 

**Output** The soft inference values at each node  $S_n$ 

```
Initialize S_n = 0
     Find topological order T of S
    for each node n \in S from T do
         if n is a leaf node then
              Let Sc(n) = \{X_k\}, p_n(x) be n's fdp and \hat{p}_n be p_n's mode
 5:
             if X_k \in X then
 6:
 7:
                   Let x_k be X_k's value in X
 8:
                   S_n \leftarrow p_n(x_k)
             else
 9:
                   S_n \leftarrow \hat{p}_n
10:
         else if n is sum node then
11:
12:
             for all j \in Ch(n) do
                   S_n \leftarrow S_n + w_{n,j}S_j
13:
         else
14:
             for all j \in Ch(n) do
15:
```

#### Algorithm 2 HardInference: Computes an approximation of the MAP in SPNs

**Input** A valid SPN *S* with normalized weights and a valuation *X* 

**Output** The hard inference values at each node  $M_n$ 

 $S_n \leftarrow S_n \cdot S_i$ 

17: **return** each  $S_n$  node value

```
Let M be S's MPN
     Initialize M_n = 0
     Find topological order T of M
 4: for each node n \in M from T do
        if n is a leaf node then
              Let Sc(n) = \{X_k\}, p_n(x) be n's fdp and \hat{p}_n be p_n's mode
 6:
             if X_k \in X then
 7:
                  Let x_k be X_k's value in X
 8:
 9:
                   M_n \leftarrow p_n(x_k)
             else
10:
                   M_n \leftarrow \hat{p}_n
11:
        else if n is sum node then
12:
             for all j \in Ch(n) do
13:
                   M_n \leftarrow \max(M_n, w_{n,j}M_j)
14:
        else
15:
             for all j \in Ch(n) do
16:
                   M_n \leftarrow M_n \cdot M_i
17:
18: return each M_n node value
```

Finally, we show how to algorithmically compute the MPE given some evidence.

#### Algorithm 3 ArgMaxSPN: Finds the MPE of a valuation on an SPN

**Input** A valid SPN S with normalized weights and a valuation X **Output** The arg max values of each variable according to X

```
1: M \leftarrow \mathsf{HardInference}(S, X)
2: Let Y be a copy of X
3: Let Q be a queue
4: Push S into Q
5: for each node n \in M in Q do
        if n is a leaf node then
6:
             Let Sc(n) = \{X_k\} and p_n(x) be n's fdp
7:
             Let \hat{x} = \arg \max_{x_k} p_n(x_k) be p_n's maximum valuation
8:
            if X_k \notin X then
9:
                  Y \leftarrow Y \cup \{X_k = \hat{x}\}\
10:
        else if n is sum node then
11:
             Push maximum child M_j, j \in Ch(n) into Q
12:
        else
13:
             Push all children j \in Ch(n) into Q
14:
15: return Y
```

## **Chapter 3**

### Parameter learning

The objective of this chapter is to expose the ideas behind generative and discriminative gradient descent for parameter learning of sum-product networks. We first show how to derive the SPN with respect to its nods and weights so that we can find the gradient of the SPN wrt its parameters (i.e. weights). This allows us to find the weight updates needed for gradient descent on SPNs. We then describe how to perform generative stochastic gradient descent, and finally discriminative gradient descent.

#### 3.1 Derivatives

Let *S* be an SPN. We are only interested in finding the derivative of internal nodes, as leaf nodes have no weights to be updated. Our objective is to find the gradient  $\partial S/\partial W$  by computing each component  $\partial S/\partial W_{n,j}$ , allowing us to find each weight update on the SPN.

At each weighted edge  $(n \to j, w_{n,j})$ , the derivative  $\partial S/\partial w_{n,j}$  takes the form

$$\frac{\partial S}{\partial w_{n,j}}(X) = \frac{\partial S}{\partial S_n} \frac{\partial S_n}{\partial w_{n,j}}(X) = \frac{\partial S}{\partial S_n} \frac{\partial}{\partial w_{n,j}} \left( \sum_{i \in Ch(n)} w_{n,i} S_i(X) \right) = \frac{\partial S}{\partial S_n} S_j(X). \tag{3.1}$$

The term  $\partial S/\partial S_n$  appears because of chain rule, since  $S_n$  is a function of S. This can be intuitively interpreted as taking into account the change in all nodes "above" n. So to compute the derivative wrt a weight, we need to find the derivative  $\partial S/\partial S_j$  for each internal node j.

Finding  $\partial S/\partial S_j$  requires analyzing two possible cases: sum and product parents of j. We now that S is a multilinear function of X, since in reality S is just a function made of sums and products. In particular, if we apply chain rule on  $\partial S/\partial S_j$ , we have that

$$\frac{\partial S}{\partial S_{j}}(X) = \underbrace{\sum_{\substack{n \in \operatorname{Pa}(j) \\ n: \text{ sum}}} \frac{\partial S}{\partial S_{n}} \frac{\partial S_{n}}{\partial S_{j}}(X)}_{(*)} + \underbrace{\sum_{\substack{n \in \operatorname{Pa}(j) \\ n: \text{ product}}} \frac{\partial S}{\partial S_{n}} \frac{\partial S_{n}}{\partial S_{j}}(X).$$

We expand each term at a time. Starting with the sum parents case, we can substitute the value of  $S_n(X)$  with the corresponding expansion.

$$(*) = \sum_{\substack{n \in \text{Pa}(j) \\ n: \text{ sum}}} \frac{\partial S}{\partial S_n} \frac{\partial}{\partial S_j} \left( \sum_{i \in \text{Ch}(n)} w_{n,i} S_i(X) \right) = \sum_{\substack{n \in \text{Pa}(j) \\ n: \text{ sum}}} \frac{\partial S}{\partial S_n} w_{n,j}$$

We do the same for the product case.

$$(**) = \sum_{\substack{n \in \text{Pa}(j) \\ n: \text{ product}}} \frac{\partial S}{\partial S_n} \frac{\partial}{\partial S_j} \left( \prod_{i \in \text{Ch}(n)} S_i(X) \right) = \sum_{\substack{n \in \text{Pa}(j) \\ n: \text{ product}}} \frac{\partial S}{\partial S_n} \prod_{k \in \text{Ch}(n) \setminus \{j\}} S_k$$

Which brings us to the final form.

$$\frac{\partial S}{\partial S_{j}}(X) = \sum_{\substack{n \in \text{Pa}(j) \\ n: \text{ sum}}} \frac{\partial S}{\partial S_{n}} w_{n,j} + \sum_{\substack{n \in \text{Pa}(j) \\ n: \text{ product}}} \frac{\partial S}{\partial S_{n}} \prod_{k \in \text{Ch}(n) \setminus \{j\}} S_{k}$$
(3.2)

Note how each  $\partial S/\partial S_i$  depends on the derivative of its parents. This dependency goes all the way up to the root, where  $\partial S/\partial S=1$ . This derivation lends itself neatly to an algorithmic format.

#### **Algorithm 4** Backprop: Backpropagation derivation on SPNs

**Input** A valid SPN S with pre-computed probabilities  $S_n(X)$ 

**Output** Partial derivatives of *S* with respect to every node and weight

- 1: Înitialize  $\frac{\partial S}{\partial S_n} = 0$  except  $\frac{\partial S}{\partial S} = 1$ 2: **for** each node  $n \in S$  in top-down order **do**
- **if** *n* is sum node **then** 3:
- 4:
- $\frac{\partial S}{\partial S_j} \leftarrow \frac{\partial S}{\partial S_j} + w_{n,j} \frac{\partial S}{\partial S_n}$   $\frac{\partial S}{\partial w_{n,i}} \leftarrow \frac{\partial S}{\partial S_n} S_j$ 5:
- 6:
- else 7:
- **for** all  $j \in Ch(n)$  **do** 8:
- $\frac{\partial S}{\partial S_i} \leftarrow \frac{\partial S}{\partial S_i} + \frac{\partial S}{\partial S_n} \prod_{k \in Ch(n) \setminus \{j\}} S_k$ 9:

Computing all derivatives and forward passes is fast, as it takes linear time in the

number of edges. However, these values suffer from gradient diffusion, as their signal dwindles the deeper the network, eventually becoming zero.

A possible solution to this issue is replacing soft derivation with hard derivation. This is done by finding the derivatives of the MPN of the network instead of the SPN. This guarantees that the signal remains constant throughout the structure, at the cost of slower convergence rate. We call this hard inference derivation, as opposed to the regular soft inference derivation we covered earlier.

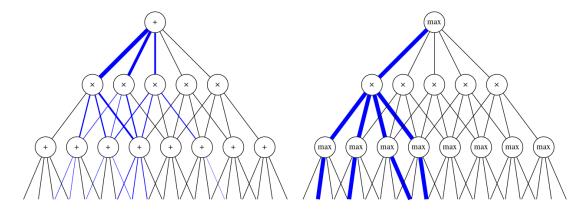


Figure 3.1: Signal difference between soft and hard derivation.

Figure 3.1 gives a visual representation of the difference between soft and hard derivation in gradient descent. MPNs preserve the signal, as the resulting gradient is constant.

To compute the hard derivatives of an SPN, we take its MPN and find its derivatives in a similar way as in soft derivation. Let M be an MPN. We shall call W the multiset of weights that a forward pass through M visits. The value of M is  $M(X) = \prod_{w_i \in W} w_i^{c_i}$ , where  $c_i$  is the number of times  $w_i$  appears in W. We can then take the logarithm of the MPN to end up with a friendlier expression.

$$\frac{\partial \log M}{\partial w_{n,j}} = \frac{\partial}{\partial w_{n,j}} \log \left( \prod_{w_i \in W} w_i^{c_i} \right) = \frac{1}{\prod_{w_i \in W} w_i^{c_i}} \cdot c_{n,j} w_{n,j}^{c_{n,j}-1} \cdot \prod_{w_i \in W \setminus \{w_{n,j}\}} w_i^{c_i}$$

If we assume that weights are strictly positive, the resulting expression results in the final hard derivative

$$\frac{\partial \log M}{\partial w_{n,j}} = c_{n,j} \frac{w_{n,j}^{c_{n,j}-1}}{w_{n,j}^{c_{n,j}}} = \frac{c_{n,j}}{w_{n,j}}.$$
(3.3)

Although not needed for the gradient, we can also compute the derivative in each internal node. The process is similar to soft derivation. There is no change for parent product nodes. For parent max nodes, we sum only contributions where  $w_{n,j} \in W$ .

$$\frac{\partial M}{\partial M_{j}} = \sum_{\substack{n \in \text{Pa}(j) \\ n: \text{ max}}} \begin{cases} w_{k,n} \frac{\partial M}{\partial M_{k}} & \text{if } w_{k,n} \in W \\ 0 & \text{otherwise} \end{cases} + \sum_{\substack{n \in \text{Pa}(j) \\ n: \text{ product}}} \frac{\partial M}{\partial M_{n}} \prod_{k \in \text{Ch}(n) \setminus \{j\}} M_{k}$$
(3.4)

Computing each derivative  $\partial \log M/\partial w_{n,j}$  means finding each  $c_{n,j}$  count at each weight. This is done through an initial forward pass on M to find each MAP, and then finding each maximal edge in W through a backwards pass. Algorithm 5 computes the total number of occurences  $c_{n,j}$  for each maximal edge  $w_{n,j}$ .

```
Algorithm 5 HardBackprop: Hard backpropagation derivation on SPNs
```

```
Input A valid SPN S with pre-computed MAP probabilities M_n(X) Output Counts c_{n,j} of each derivative \frac{\partial \log M}{\partial w_{n,j}}
```

```
1: Initialize c_{n,j} = 0
2: Let Q be a queue
3: Push M into Q
4: for each node n \in M in queue Q do
        if n is max node then
5:
            Let j = \arg \max_{i \in Ch(n)} w_{n,i} M_i(X) the maximum weighted child
6:
7:
            c_{n,j} \leftarrow c_{n,j} + 1
            Push M_j into Q
8:
9:
        else if n is product node then
            Push all children j \in Ch(n) into Q
10:
11: return all counts c_{n,j}
```

In summary, the derivatives of an SPN with respect to its internal nodes take values according to Table 3.1. The gradient components are shown in Table 3.2.

Inference	Partial derivatives wrt internal node j					
Soft	$\frac{\partial S}{\partial S_j} = \sum_{\substack{n \in \operatorname{Pa}(j) \\ n: \text{ sum}}} w_{n,j} \frac{\partial S}{\partial S_n} + \sum_{\substack{n \in \operatorname{Pa}(j) \\ n: \text{ product}}} \frac{\partial S}{\partial S_n} \prod_{k \in \operatorname{Ch}(n) \setminus \{j\}} S_k$					
Hard	$\frac{\partial M}{\partial M_{j}} = \sum_{\substack{n \in \operatorname{Pa}(j) \\ n : \max}} \begin{cases} w_{k,n} \frac{\partial M}{\partial M_{k}} & \text{if } w_{k,n} \in W, \\ 0 & \text{otherwise.} \end{cases} + \sum_{\substack{n \in \operatorname{Pa}(j) \\ n : \text{ product}}} \frac{\partial M}{\partial M_{n}} \prod_{k \in \operatorname{Ch}(n) \setminus \{j\}} M_{k}$					

**Table 3.1:** Partial derivatives for the SPN wrt internal nodes.

Inference	Partial derivatives wrt weight $w_{n,j}$		
Soft	$\frac{\partial S}{\partial w_{n,j}} = S_j \frac{\partial S}{\partial S_n}$		
Hard	$\frac{\partial M}{\partial w_{n,j}} = M_j \frac{\partial M}{\partial M_n}$		

**Table 3.2:** *Partial derivatives for the SPN wrt weights.* 

#### 3.2 Generative gradient descent

Once computed all derivatives, we update each node with the resulting gradient component. For generative gradient descent, where we are learning a joint probability distribution P(X, Y), our objective is to find the gradient of the log-likelihood

$$\frac{\partial}{\partial W}\log P(X,Y) = \frac{\partial}{\partial W}\log S(X,Y) = \frac{1}{S(X,Y)}\frac{\partial S}{\partial W}(X,Y) \propto \frac{\partial S}{\partial W}(X,Y).$$

Since the gradient is proportional to the derivative of the weights, our weight update becomes

$$\Delta w_{n,j} = \eta \frac{\partial S}{\partial w_{n,i}}(X,Y),$$

where  $\eta$  is the learning rate. An L2 regularization factor can be added to the expression above, leaving us with the final generative gradient descent weight update

$$\Delta w_{n,j} = \eta \frac{\partial S}{\partial w_{n,j}}(X, Y) - 2\lambda w_{n,j}, \tag{3.5}$$

where  $\lambda$  is the regularization constant. We call this soft generative gradient descent. It is now easy to visualize why gradient diffusion occurs with soft derivation. Component  $\partial S/\partial w_{n,j}$  depends on partial derivative  $\partial S/\partial S_n$ . Assuming normalized weights, the root node derivative  $\partial S/\partial S=1$  and each subsequent descendant node becomes smaller and smaller.

Weight update for hard derivation comes directly from Equation 3.3. Since we are interested in the log-likelihood of the joint distribution

$$\frac{\partial}{\partial W}\log P(X,Y) = \frac{\partial}{\partial W}\log M(X,Y),$$

we get, for each component  $w_{n,j}$ , the weight update

$$\Delta w_{n,j} = \eta \frac{c_{n,j}}{w_{n,j}}.$$

In a similar fashion to soft generative gradient descent, we can apply L2 regularization to each weight update.

$$\Delta w_{n,j} = \eta \frac{c_{n,j}}{w_{n,j}} - 2\lambda w_{n,j} \tag{3.6}$$

So for generative gradient descent we get the following weight updates.

Inference	Weight updates			
Soft	$\Delta w_{n,j} = \eta \frac{\partial S}{\partial w_{n,j}}(X, Y) - 2\lambda w_{n,j}$			
Hard	$\Delta w_{n,j} = \eta \frac{c_{n,j}}{w_{n,j}} - 2\lambda w_{n,j}$			

**Table 3.3:** *Generative gradient descent weight updates with L2 regularization.* 

Algorithm 6 and Algorithm 7 show pseudocode for both soft and hard generative stochastic gradient descent, though it is easy to extend both to mini-batch versions. From now on we denote soft generative gradient descent and hard generative gradient descent as SGGD and HGGD for short.

#### Algorithm 6 SoftGenGD: Soft generative stochastic gradient descent for SPNs

**Input** A valid SPN S, learning rate  $\eta$ , regularization constant  $\lambda$  and a dataset D **Output** S with learned weights

```
1: repeat
2: for each instance I \in D do
3: Compute SoftInference(S, I)
4: Compute Backprop(S)
5: for each sum node n \in S do
6: w_{n,j} \leftarrow \eta \frac{\partial S}{\partial w_{n,j}} - 2\lambda w_{n,j}
7: Normalize weights
```

8: until convergence

#### Algorithm 7 HardGenGD: Hard generative stochastic gradient descent for SPNs

**Input** A valid SPN S, learning rate  $\eta$ , regularization constant  $\lambda$  and a dataset D **Output** S with learned weights

```
1: repeat
2: for each instance I \in D do
3: Compute HardInference(S, I)
4: Compute HardBackprop(S)
5: for each sum node n \in S do
6: w_{n,j} \leftarrow \eta \frac{c_{n,j}}{w_{n,j}} - 2\lambda w_{n,j}
7: Normalize weights
```

8: until convergence

#### 3.3 Discriminative gradient descent

The goal of discriminative learning is optimizing the conditional probability distribution P(Y|X), where Y and X are query and evidence variables. To compute the gradient of this distribution we maximize the conditional log-likelihood (Gens and Domingos, 2012).

$$\frac{\partial}{\partial W} \log P(Y|X) = \frac{\partial}{\partial W} \log \left( \frac{P(Y,X)}{P(X)} \right) = \frac{\partial}{\partial W} \log P(Y,X) - \frac{\partial}{\partial W} \log P(X)$$

Through chain rule, we get the form

$$\frac{\partial}{\partial W} \log P(Y, X) - \frac{\partial}{\partial W} \log P(X) = \frac{1}{P(Y, X)} \frac{\partial}{\partial W} P(Y, X) - \frac{1}{P(X)} \frac{\partial}{\partial W} P(X) =$$

$$= \frac{1}{S(Y, X)} \frac{\partial}{\partial W} S(Y, X) - \frac{1}{S(Y, X)} \frac{\partial}{\partial W} S(X).$$

We can update our weights discriminatively by taking each gradient component

$$\Delta w_{n,j} = \eta \left( \frac{1}{S(Y,X)} \frac{\partial S(Y,X)}{\partial w_{n,j}} - \frac{1}{S(X)} \frac{\partial S(X)}{\partial w_{n,j}} \right).$$

With L2 regularization, soft discriminative gradient descent has the following form.

$$\Delta w_{n,j} = \eta \left( \frac{1}{S(Y,X)} \frac{\partial S(Y,X)}{\partial w_{n,j}} - \frac{1}{S(X)} \frac{\partial S(X)}{\partial w_{n,j}} \right) - 2\lambda w_{n,j}$$
(3.7)

For hard inference we want to optimize the following expression.

$$\frac{\partial}{\partial W} \log \tilde{P}(Y|X) = \frac{\partial}{\partial W} \log \left( \frac{\tilde{P}(Y,X)}{\tilde{P}(X)} \right) = \frac{\partial}{\partial W} \log \left( \frac{M(Y,X)}{M(X)} \right)$$

Where  $\tilde{P}$  is the MAP probability of the distribution. As usual, we apply chain rule, yielding

$$\frac{\partial}{\partial W}\log\left(\frac{M(Y,X)}{M(X)}\right) = \frac{\partial}{\partial W}\log M(Y,X) - \frac{\partial}{\partial W}\log M(X).$$

But we know from Equation 3.3 that the derivatives of the logs have a particular expression based on the counts of visited weights. We substitute the equation above with the earlier results from hard derivation, giving us the following equation for each gradient component.

$$\frac{\partial}{\partial w_{n,j}} \log \left( \frac{M(Y,X)}{M(X)} \right) = \frac{\partial}{\partial w_{n,j}} \log M(Y,X) - \frac{\partial}{\partial w_{n,j}} \log M(X) = \frac{\Delta c_{n,j}}{w_{n,j}}$$

Where  $\Delta c_{n,j}$  is the difference between the first counting, restricted to (Y, X), and the second restricted to only X.

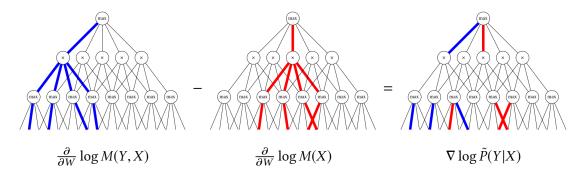


Figure 3.2: Hard discriminative gradient descent counts visualization.

Figure 3.2 shows the hard discriminative gradient descent difference derived from  $\frac{\partial}{\partial W} \log \tilde{P}(Y|X)$ . The first pass, shown in the image with blue edges, counts the maximum edges given the Y, X valuation. The second pass, in red, is the evidence pass on X. The gradient is then computed by finding the difference between the two countings. On the right-hand side of the expression portrayed in Figure 3.2, blue edges mean a positive count  $c_{n,i}$  and red edges represent a negative count.

The actual weight update has a similar form to hard gradient descent.

$$\Delta w_{n,j} = \eta \frac{\Delta c_{n,j}}{w_{n,j}}$$

With L2 regularization we get

$$\Delta w_{n,j} = \eta \frac{\Delta c_{n,j}}{w_{n,j}} - 2\lambda w_{n,j}. \tag{3.8}$$

In a similar fashion to generative gradient descent, we denote by HDGD and SDGD hard discriminative gradient descent and soft discriminative gradient descent respectively.

We now build a discriminative gradient descent table for each inference type. Just like in generative gradient descent, we add an L2 term to it.

Inference	Weight updates		
Soft	$\Delta w_{n,j} = \eta \left( \frac{1}{S(Y,X)} \frac{\partial S(Y,X)}{\partial w_{n,j}} - \frac{1}{S(X)} \frac{\partial S(X)}{\partial w_{n,j}} \right) - 2\lambda w_{n,j}$		
Hard	$\Delta w_{n,j} = \eta \frac{\Delta c_{n,j}}{w_{n,j}} - 2\lambda w_{n,j}$		

**Table 3.4:** Discriminative gradient descent weight updates with L2 regularization.

We now finally show an algorithmic form to HDGD and SDGD. Note how in discriminative gradient descent we have two passes through the network. We can avoid recomputing node values by memoizing nodes that have no query variables in descendant's scopes (Gens and Domingos, 2012).

#### Algorithm 8 SoftDiscGD: Soft discriminative stochastic gradient descent for SPNs

**Input** A valid SPN S, query variables Y, learning rate  $\eta$ , regularization constant  $\lambda$  and a dataset D

**Output** *S* with learned weights

```
1: repeat
```

3:

**for** each instance  $I \in D$  **do** 

Compute SoftInference(S, I) and store them in  $S_n^+$  for each node n

Compute Backprop( $S^+$ ) and store them in  $\frac{\partial S_n^+}{\partial w_{n,j}}$ 4:

Compute SoftInference( $S, I \setminus Y$ ) and store them in  $S_n^-$  for each node n

Compute Backprop( $S^-$ ) and store them in  $\frac{\partial S_n^-}{\partial w_n}$ 

7:

7: **for** each sum node 
$$n \in S^- \cup S^+$$
 **do**  
8:  $w_{n,j} \leftarrow \eta \left( \frac{1}{S^+} \frac{\partial S^+}{\partial w_{n,j}} - \frac{1}{S^-} \frac{\partial S^-}{\partial w_{n,j}} \right) - 2\lambda w_{n,j}$ 

Normalize weights

10: **until** convergence

#### Algorithm 9 HardDiscGD: Hard discriminative stochastic gradient descent for SPNs

**Input** A valid SPN S, query variables Y, learning rate  $\eta$ , regularization constant  $\lambda$  and a dataset D

**Output** *S* with learned weights

10: until convergence

```
1: repeat
         for each instance I \in D do
2:
               Compute \operatorname{HardInference}(S, I) and store them in M_n^+ for each node n
3:
               Compute \operatorname{HardBackprop}(M^+) and store them in c_{n,j}^+
4:
               Compute \operatorname{HardInference}(S, I \setminus Y) and store them in M_n^- for each node n
5:
               Compute \operatorname{HardBackprop}(M^-) and store them in c_{n,j}^-
6:
              for each sum node n \in S do w_{n,j} \leftarrow \eta \left(\frac{c_{n,j}^+ - c_{n,j}^-}{w_{n,j}}\right) - 2\lambda w_{n,j}
7:
8:
              Normalize weights
9:
```

**Chapter 4** 

**Structure learning** 

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