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Cumulative Distribution Networks and the Derivative-sum-product Algorithm: Models and Inference for Cumulative Distribution Functions on Graphs

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Abstract

We present a class of graphical models for directly representing the joint cumulative distribution function (CDF) of many random variables, called *cumulative distribution networks* (CDNs). Unlike graphs for probability density and mass functions, for CDFs the marginal probabilities for any subset of variables are obtained by computing limits of functions in the model, and conditional probabilities correspond to computing mixed derivatives. We will show that the conditional independence properties in a CDN are distinct from the conditional independence properties of directed, undirected and factor graphs, but include the conditional independence properties of bi-directed graphs. In order to perform inference in such models, we describe the 'derivative-sum-product' (DSP) message-passing algorithm in which messages correspond to derivatives of the joint CDF. We will then apply CDNs to the problem of learning to rank players in multiplayer team-based games and suggest several future directions for research.

Keywords: graphical models, cumulative distribution function, message-passing algorithm, inference

1. Introduction

Probabilistic graphical models provide a pictorial means of specifying a joint probability density function (PDF) defined over many continuous random variables, the joint probability mass function (PMF) of many discrete random variables, or a joint probability distribution defined over a mixture of continuous and discrete variables. Each variable in the model corresponds to a node in a graph and edges between nodes in the graph convey statistical dependence relationships between the variables in the model. The graphical formalism allows one to obtain the independence relationships between random variables in a model by inspecting the corresponding graph, where the separation of nodes in the graph implies a particular conditional independence relationship between the corresponding variables.

A consequence of representing independence constraints between subsets of variables using a graph is that the joint probability often factors into a product of functions defined over subsets of neighboring nodes in the graph. Typically, this allows us to decompose a large multivariate distribution into a product of simpler functions, so that the task of inference and estimation of such models can also be simplified and efficient algorithms for performing these tasks can be implemented. Often, a complex distribution over observed variables can be constructed using a graphical model with latent variables introduced, where the joint probability over the observed variables is obtained by marginalization over the latent variables. The model with additional latent variables has the advantage of having a more compact factorized form as compared to that for the joint probability over the observed variables. However, this often comes at the cost of a significantly higher computational cost for estimation and inference, as additional latent variables often require one to either approximate intractable marginalization operations (Minka, 2001) or to sample from the model using Markov Chain Monte Carlo (MCMC) methods (Neal, 1993). Furthermore, there is also the problem that there are possibly an infinite number of latent variable models associated with any given model defined over observable variables, so that adding latent variables for any given application can often present difficulties in terms of model identifiability, which may be desirable when model parameters are to be interpreted. These issues may hamper the applicability of graphical models for many real-world problems in the presence of latent variables.

Another possible limitation of many graphical models is that the joint PDF/PMF itself might not be appropriate as a probability model for certain applications. For example, in learning to rank, the *cumulative distribution function* (CDF) is a probabilistic representation that arises naturally as a probability of inequality events of the type $\{X \leq x\}$. The joint CDF lends itself to such problems that are easily described in terms of inequality events in which statistical dependence relationships also exist among events. An example of this type of problem is that of predicting multiplayer game outcomes with a team structure (Herbrich, Minka and Graepel, 2007). In contrast to the canonical problems of classification or regression, in learning to rank we are required to learn some mapping from inputs to inter-dependent output variables so that we may wish to model both stochastic orderings between variable states and statistical dependence relationships between variables.

Given the above, here we present a class of graphical models called *cumulative distribution networks* (CDN) in which we represent the joint CDF of a set of observed variables. As we will show, CDNs can be viewed as providing a means to construct multivariate distributions over observed variables without the need to explicitly introduce latent variables and then marginalize. The resulting model consists of a factorized form for the joint CDF, where the principal operations required for answering probabilistic queries and for marginalization consist of differentiation and computing limits respectively, in contrast to summation/integration in graphical models for PDFs with latent variables. Furthermore, the parametrization of the model as a joint CDF has the advantage that the global normalization constraint can be enforced locally for each function in the CDN, unlike the case of undirected graphical models for PDF/PMFs. We will present the basic properties of CDNs and show that the rules for ascertaining conditional independence relationships among variables in a CDN are distinct from the rules in directed, undirected and factor graphs (Pearl, 1988; Lauritzen, 1996; Kschischang, Frey and Loeliger, 2001). We will show that the conditional independence properties in a CDN include, but are not limited to, the conditional independence properties for bi-directed graphs (Drton and Richardson, 2008; Richardson and Spirtes, 2002; Richardson, 2003).

We will then discuss the problem of performing inference under CDNs in which the principal challenge is to compute the derivatives of the joint CDF. To this end we will describe a message-passing algorithm for inference in CDNs called the *derivative-sum-product algorithm* based on previous work (Huang and Frey, 2008; Huang, 2009). To demonstrate the applicability of CDNs, we will use the message-passing algorithm for inference in order to apply CDNs to the problem of learning to rank, where we will show that CDFs arise naturally as a probability models in which it is easy to specify stochastic ordering constraints among variables in the model.

1.1 Notation

Before we proceed, we will establish some notation to be used throughout the paper. We will denote bipartite graphs as $\mathcal{G} = (V, S, E)$ where V, S are two disjoint sets of nodes and $E \subseteq \{V \times S, S \times V\}$ is a set of edges that correspond to ordered pairs (α, s) or (s, α) for $\alpha \in V$ and $s \in S$. We will denote neighboring sets $\mathcal{N}(\alpha)$ and $\mathcal{N}(s)$ as

$$\mathcal{N}(\alpha) = \{s \in S : (\alpha, s) \in E\},$$
$$\mathcal{N}(s) = \{\alpha \in V : (\alpha, s) \in E\}.$$

Furthermore, let $\mathcal{N}(A) = \cup_{\alpha \in A} \mathcal{N}(\alpha)$.

Throughout the paper we will use boldface notation to denote vectors and/or matrices. Scalar and vector random variables will be denoted as X_α and $\mathbf{X}_A$ respectively where α is a node in a graph $\mathcal{G}$ and A denotes a set of nodes in $\mathcal{G}$. The notation $|A|, |\mathbf{x}|, |\mathbf{X}|$ will denote the cardinality, or number of elements, in set A and vectors $\mathbf{x}, \mathbf{X}$ respectively. We will also denote the mixed partial derivative/finite difference as $\partial_{\mathbf{x}_A}\Big[\cdot\Big]$, where the mixed derivative here is taken with respect to arguments $x_\alpha \; \forall \; \alpha \in A$. Throughout the paper we assume hat sets consist of unique elements such that for any set A and for any element $\alpha \in A$, $A \cap \alpha = \alpha$, so that $\partial_{\mathbf{x}_A}\Big[\cdot\Big]$ consists of the mixed derivative with respect to unique variable arguments $X_\alpha \in \mathbf{X}_A$. For example, $\partial_{x_{1,2,3}}\Big[F(x_1, x_2, x_3)\Big] \equiv \frac{\partial^3 F}{\partial x_1 \partial x_2 \partial x_3}$.

1.2 Cumulative Distribution Functions

Here we provide a brief definition for the joint CDF $F(\mathbf{x})$ defined over random variables $\mathbf{X}$, denoted individually as X_α. The joint *cumulative distribution function* $F(\mathbf{x})$ is then defined as the function $F : \mathbb{R}^{|\mathbf{X}|} \mapsto [0, 1]$ such that

$$F(\mathbf{x}) = \mathbb{P}\left[\bigcap_{X_\alpha \in \mathbf{X}} \{X_\alpha \leq x_\alpha\}\right] \equiv \mathbb{P}\big[\mathbf{X} \leq \mathbf{x}\big].$$

Thus the CDF is a probability of events $\{X_\alpha \leq x_\alpha\}$. Alternately, the CDF can be defined in terms of the joint probability density function (PDF) or probability mass function (PMF) $P(\mathbf{x})$ via

$$F(\mathbf{x}) = \int_{-\infty}^{\mathbf{x}} P(\mathbf{u}) \, d\mathbf{u},$$

where $P(\mathbf{x})$, if it exists, satisfies $P(\mathbf{x}) \geq 0$, $\int_{\mathbf{x}} P(\mathbf{x}) \, d\mathbf{x} = 1$ and $P(\mathbf{x}) = \partial_{\mathbf{x}}\Big[F(\mathbf{x})\Big]$ where $\partial_{\mathbf{x}}\Big[\cdot\Big]$ denotes the higher-order mixed derivative operator $\partial_{x_1, \cdots, x_K}\Big[\cdot\Big] \equiv \dfrac{\partial^K}{\partial x_1 \cdots \partial x_K}$ for $\mathbf{x} = [x_1 \; \cdots \; x_K] \in \mathbb{R}^K$.

A function F is a CDF for some probability $\mathbb{P}$ if and only if F satisfies the following conditions:

1. The CDF $F(\mathbf{x})$ converges to unity as all of its arguments tend to ∞, or

$$F(\infty) \equiv \lim_{\mathbf{x} \to \infty} F(\mathbf{x}) = 1.$$

2. The CDF $F(\mathbf{x})$ converges to 0 as any of its arguments tends to $-\infty$, or

$$F(-\infty, \mathbf{x} \setminus x_\alpha) \equiv \lim_{x_\alpha \to -\infty} F(x_\alpha, \mathbf{x} \setminus x_\alpha) = 0 \quad \forall X_\alpha \in \mathbf{X}.$$

3. The CDF $F(\mathbf{x})$ is monotonically non-decreasing, so that

$$F(\mathbf{x}) \leq F(\mathbf{y}) \; \forall \, \mathbf{x} \leq \mathbf{y}, \; \mathbf{x}, \mathbf{y} \in \mathbb{R}^{|\mathbf{X}|}.$$

   where $\mathbf{x} \leq \mathbf{y}$ denotes element-wise inequality of all the elements in vectors $\mathbf{x}, \mathbf{y}$.

4. The CDF $F(\mathbf{x})$ is right-continuous, so that

$$\lim_{\boldsymbol{\epsilon} \to \mathbf{0}^+} F(\mathbf{x} + \boldsymbol{\epsilon}) \equiv F(\mathbf{x}) \; \forall \, \mathbf{x} \in \mathbb{R}^{|\mathbf{X}|}.$$

A proof of forward implication in the above can be found in Wasserman (2004) and Papoulis and Pillai (2001).

Proposition 1 *Let $F(\mathbf{x}_A, \mathbf{x}_B)$ be the joint CDF for variables $\mathbf{X}$ where $\mathbf{X}_A, \mathbf{X}_B$ for a partition of the set of variables $\mathbf{X}$. The joint probability of the event $\{\mathbf{X}_A \leq \mathbf{x}_A\}$ is then given in terms of $F(\mathbf{x}_A, \mathbf{x}_B)$ as*

$$F(\mathbf{x}_A) \equiv \mathbb{P}\Big[\mathbf{X}_A \leq \mathbf{x}_A\Big] = \lim_{\mathbf{x}_B \to \infty} F(\mathbf{x}_A, \mathbf{x}_B).$$

□

The above proposition follows directly from the definition of a CDF in which

$$\lim_{\mathbf{x}_B \to \infty} F(\mathbf{x}_A, \mathbf{x}_B) = \mathbb{P}\left[\left[\bigcap_{\alpha \in A} \{X_\alpha \leq x_\alpha\}\right] \cap \left[\bigcap_{\beta \in B} \{X_\beta \leq \infty\}\right]\right] = \mathbb{P}\left[\bigcap_{\alpha \in A} \{X_\alpha \leq x_\alpha\}\right] = F(\mathbf{x}_A).$$

Thus, marginal CDFs of the form $F(\mathbf{x}_A)$ can be computed from the joint CDF by computing limits.

1.3 Conditional Cumulative Distribution Functions

In the sequel we will be making use of the concept of a conditional CDF for some subset of variables $\mathbf{X}_A$ conditioned on event M. We formally define the conditional CDF below.

Definition 2 *Let M be an event with $\mathbb{P}[M] > 0$. The conditional CDF $F(\mathbf{x}_A \mid M)$ conditioned on event M is defined as*

$$F(\mathbf{x}_A \mid M) \equiv \mathbb{P}\Big[\mathbf{X}_A \leq \mathbf{x}_A \mid M\Big] = \frac{\mathbb{P}\Big[\{\mathbf{X}_A \leq \mathbf{x}_A\} \cap M\Big]}{\mathbb{P}\Big[M\Big]}.$$

□

We will now find the above conditional CDF for different types of events M.

Lemma 3 *Let $F(\mathbf{x}_C)$ be a marginal CDF obtained from the joint CDF $F(\mathbf{x})$ as given by Proposition 1 for some $\mathbf{X}_C \subseteq \mathbf{X}$. Consider some variable set $\mathbf{X}_A \subseteq \mathbf{X}$ where $\mathbf{X}_A \bigcap \mathbf{X}_C = \emptyset$. Let $M = \omega(\mathbf{x}_C) \equiv \{\mathbf{X}_C \leq \mathbf{x}_C\}$ for $\mathbf{X}_C \subset \mathbf{X}$. If $F(\mathbf{x}_C) > 0$, then $F(\mathbf{x}_A | \omega(\mathbf{x}_C)) \equiv F(\mathbf{x}_A | \mathbf{X}_C \leq \mathbf{x}_C) = \dfrac{F(\mathbf{x}_A, \mathbf{x}_C)}{F(\mathbf{x}_C)}$.* □

Thus a conditional CDF of the form $F(\mathbf{x}_A|\omega(\mathbf{x}_C))$ can be obtained by taking ratios of joint CDFs, which consists of computing limits to obtain the required marginal CDFs. It follows from Lemma 3 that marginalization over variables $\mathbf{X}_C$ can be viewed as a special case of conditioning on $\mathbf{X}_C < \infty$.

To compute conditional CDFs of the form $F(\mathbf{x}_A|x_\beta)$ where we instead condition on x_β, we need to *differentiate* the joint CDF, as we now show.

Lemma 4 *Consider some variable set* $\mathbf{X}_A \subseteq \mathbf{X}$. *Let* $M = \{x_\beta < X_\beta \leq x_\beta + \varepsilon\}$ *with* $\varepsilon > 0$ *for some scalar random variable* $X_\beta \notin \mathbf{X}_A$. *If* $F(x_\beta)$ *and* $F(\mathbf{x}_A, x_\beta)$ *are differentiable with respect to* x_β *so that* $\partial_{x_\beta}\Big[F(x_\beta)\Big]$ *and* $\partial_{x_\beta}\Big[F(\mathbf{x}_A, x_\beta)\Big]$ *exist with* $\partial_{x_\beta}\Big[F(x_\beta)\Big] > 0$, *then the conditional CDF* $F(\mathbf{x}_A|x_\beta) \equiv \lim_{\varepsilon\to 0^+} F(\mathbf{x}_A|x_\beta < X_\beta < x_\beta + \varepsilon) = \lim_{\varepsilon\to 0^+} \frac{\mathbb{P}\Big[\{\mathbf{X}_A \leq \mathbf{x}_A\} \cap \{x_\beta < X_\beta \leq x_\beta + \varepsilon\}\Big]}{\mathbb{P}\Big[x_\beta < X_\beta \leq x_\beta + \varepsilon\Big]}$ *is given by*

$$F(\mathbf{x}_A|x_\beta) = \frac{\partial_{x_\beta}\Big[F(\mathbf{x}_A, x_\beta)\Big]}{\partial_{x_\beta}\Big[F(x_\beta)\Big]} \propto \partial_{x_\beta}\Big[F(\mathbf{x}_A, x_\beta)\Big].$$

Proof We can write

$$\begin{aligned} F(\mathbf{x}_A|x_\beta < X_\beta \leq x_\beta + \varepsilon) &= \frac{\mathbb{P}\Big[\{\mathbf{X}_A \leq \mathbf{x}_A\} \cap \{x_\beta < X_\beta \leq x_\beta + \varepsilon\}\Big]}{\mathbb{P}\Big[x_\beta < X_\beta \leq x_\beta + \varepsilon\Big]} \\ &= \frac{\frac{1}{\varepsilon}\mathbb{P}\Big[\{\mathbf{X}_A \leq \mathbf{x}_A\} \cap \{x_\beta < X_\beta \leq x_\beta + \varepsilon\}\Big]}{\frac{1}{\varepsilon}\mathbb{P}\Big[x_\beta < X_\beta \leq x_\beta + \varepsilon\Big]} = \frac{\frac{F(\mathbf{x}_A, x_\beta+\varepsilon) - F(\mathbf{x}_A, x_\beta)}{\varepsilon}}{\frac{F(x_\beta+\varepsilon) - F(x_\beta)}{\varepsilon}}. \end{aligned}$$

Taking limits, and given differentiability of both $F(x_\beta)$ and $F(\mathbf{x}_A, x_\beta)$ with respect to x_β, the conditional CDF $F(\mathbf{x}_A|x_\beta)$ is given by

$$F(\mathbf{x}_A|x_\beta) \equiv \frac{\lim_{\varepsilon\to 0^+} \frac{F(\mathbf{x}_A, x_\beta+\varepsilon) - F(\mathbf{x}_A, x_\beta)}{\varepsilon}}{\lim_{\varepsilon\to 0^+} \frac{F(x_\beta+\varepsilon) - F(x_\beta)}{\varepsilon}} = \frac{\partial_{x_\beta}\Big[F(\mathbf{x}_A, x_\beta)\Big]}{\partial_{x_\beta}\Big[F(x_\beta)\Big]} \propto \partial_{x_\beta}\Big[F(\mathbf{x}_A, x_\beta)\Big],$$

where the proportionality constant does not depend on $\mathbf{x}_A$. ■

The generalization of the above lemma to conditioning on sets of variables $\mathbf{X}_C \subseteq \mathbf{X}$ can be found in the Appendix.

2. Cumulative Distribution Networks

Graphical models allow us to simplify the computations required for obtaining conditional probabilities of the form $P(\mathbf{x}_A|\mathbf{x}_B)$ or $P(\mathbf{x}_A)$ by allowing us to model conditional independence constraints in terms of graph separation constraints. However, for many applications it may be desirable to compute other conditional and marginal probabilities such as probabilities of events of the type $\{\mathbf{X} \leq \mathbf{x}\}$. Here we will present the cumulative distribution network (CDN), which is a graphical framework for directly modeling the joint cumulative distribution function, or CDF. With the CDN, we can thus expand the set of possible probability queries so that in addition to formulating queries as conditional/marginal probabilities of the form $P(\mathbf{x}_A)$ and $P(\mathbf{x}_A|\mathbf{x}_B)$, we can also compute probabilities of the form $F(\mathbf{x}_A|\omega(\mathbf{x}_B)), F(\mathbf{x}_A|\mathbf{x}_B), P(\mathbf{x}_A|\omega(\mathbf{x}_B))$ and $F(\mathbf{x}_A)$, where $F(\mathbf{u}) \equiv \mathbb{P}\Big[\mathbf{U} \leq \mathbf{u}\Big]$ is a CDF and we denote the inequality event $\{\mathbf{U} \leq \mathbf{u}\}$ using $\omega(\mathbf{x}_U)$. Examples of this new type of query could be "Given that the drug dose was less than 1 mg, what is the probability of the patient living at least another year?", or "Given that a person prefers one brand of soda over another, what is the probability of that person preferring one type of chocolate over another?". A significant advantage with CDNs is that the graphical representation of the joint CDF may naturally allow for queries which would otherwise be difficult, if not intractable, to compute under directed, undirected and factor graphical models for PDFs/PMFs.

Here we provide a formal definition of the CDN and we will show that the conditional independence properties in such graphical models are distinct from the properties for directed, undirected and factor graphs. We will then show that the conditional independence properties in CDNs include the properties of bi-directed graphs (Drton and Richardson, 2008; Richardson, 2003). Finally, we will show that CDNs provide a tractable means of parameterizing models for learning to rank in which we can construct multivariate CDFs from a product of CDFs defined over subsets of variables.

Definition 5 *The cumulative distribution network (CDN) is an undirected bipartite graphical model consisting of a bipartite graph $\mathcal{G} = (V, S, E)$, where V denotes variable nodes and S denotes factor nodes, with edges in E connecting factor nodes to variable nodes. The CDN also includes a specification of functions $\phi_s(\mathbf{x}_s)$ for each function node $s \in S$, where $\mathbf{x}_s \equiv \mathbf{x}_{\mathcal{N}(s)}, \cup_{s\in S}\mathcal{N}(s) = V$ and each function $\phi_s : \mathbb{R}^{|\mathcal{N}(s)|} \mapsto [0,\ 1]$ satisfies the properties of a CDF. The joint CDF over the variables in the CDN is then given by the product over CDFs $\phi_s : \mathbb{R}^{|\mathcal{N}(s)|} \mapsto [0,\ 1]$, or*

$$F(\mathbf{x}) = \prod_{s\in S} \phi_s(\mathbf{x}_s),$$

where each CDF ϕ_s is defined over neighboring variable nodes $\mathcal{N}(s)$. □

An example of a CDN defined over three variable nodes with four CDN function nodes is shown in Figure 1, where the joint CDF over three variables X, Y, Z is given by

$$F(x, y, z) = \phi_a(x, y)\phi_b(x, y, z)\phi_c(y, z)\phi_d(z).$$

In the CDN, each function node (depicted as a diamond) corresponds to one of the functions $\phi_s(\mathbf{x}_s)$ in the model for the joint CDF $F(\mathbf{x})$. Thus, one can think of the CDN as a factor graph for modeling the joint CDF instead of the joint PDF. However, as we will see shortly, this leads to a different set of conditional independence properties as compared to the conditional independence properties of directed, undirected and factor graphs.

Since the CDN is a graphical model for the joint CDF, the functions in the CDN must be such that $F(\mathbf{x})$ is a CDF for some probability $\mathbb{P}$. The following lemma establishes a sufficient condition that the CDN functions ϕ_s be themselves CDFs in order for F to be a CDF.

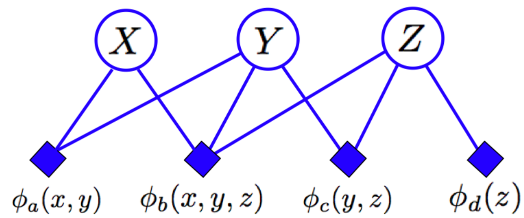


Figure 1: A cumulative distribution network (CDN) defined over three variables and four functions.

Lemma 6 *If all functions $\phi_s(\mathbf{x}_s)$ satisfy the properties of a CDF, then the product $\prod_{s\in S}\phi_s(\mathbf{x}_s)$ also satisfies the properties of a CDF.* □

Proof If for all $s \in S$, we have $\lim_{\mathbf{x}_s\to\infty}\phi_s(\mathbf{x}_s) = 1$, then $\lim_{\mathbf{x}\to\infty}\prod_{s\in S}\phi_s(\mathbf{x}_s) = 1$. Furthermore, if for any given $\alpha \in V$ and for $s \in \mathcal{N}(\alpha)$, we have $\lim_{x_\alpha\to-\infty}\phi_s(\mathbf{x}_s) = 0$, then $\lim_{x_\alpha\to-\infty}\prod_{s\in S}\phi_s(\mathbf{x}_s) = 0$.

To show that the product of monotonically non-decreasing functions is monotonically non-decreasing, we note that $\mathbf{x}_s < \mathbf{y}_s$ for all $s \in S$ if and only if $\mathbf{x} < \mathbf{y}$, since $\cup_{s\in S}\mathcal{N}(s) = V$. Thus if we have $\phi_s(\mathbf{x}_s) \leq \phi_s(\mathbf{y}_s)\ \forall\, \mathbf{x}_s < \mathbf{y}_s$ for all $s \in S$, we can then write

$$F(\mathbf{x}) = \prod_{s\in S}\phi_s(\mathbf{x}_s) \leq \prod_{s\in S}\phi_s(\mathbf{y}_s) = F(\mathbf{y}).$$

Finally, a product of right-continuous functions is also right-continuous. Thus if all of the functions $\phi_s(\mathbf{x}_s)$ satisfy the properties of a CDF, then the product of such functions also satisfies the properties of a CDF. ■

Although the condition that each of the ϕ_s functions be a CDF is sufficient for the overall product to satisfy the properties of a CDF, we emphasize that it is not a necessary condition, as one could construct a function that satisfies the properties of a CDF from a product of functions that are not CDFs. The sufficient condition above ensures, however, that we can construct CDNs by multiplying together CDFs to obtain another CDF. Furthermore, the above definition and theorem do not assume differentiability of the joint CDF or of the CDN functions: the following proposition shows that differentiability and non-negativity of the derivatives of functions ϕ_s with respect to all neighboring variables in $\mathcal{N}(s)$ imply both differentiability and monotonicity of the joint CDF $F(\mathbf{x})$. In the sequel we will assume that whenever CDN functions are differentiable, derivatives are invariant to the order in which they are computed (Schwarz' Theorem).

Proposition 7 *If the mixed derivatives $\partial_{\mathbf{x}_A}\Big[\phi_s(\mathbf{x}_s)\Big]$ satisfy $\partial_{\mathbf{x}_A}\Big[\phi_s(\mathbf{x}_s)\Big] \geq 0$ for all $s \in S$ and $A \subseteq \mathcal{N}(s)$, then*

- $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x})\Big] \geq 0$ *for all* $C \subseteq V$,
- $F(\mathbf{x}) \leq F(\mathbf{y})$ *for all* $\mathbf{x} < \mathbf{y}$,
- $F(\mathbf{x})$ *is differentiable.*

□

Proof A product of differentiable functions is differentiable and so $F(\mathbf{x})$ is differentiable. To show that $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x})\Big] \geq 0 \;\forall\, C \subseteq V$, we can group the functions $\phi_s(\mathbf{x}_s)$ arbitrarily into two functions $g(\mathbf{x})$ and $h(\mathbf{x})$ so that $F(\mathbf{x}) = g(\mathbf{x})h(\mathbf{x})$. The goal here will be to show that if all derivatives $\partial_{\mathbf{x}_A}\Big[g(\mathbf{x})\Big]$ and $\partial_{\mathbf{x}_A}\Big[h(\mathbf{x})\Big]$ are non-negative, then $\partial_{\mathbf{x}_A}\Big[F(\mathbf{x})\Big]$ must also be non-negative. For all $C \subseteq V$, applying the product rule to $F(\mathbf{x}) = g(\mathbf{x})h(\mathbf{x})$ yields

$$\partial_{\mathbf{x}_C}\Big[F(\mathbf{x})\Big] = \sum_{A \subseteq C} \partial_{\mathbf{x}_A}\Big[g(\mathbf{x})\Big]\partial_{\mathbf{x}_{C\setminus A}}\Big[h(\mathbf{x})\Big],$$

so if $\partial_{\mathbf{x}_A}\Big[g(\mathbf{x})\Big], \partial_{\mathbf{x}_{C\setminus A}}\Big[h(\mathbf{x})\Big] \geq 0$ for all $A \subseteq C$ then $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x})\Big] \geq 0$. By recursively applying this rule to each of the functions $g(\mathbf{x}), h(\mathbf{x})$ until we obtain sums over terms involving $\partial_{\mathbf{x}_A}\Big[\phi_s(\mathbf{x}_s)\Big] \;\forall\, A \subseteq \mathcal{N}(s)$, we see that if $\partial_{\mathbf{x}_A}\Big[\phi_s(\mathbf{x}_s)\Big] \geq 0$, then $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x})\Big] \geq 0 \;\forall\, C \subseteq V$.

Now, $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x})\Big] \geq 0$ for all $C \subseteq V$ implies that $\partial_{x_\alpha}\Big[F(\mathbf{x})\Big] \geq 0$ for all $\alpha \in V$. By the Mean Value Theorem for functions of several variables, it then follows that if $\mathbf{x} < \mathbf{y}$, then

$$F(\mathbf{y}) - F(\mathbf{x}) = \sum_{\alpha \in V} \partial_{z_\alpha}\Big[F(\mathbf{z})\Big](y_\alpha - x_\alpha) \geq 0,$$

and so $F(\mathbf{x})$ is monotonic. ■

The above ensures differentiability and monotonicity of the joint CDF through constraining the derivatives of each of the CDN functions. We note that although it is merely sufficient for the first-order derivatives to be non-negative in order for $F(\mathbf{x})$ to be monotonic, the condition that the higher-order mixed derivatives $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x})\Big]$ of the functions $\phi_s(\mathbf{x}_s)$ be non-negative also implies non-negativity of the first-order derivatives. Thus in the sequel, whenever we assume differentiability of CDN functions, we will assume that for all $s \in S$, all mixed derivatives of $\phi_s(\mathbf{x}_s)$ with respect to any and all subsets of argument variables are non-negative.

Having described the above conditions on CDN functions, we will now provide some examples of CDNs constructed from a product of CDFs.

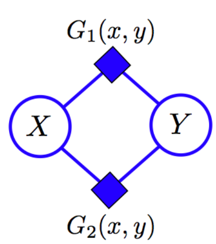
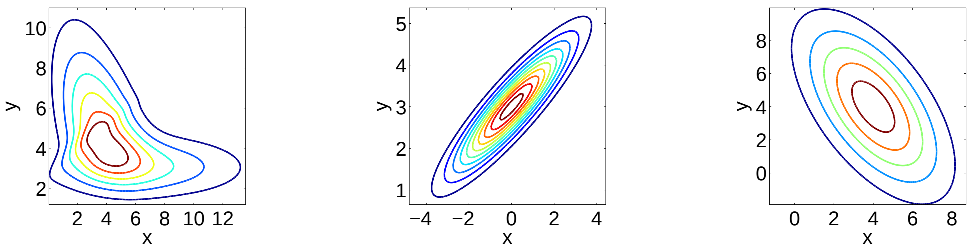


Figure 2: A CDN defined over two variables X and Y with functions $G_1(x,y), G_2(x,y)$.

Example 1 (Product of bivariate Gaussian CDFs) *As a simple example of a CDN, consider two random variables X and Y with joint CDF modeled by the CDN in Figure 2, so that $F(x,y) =$*



(a) (b) (c)

Figure 3: a) Joint probability density function $P(x,y)$ corresponding to the distribution function $F(x,y)$ using bivariate Gaussian CDFs as CDN functions; b),c) The PDFs corresponding to $\partial_{x,y}\Big[G_1(x,y)\Big]$ and $\partial_{x,y}\Big[G_2(x,y)\Big]$.

$G_1(x,y)G_2(x,y)$ *with*

$$G_1(x,y) = \Phi\left(\begin{bmatrix} x \\ y \end{bmatrix}; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1\right), \quad \boldsymbol{\mu}_1 = \begin{bmatrix} \mu_{x,1} \\ \mu_{y,1} \end{bmatrix}, \qquad \boldsymbol{\Sigma}_1 = \begin{bmatrix} \sigma_{x,1}^2 & \rho_1\sigma_{x,1}\sigma_{y,1} \\ \rho_1\sigma_{x,1}\sigma_{y,1} & \sigma_{y,1}^2 \end{bmatrix},$$

$$G_2(x,y) = \Phi\left(\begin{bmatrix} x \\ y \end{bmatrix}; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2\right), \quad \boldsymbol{\mu}_2 = \begin{bmatrix} \mu_{x,2} \\ \mu_{y,2} \end{bmatrix}, \qquad \boldsymbol{\Sigma}_2 = \begin{bmatrix} \sigma_{x,2}^2 & \rho_2\sigma_{x,2}\sigma_{y,2} \\ \rho_2\sigma_{x,2}\sigma_{y,2} & \sigma_{y,2}^2 \end{bmatrix},$$

where $\Phi(\cdot;\mathbf{m},\mathbf{S})$ *is the multivariate Gaussian CDF with mean vector* $\mathbf{m}$ *and covariance* $\mathbf{S}$*. Taking derivatives, the density* $P(x,y)$ *is given by*

$$\begin{aligned} P(x,y) &= \partial_{x,y}\Big[F(x,y)\Big] = \partial_{x,y}\Big[G_1(x,y)G_2(x,y)\Big] \\ &= G_1(x,y)\partial_{x,y}\Big[G_2(x,y)\Big] + \partial_x\Big[G_1(x,y)\Big]\partial_y\Big[G_2(x,y)\Big] \\ &\quad + \partial_y\Big[G_1(x,y)\Big]\partial_x\Big[G_2(x,y)\Big] + \partial_{x,y}\Big[G_1(x,y)\Big]G_2(x,y). \end{aligned}$$

As functions G_1, G_2 *are Gaussian CDFs, the above derivatives can be expressed in terms of Gaussian CDF and PDFs. For example,*

$$\begin{aligned} \partial_x\Big[G_1(x,y)\Big] &= \int_{-\infty}^{y} Gaussian\left(\begin{bmatrix} x \\ t \end{bmatrix}; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1\right) dt \\ &= Gaussian(x;\mu_{x,1},\sigma_{x,1}^2)\int_{-\infty}^{y} Gaussian(t;\mu_{y|x,1},\sigma_{y|x,1}^2)\,dt \\ &= Gaussian(x;\mu_{x,1},\sigma_{x,1}^2)\Phi(y;\mu_{y|x,1},\sigma_{y|x,1}^2), \end{aligned}$$

where

$$\begin{aligned} \mu_{y|x,1} &= \mu_{y,1} + \rho_1\frac{\sigma_{y,1}}{\sigma_{x,1}}(x-\mu_{x,1}), \\ \sigma_{y|x,1}^2 &= (1-\rho_1^2)\sigma_{y,1}^2. \end{aligned}$$

Other derivatives can be obtained similarly. The resulting joint PDF $P(x,y)$ obtained by differentiating the CDF is shown in Figure 3(a), where the CDN function parameters are given by $\mu_{x,1}=0,\mu_{x,2}=4,\mu_{y,1}=3,\mu_{y,2}=4,\sigma_{x,1}=\sqrt{3},\sigma_{x,2}=\sqrt{5},\sigma_{y,1}=1,\sigma_{y,2}=\sqrt{10},\rho_1=0.9,\rho_2=-0.6$. The PDFs corresponding to $\partial_{x,y}\Big[G_1(x,y)\Big]$ and $\partial_{x,y}\Big[G_2(x,y)\Big]$ are shown in Figures 3(b) and 3(c). $\square$

The next example provides an illustration of the use of copula functions for constructing multivariate CDFs under the framework of CDNs.

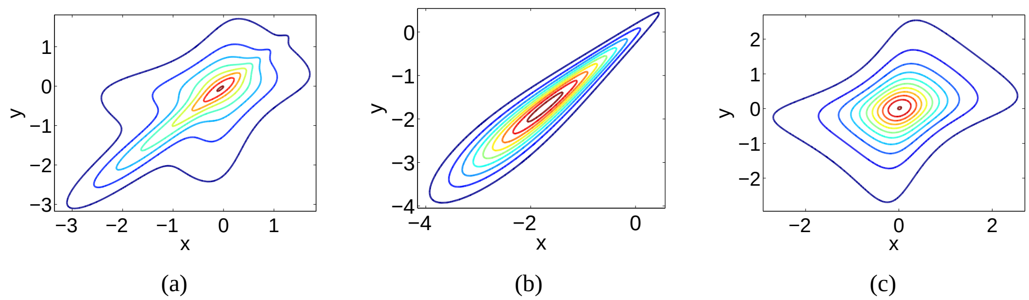


Figure 4: a) Joint probability density function $P(x,y)$ corresponding to the distribution function $F(x,y)$ using bivariate Gumbel copulas as CDN functions, with Student's-t and Gaussian marginal input CDFs; b),c) The PDFs corresponding to $\partial_{x,y}\Big[G_1(x,y)\Big]$ and $\partial_{x,y}\Big[G_2(x,y)\Big]$.

Example 2 (Product of copulas) *We can repeat the above for the case where each CDN function consists of a copula function (Nelsen, 1999). Copula functions provide a flexible means to construct CDN functions ϕ_s whose product yields a joint CDF under Lemma 6. Copula functions allow one to construct a multivariate CDF ϕ_s from marginal CDFs $\{F(x_\alpha)\}_{\alpha\in\mathcal{N}(s)}$ so that*

$$\phi_s(\mathbf{x}_s)=\zeta_s\Big(\{F(x_\alpha)\}_{\alpha\in\mathcal{N}(s)}\Big),$$

where ζ_s is a copula defined over variables $X_\alpha,\alpha\in\mathcal{N}(s)$. For the CDN shown in Figure 2, we can set the CDN functions G_1,G_2 to Gumbel copulas so that

$$G_1(x,y)=\zeta_1(H_{1,x}(x),H_{1,y}(y))=\exp\left(-\left((-\log H_{1,x}(x))^{\frac{1}{\theta_1}}+(-\log H_{1,y}(y))^{\frac{1}{\theta_1}}\right)^{\theta_1}\right),$$
$$G_2(x,y)=\zeta_2(H_{2,x}(x),H_{2,y}(y))=\exp\left(-\left((-\log H_{2,x}(x))^{\frac{1}{\theta_2}}+(-\log H_{2,y}(y))^{\frac{1}{\theta_2}}\right)^{\theta_2}\right),$$

with $H_{1,x},H_{2,x}$ set to univariate Gaussian CDFs with parameters $\mu_{1,x},\mu_{2,x},\sigma_{1,x},\sigma_{2,x}$ and $H_{1,y},H_{2,y}$ set to univariate Student's-t CDFs with parameters $\nu_{1,y},\nu_{2,y}$. One can then verify that the functions G_1,G_2 satisfy the properties of a copula function (Nelsen, 1999) and so the product of G_1,G_2 yields the CDF $F(x,y)$. An example of the resulting joint probability density $P(x,y)$ obtained by differentiation of $F(x,y)$ for parameters $\mu_{1,x}=\mu_{2,x}=-2,\sigma_{1,x}=\sigma_{2,x}=1,\ \nu_{1,y}=\nu_{2,y}=0.5,\theta_1=0.25,\theta_2=0.5$

is shown in Figure 4(a), with the PDFs corresponding to $\partial_{x,y}\Big[G_1(x,y)\Big]$ *and* $\partial_{x,y}\Big[G_2(x,y)\Big]$ *shown in Figures 4(b) and 4(c).* □

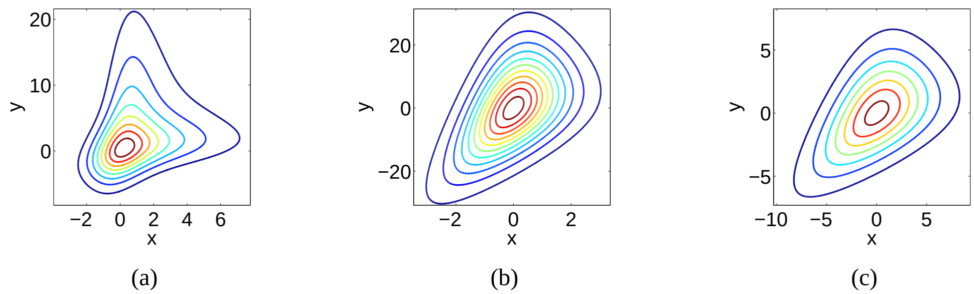


Figure 5: a) Joint probability density function $P(x,y)$ corresponding to the distribution function $F(x,y)$ using bivariate sigmoidal functions as CDN functions; b),c) The PDFs corresponding to $\partial_{x,y}\Big[G_1(x,y)\Big]$ and $\partial_{x,y}\Big[G_2(x,y)\Big]$.

Example 3 (Product of bivariate sigmoids) *As another example of a probability density function constructed using a CDN, consider the case in which functions* $G_1(x,y)$ *and* $G_1(x,y)$ *in the CDN of Figure 2 are set to be multivariate sigmoids of the form*

$$G_1(x,y) = \frac{1}{1+\exp(-w_x^1 x)+\exp(-w_y^1 y)},$$
$$G_2(x,y) = \frac{1}{1+\exp(-w_x^2 x)+\exp(-w_y^2 y)},$$

with $w_x^1, w_y^1, w_x^2, w_y^2$ *non-negative. An example of the resulting joint probability density* $P(x,y)$ *obtained by differentiation of* $F(x,y) = G_1(x,y)G_2(x,y)$ *for parameters* $w_x^1 = 12.5, w_y^1 = 0.125, w_x^2 = 0.4, w_y^2 = 0.5$ *is shown in Figure 5(a), with the PDFs corresponding to* $\partial_{x,y}\Big[G_1(x,y)\Big]$ *and* $\partial_{x,y}\Big[G_2(x,y)\Big]$ *shown in Figures 5(b) and 5(c).* □

The above examples demonstrate that one can construct multivariate CDFs by taking a product of CDFs defined over subsets of variables in the graph.

2.1 Conditional and Marginal Independence Properties of CDNs

In this section, we will derive the marginal and conditional independence properties for a CDN, which we show to be distinct from those of Bayesian networks, Markov random fields or factor graphs. As with these graphical models, marginal and conditional independence relationships can be gleaned by inspecting whether variables are separated with respect to the graph. In a bipartite graph $\mathcal{G} = (V,S,E)$, a (undirected) path of length K between two variable nodes $\alpha,\beta \in V$ consists of a sequence of distinct variable and function nodes $\alpha_0, s_0, \alpha_1, s_1, \cdots, s_K, \alpha_K$ such that $\alpha_0 = \alpha, \alpha_K = \beta$ and $(\alpha_k, s_k) = (s_k, \alpha_k) \in E$ for all $k = 0, \cdots, K$. A set $C \subseteq V$ is said to separate two variable nodes

$\alpha, \beta \in V \setminus C$ with respect to $\mathcal{G}$ if all paths from α to β intersect C. Two variable nodes $\alpha, \beta \in V$ are said to be separated if there exists any non-empty set C that separates them with respect to $\mathcal{G}$. Similarly, a set $C \subseteq V$ is said to separate two variable node sets $A, B \subseteq V \setminus C$ with respect to $\mathcal{G}$ if all paths from any variable node $\alpha \in A$ to any variable node $\beta \in B$ intersect C. Disjoint variable sets $A, B \in V$ are said to be separated if all pairs of nodes (α, β) for $\alpha \in A, \beta \in B$ are separated.

Having defined graph separation for bipartite graphs, we begin with the conditional inequality independence property of CDNs, from which other marginal and conditional independence properties for a CDN will follow.

Theorem 8 (Conditional inequality independence in CDNs) *Let $\mathcal{G} = (V, S, E)$ be a CDN and let $A, B \subseteq V$ be disjoint sets of variable nodes. If A and B are separated with respect to $\mathcal{G}$, then for any $W \subseteq V \setminus (A \cup B)$ $A \perp\!\!\!\perp B | \omega(\mathbf{x}_W)$ where $\omega(\mathbf{x}_W) \equiv \{\mathbf{X}_W \leq \mathbf{x}_W\}$.*

Proof If A and B are separated with respect to $\mathcal{G}$, then we can write

$$F(\mathbf{x}_A, \mathbf{x}_B, \mathbf{x}_{V \setminus (A \cup B)}) = g(\mathbf{x}_A, \mathbf{x}_{V \setminus (A \cup B)}) h(\mathbf{x}_B, \mathbf{x}_{V \setminus (A \cup B)})$$

for some functions g, h that satisfy the conditions of Lemma 6. This means that $F(\mathbf{x}_A, \mathbf{x}_B | \omega(\mathbf{x}_W))$ is given by

$$\begin{aligned} F(\mathbf{x}_A, \mathbf{x}_B | \omega(\mathbf{x}_W)) &= \frac{\lim\limits_{\mathbf{x}_{V \setminus (A \cup B \cup W)} \to \infty} F(\mathbf{x}_A, \mathbf{x}_B, \mathbf{x}_{V \setminus (A \cup B)})}{\lim\limits_{\mathbf{x}_{V \setminus W} \to \infty} F(\mathbf{x}_A, \mathbf{x}_B, \mathbf{x}_{V \setminus (A \cup B)})} \\ &\propto F(\mathbf{x}_A, \mathbf{x}_B, \mathbf{x}_W) = g(\mathbf{x}_A, \mathbf{x}_W) h(\mathbf{x}_B, \mathbf{x}_W), \end{aligned}$$

which implies $A \perp\!\!\!\perp B | \omega(\mathbf{x}_W)$. ■

We show that if a CDF $F(\mathbf{x})$ satisfies the conditional independence property of Theorem 8 for a given CDN, then F can be written as a product over functions $\phi_s(\mathbf{x}_s)$.

Theorem 9 (Factorization property of a CDN) *Let $\mathcal{G} = (V, S, E)$ be a bipartite graph and let the CDF $F(\mathbf{x})$ satisfy the conditional independence property implied by the CDN described by $\mathcal{G}$, so that graph separation of A and B by $V \setminus (A \cup B)$ with respect to $\mathcal{G}$ implies $A \perp\!\!\!\perp B | \omega(\mathbf{x}_W)$ for any $W \subseteq V \setminus (A \cup B)$ and for any $\mathbf{x}_W \in \mathbb{R}^{|W|}$. Then there exist functions $\phi_s(\mathbf{x}_s), s \in S$ that satisfy the properties of a CDF such that the joint CDF $F(\mathbf{x})$ factors as $\prod_{s \in S} \phi_s(\mathbf{x}_s)$.*

Proof The proof here parallels that for the Hammersley-Clifford theorem for undirected graphical models (Lauritzen, 1996). We begin our proof by defining $\psi_U(\mathbf{x}), \zeta_U(\mathbf{x})$ as functions that depend only on variable nodes in some set $U \subseteq V$ and that form a Möbius transform pair

$$\begin{aligned} \psi_U(\mathbf{x}) &= \sum_{W \subseteq U} \zeta_W(\mathbf{x}), \\ \zeta_U(\mathbf{x}) &= \sum_{W \subseteq U} (-1)^{|U \setminus W|} \psi_W(\mathbf{x}), \end{aligned}$$

where we take $\psi_U(\mathbf{x}) \equiv \log F(\mathbf{x}_U)$. Now, we note that $F(\mathbf{x})$ can always be written as a product of functions $\prod_{U \subseteq V} \phi_U(\mathbf{x})$ where each function ϕ_U satisfies the properties of a CDF: a trivial example of this is to set $\phi_V(\mathbf{x}) = F(\mathbf{x})$ and $\phi_U(\mathbf{x}) = 1$ for all $U \subset V$. Since by hypothesis F satisfies all of the conditional independence properties implied by the CDN described by $\mathcal{G}$, if we take $\phi_U(\mathbf{x}) = \exp\big(\zeta_U(\mathbf{x})\big)$, then it suffices to show that $\zeta_U(\mathbf{x}) \equiv 0$ for subsets of variable nodes U for which any two non-neighboring variable nodes $\alpha, \beta \in U$ are separated such that $\alpha \perp\!\!\!\perp \beta | \omega(\mathbf{x}_W)$ for any $W \subseteq U \setminus (\alpha, \beta)$. Observe that we can write $\zeta_U(\mathbf{x})$ as

$$\begin{aligned}\zeta_U(\mathbf{x}) &= \sum_{W \subseteq U} (-1)^{|U \setminus W|} \psi_W(\mathbf{x}) \\ &= \sum_{W \subseteq U \setminus (\alpha \cup \beta)} (-1)^{|U \setminus W|} \Big(\psi_W(\mathbf{x}) - \psi_{W \cup \alpha}(\mathbf{x}) - \psi_{W \cup \beta}(\mathbf{x}) + \psi_{W \cup \alpha \cup \beta}(\mathbf{x}) \Big).\end{aligned}$$

If $\alpha, \beta \in U$ are separated and $W \subseteq U \setminus (\alpha \cup \beta)$, then $\alpha \perp\!\!\!\perp \beta | \omega(\mathbf{x}_W)$ and

$$\begin{aligned}\psi_{W \cup \alpha \cup \beta}(\mathbf{x}) - \psi_{W \cup \alpha}(\mathbf{x}) &= \log \frac{F(x_\alpha, x_\beta, \mathbf{x}_W)}{F(x_\alpha, \mathbf{x}_W)} = \log \frac{F(x_\alpha | \omega(\mathbf{x}_W)) F(x_\beta | \omega(\mathbf{x}_W)) F(\mathbf{x}_W)}{F(x_\alpha | \omega(\mathbf{x}_W)) F(\mathbf{x}_W)} \\ &= \log \frac{F(x_\beta | \omega(\mathbf{x}_W)) F(\mathbf{x}_W)}{F(\mathbf{x}_W)} \\ &= \log F(x_\beta, \mathbf{x}_W) - \log F(\mathbf{x}_W) \\ &= \psi_{W \cup \beta}(\mathbf{x}) - \psi_W(\mathbf{x}).\end{aligned}$$

Thus if U is any set where nodes $\alpha, \beta \in U$ are separated, then for all $W \subseteq U \setminus (\alpha \cup \beta)$ we must have $\psi_W(\mathbf{x}) - \psi_{W \cup \alpha}(\mathbf{x}) - \psi_{W \cup \beta}(\mathbf{x}) + \psi_{W \cup \alpha \cup \beta}(\mathbf{x}) \equiv 0$ and so $\zeta_U(\mathbf{x}) = 0$. Since $F(\mathbf{x}) = \exp(\psi_V(\mathbf{x})) = \exp\Big(\sum_U \zeta_U(\mathbf{x})\Big) = \prod_U \phi_U(\mathbf{x})$ where the product is taken over subsets of variable nodes U that are not separated. Now, we note that for any U that is not separated, we must have $U \subseteq \mathcal{N}(s)$ (as $U = \mathcal{N}(s) \cup A$ for some A with $\mathcal{N}(s) \cap A = \emptyset$ implies that U is not separated) for some $s \in S$ and so we can write $F(\mathbf{x}) = \prod_U \phi_U(\mathbf{x}) = \prod_{s \in S} \prod_{U \subseteq \mathcal{N}(s)} \phi_U(\mathbf{x}) = \prod_{s \in S} \phi_s(\mathbf{x}_s)$, where $\phi_s(\mathbf{x}_s) = \prod_{U \subseteq \mathcal{N}(s)} \phi_U(\mathbf{x})$ satisfies the properties of a CDF given that functions $\phi_U(\mathbf{x})$ each satisfy the properties of a CDF. Thus we can write $F(\mathbf{x}) = \prod_{s \in S} \phi_s(\mathbf{x}_s)$, where each function ϕ_s is defined over the set of variable nodes $\mathcal{N}(s)$. ■

Thus, if $F(\mathbf{x})$ satisfies the conditional independence property where graph separation of A and B with respect to $\mathcal{G}$ implies $A \perp\!\!\!\perp B | \omega(\mathbf{x}_W)$ for any $W \subseteq V \setminus (A, B)$, then F can be written as a product of functions of the form $\prod_{s \in S} \phi_s(\mathbf{x}_s)$. The above theorem then demonstrates equivalence between the conditional independence property $A \perp\!\!\!\perp B | \omega(\mathbf{x}_W)$ and the factored form for $F(\mathbf{x})$.

The conditional inequality independence property for CDNs then implies that variables that are separated in the CDN are marginally independent. An example of the marginal independence property for a three-variable CDN in Figure 6, where variables X and Y are separated by variable Z with respect to graph $\mathcal{G}$, and so are marginally independent. In a CDN, variables that share no neighbors in the CDN graph are marginally independent: we formalize this with the following theorem.

Theorem 10 (Marginal Independence) *Let $\mathcal{G} = (V, S, E)$ be a CDN and let $A, B \subseteq V$ be disjoint sets of variables. Then $A \perp\!\!\!\perp B$ if $\mathcal{N}(A) \bigcap \mathcal{N}(B) = \emptyset$.* □

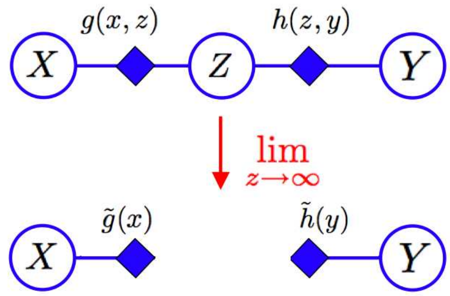


Figure 6: Marginal independence property of CDNs: if two variables X and Y share no common function nodes, they are marginally independent.

Proof Follows from Theorem 8 with $\mathbf{x}_W \to \infty$. ■

Note that the converse to the above does not generally hold: if disjoint sets A and B do share functions in S, they can still be marginally independent, as one can easily construct a bipartite graph in which variable nodes are not separated in the graph but the function nodes connecting A to B correspond to factorized functions so that $A \perp\!\!\!\perp B$. Given the above marginal independence property in a CDN, we now consider the conditional independence property of a CDN. To motivate this, we first present a toy example in Figure 7 in which we are given CDNs for variables X,Y,Z,W and we condition on variable Z. Here the separation of X and Y by unobserved variable W implies $X \perp\!\!\!\perp Y|Z$, but separation of X and Y by Z only implies the marginal independence relationship $X \perp\!\!\!\perp Y$. In general, variable sets that are separated in a CDN by unobserved variables will be conditionally independent given all other variables: thus, as long as two variables are separated by some unobserved variables they are independent, irrespective of the fact that other variables may be observed as well. We formalize this conditional independence property with the following theorem.

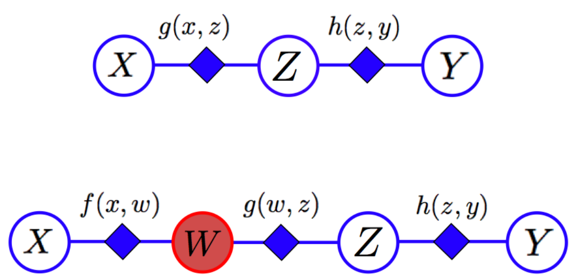


Figure 7: Conditional independence in CDNs. Two variables X and Y that are separated with respect to the graph are marginally independent (*top*). When an unobserved variable W (shaded to denote its unobserved status) separates X from Y, X,Y are conditionally independent given Z (*bottom*). The bottom graph thus implies $X \perp\!\!\!\perp Y$,$X \perp\!\!\!\perp Z$, $W \perp\!\!\!\perp Y$, $X \perp\!\!\!\perp Y|W$ and $X \perp\!\!\!\perp Y|Z$.

Theorem 11 (Conditional independence in CDNs) *Let $\mathcal{G} = (V,S,E)$ be a CDN. For all disjoint sets of $A,B,C \subseteq V$, if C separates A from B relative to graph $\mathcal{G}$ then*

$$A \perp\!\!\!\perp B | V \setminus (A \cup B \cup C).$$

$\square$.

Proof If C separates A from B, then marginalizing out variables in C yields two disjoint subgraphs with variable sets A', B', with $A \subseteq A', B \subseteq B'$, $A' \cup B' = V \setminus C$ and $\mathcal{N}(A') \bigcap \mathcal{N}(B') = \emptyset$. From Theorem 10, we therefore have $A' \perp\!\!\!\perp B'$. Now consider the set $V \setminus (A \cup B \cup C)$ and let $\tilde{A}, \tilde{B}$ denote a partition of the set so that

$$\tilde{A} \cup \tilde{B} = V \setminus (A \cup B \cup C), \quad \tilde{A} \cap \tilde{B} = \emptyset,$$
$$\tilde{A} \cap B' = \emptyset, \quad \tilde{B} \cap A' = \emptyset.$$

From the semi-graphoid axioms (Lauritzen, 1996; Pearl, 1988), $A' \perp\!\!\!\perp B'$ implies $A \perp\!\!\!\perp B | V \setminus (A \cup B \cup C)$ since $\tilde{A} \subset A'$ and $\tilde{B} \subset B'$. ■

An illustration of the proof is provided in Figures 8(a) and 8(b). The above conditional independence property is distinct from that described in Theorem 8, as in the latter we condition on inequality events of the type $\omega(\mathbf{x}_W)$, whereas in the former we condition on observations $\mathbf{x}_W$ themselves.

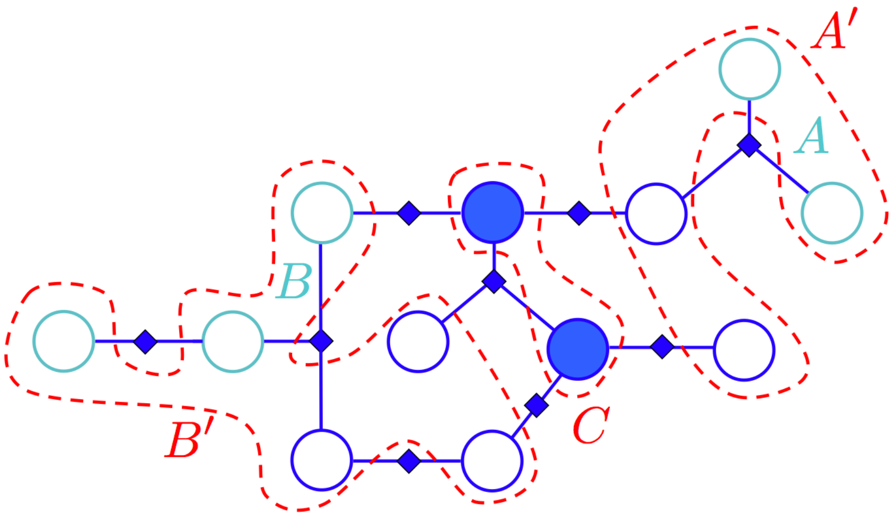
In addition to the above, both the conditional independence properties of Theorem 11 and 8 are closed under marginalization, which consists of computing limits of CDN functions. Thus if $\mathcal{G}$ is a CDN model for $F(\mathbf{x})$, then the graph for CDN for CDF $F(\mathbf{x}_A) = \lim_{\mathbf{x}_{V \setminus A} \to \infty} F(\mathbf{x}_A, \mathbf{x}_{V \setminus A})$ is given by a subgraph of $\mathcal{G}$ which then implies only a subset of the independence properties of $\mathcal{G}$. The next proposition formalizes this.

Proposition 12 *Let $\mathcal{G} = (V,S,E)$ be a CDN and let $A,B,C \subset V$ be disjoint sets of nodes with $C \subseteq V \setminus (A \cup B)$ separating A from B with respect to $\mathcal{G}$. Let $\mathcal{G}' = (V', S', E')$ be a subgraph of $\mathcal{G}$ with $V' \subseteq V, S' \subseteq S, E' \subseteq E$. Similarly, let $A' = A \cap V', B' = B \cap V', C' = C \cap V'$ be disjoint sets of nodes. Then C' separates A' from B' with respect to $\mathcal{G}'$.* $\square$

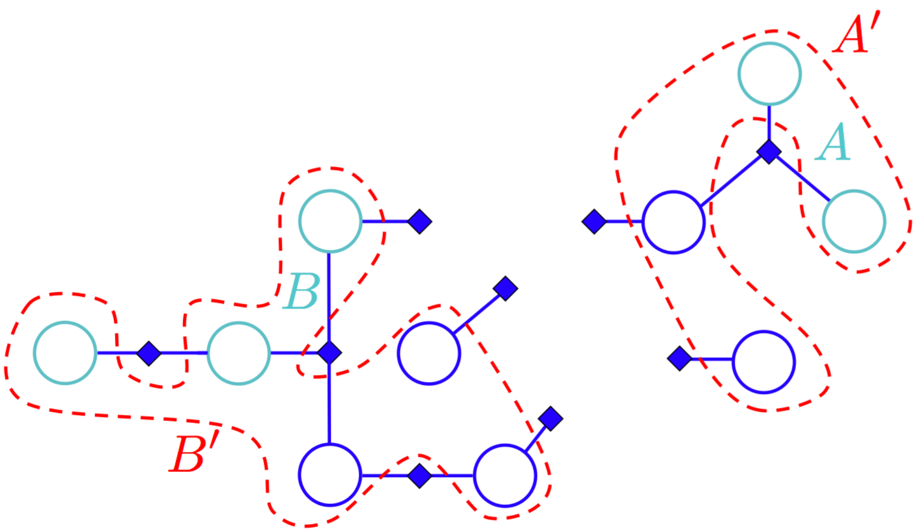
The above proposition is illustrated in Figures 9(a) and 9(b). As a result, the conditional independence relation $A' \perp\!\!\!\perp B' | V' \setminus (A' \cup B' \cup C')$ must also hold in the subgraph $\mathcal{G}'$, such that $\mathcal{G}'$ implies a subset of the independence constraints implied by $\mathcal{G}$. The above closure property under marginalization is a property that also holds for Markov random fields, but not for Bayesian networks (see Richardson and Spirtes, 2002 for an example). The above closure and conditional independence properties for CDNs have also been previously shown to hold for bi-directed graphs as well, which we will now describe.

2.2 The Relationship Between Cumulative Distribution Networks and Bi-directed Graphs

Graphical models with some of the independence properties of CDNs have in fact been studied previously in the statistics literature. The marginal independence property for CDNs is in fact identical to the global Markov property of Richardson and Spirtes (2002), which was derived in the context of bi-directed graphical models (Drton and Richardson, 2008; Richardson and Spirtes, 2002; Richardson, 2003). A bi-directed graph $G = (V,E)$ consists of nodes $\alpha \in V$ and *bi-directed* edges $e \in E$



(a)



(b)

Figure 8: Example of conditional independence due to graph separation in a CDN. a) Given bipartite graph $\mathcal{G} = (V, S, E)$, node set C separates set A from B (nodes in light blue) with respect to $\mathcal{G}$. Furthermore, we have for A', B' (nodes in red dotted line) $A \subseteq A', B \subseteq B'$, $A' \cup B' = V \setminus C$ and $\mathcal{N}(A') \bigcap \mathcal{N}(B') = \emptyset$ as shown. b) Marginalizing out variables corresponding to nodes in C yields two disjoint subgraphs of $\mathcal{G}$ and so $A \perp\!\!\!\perp B | V \setminus (A \cup B \cup C)$.

corresponding to unordered pairs of nodes α, β, denoted by (α, β). Alternately, we denote edges in

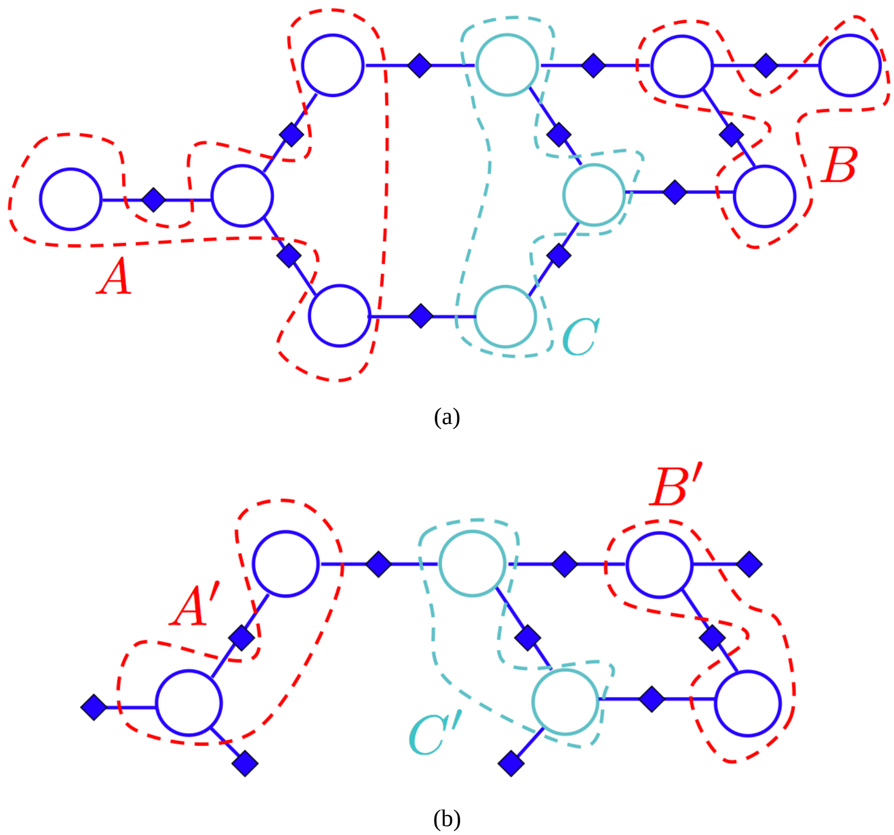


Figure 9: Example of closure under marginalization in a CDN. a) Given CDN $\mathcal{G} = (V, S, E)$, node set C separates set A from B (nodes in light blue) with respect to $\mathcal{G}$. b) For subgraph $\mathcal{G}' = (V', S', E')$ with $A' \subseteq A, B' \subseteq B, C' \subseteq C$, C' separates A' from B' with respect to $\mathcal{G}'$.

a bi-directed graph as $(\alpha, \beta) \equiv \alpha \leftrightarrow \beta$.[1] In a bi-directed graph G, the *global Markov property* corresponds to two disjoint variable sets $A, B \subseteq V$ satisfying the marginal independence constraint $A \perp\!\!\!\perp B$ if there are no paths between any $\alpha \in A$ and any $\beta \in B$. It can be shown (Richardson and Spirtes, 2002) that any bi-directed graphical model corresponds to a directed graphical model with latent variables marginalized out. In particular, we define the *canonical* directed acyclic graph (DAG) for the bi-directed graph G as a directed graph $\tilde{G}$ with additional latent variables such that if $\alpha \leftrightarrow \beta$ in G, then $\alpha \leftarrow u_{\alpha,\beta} \rightarrow \beta$ in $\tilde{G}$ for some latent variable $u_{\alpha,\beta}$. Thus bi-directed graphical models can be viewed as models obtained from a corresponding canonical DAG with latent variables marginalized out, such that independence constraints between neighboring variable nodes in G can be viewed as arising from the absence of any shared latent variables in the canonical DAG $\tilde{G}$. This suggests the usefulness of bi-directed graphical models for problems where we cannot discount the presence of unobserved variables but we either A) do not have sufficient domain knowledge to specify distributions for latent variables, and/or B) we wish to avoid marginalizing over these latent variables.

1. Note that $\alpha \leftrightarrow \beta$ is *not* equivalent to having both directed edges $\alpha \rightarrow \beta$ and $\alpha \leftarrow \beta$.

In such cases, one can instead attempt to parameterize a probability defined on observed variables using a bi-directed graphical model in which independence constraints among variables are implied by both the corresponding canonical DAG and bi-directed graphs. Examples of a canonical DAG and corresponding bi-directed graph that imply the same set of independence constraints among observed variables are shown in Figures 10(a) and 10(b). Several parameterizations had been previously proposed for bi-directed graphical models. Covariance graphs (Kauermann, 1996) were proposed in which variables are jointly Gaussian with zero pairwise covariance if there is no edge connecting the two variables in the bi-directed graph. In addition, Silva and Ghahramani (2009a) proposed a mixture model with latent variables in which dependent variables in the bi-directed graph can be explained by the causal influence of common components in the mixture model. For bi-directed graphical models defined over binary variables, a parametrization was proposed based on joint probabilities over connected components of the bi-directed graph so that the joint probability of any subset of variables could be obtained by Möbius inversion (Drton and Richardson, 2008).

Suppose now that we are given a bi-directed graph G and a CDN $\mathcal{G}$ defined over the same variables nodes V. Let G and $\mathcal{G}$ have the same connectivity, such that for any pair of variable nodes $\alpha,\beta \in V$, a path between α,β exists both in G and $\mathcal{G}$. Then both G and $\mathcal{G}$ imply the same set of marginal independence constraints, as we have shown above that in a CDN, two nodes that do not share any function nodes in common are marginally independent (Theorem 10). An example of a bi-directed graph and CDN that imply the same set of marginal independence constraints is shown in Figures 10(b) and 10(c). In addition to implying the same marginal independence constraints as a bi-directed graphical model, the conditional independence property given in Theorem 11 for CDNs corresponds to the dual global Markov property of Kauermann (1996) for bi-directed graphical models, which we now present.

Theorem 13 *Let $G = (V,E)$ be a bi-directed graphical model and let $A,B,C \subseteq V$ be three disjoint node sets so that $V \setminus (A \cup B \cup C)$ separates A from B with respect to G. Then $A \perp\!\!\!\perp B | C$.* □

Note that this is identical to the conditional independence property of Theorem 11 where the separating set is set to $V \setminus (A \cup B \cup C)$ instead of C.

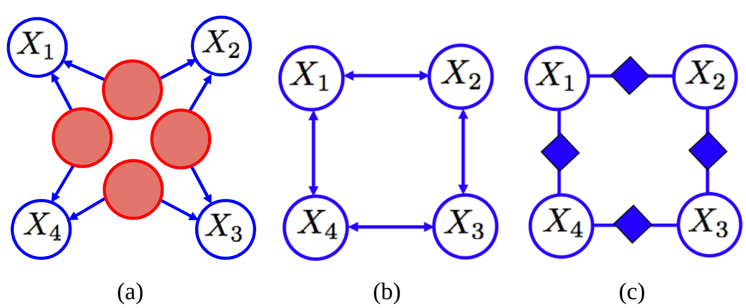


Figure 10: Graphical models over four variables X_1, X_2, X_3, X_4 in which graph separation of variable nodes imply the marginal independence relations $X_1 \perp\!\!\!\perp X_3, X_2 \perp\!\!\!\perp X_4$. a) A canonical directed acyclic graphical model with additional latent variables, shown as shaded nodes; b)A bi-directed graph; b) A corresponding CDN.

While the conditional and marginal independence constraints implied by both a bi-directed graph and a CDN of the same connectivity are identical, Theorem 8 shows that conditional independence constraints of the form $A \perp\!\!\!\perp B|\omega(\mathbf{x}_W)$ are implied in a CDN which are not included in the definition for a bi-directed graph of the same connectivity. As a result of these *additional* constraints, CDNs model a subset of the distributions that satisfy the independence constraints of a corresponding bi-directed graph with the same connectivity. In general, CDNs do not model the full set of the probability distributions that can be modeled by bi-directed graphical models with the same connectivity. The following example illustrates how the conditional inequality independence property of CDNs is in general not implied by a bi-directed graphical model with the same graph topology.

Example 4 *Consider a 3-variable covariance graph model consisting of the bi-directed graph $X_1 \leftrightarrow X_2 \leftrightarrow X_3$, where X_1, X_2, X_3 are jointly Gaussian with zero mean and covariance matrix $\mathbf{\Sigma}$. The proposed covariance graph model imposes the marginal independence constraint $X_1 \perp\!\!\!\perp X_3$, as there is no edge between variables X_1, X_3. Denoting σ_{ij} as element (i, j) of $\mathbf{\Sigma}$, this is equivalent to the constraint $\sigma_{13} = \sigma_{31} = 0$. Now suppose further that the conditional inequality independence property $X_1 \perp\!\!\!\perp X_3|\omega(x_2)$ is also implied by the covariance graph model. By Theorem 9, this implies that the joint CDF $F(x_1, x_2, x_3)$ factors as*

$$F(x_1,x_2,x_3) = \mathbf{\Phi}\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}; \mathbf{0}, \mathbf{\Sigma} \right) = g(x_1,x_2)h(x_2,x_3),$$

where $\mathbf{\Phi}(\mathbf{x}; \boldsymbol{\mu}, \mathbf{\Sigma})$ is the multivariate Gaussian CDF with mean zero and covariance matrix $\mathbf{\Sigma}$, and $g(x_1, x_2), h(x_2, x_3)$ are functions that satisfy the properties of a CDF. The constraints on functions $g(x_1, x_2), h(x_2, x_3)$ are given by marginalization with respect to subsets of variables:

$$\begin{aligned} F(x_1,x_2,\infty) &= g(x_1,x_2)h(x_2,\infty), \\ F(\infty,x_2,x_3) &= g(\infty,x_2)h(x_2,x_3), \\ F(\infty,x_2,\infty) &= g(\infty,x_2)h(x_2,\infty), \end{aligned}$$

so that and so multiplying $F(x_1, x_2, \infty)$ and $F(\infty, x_2, x_3)$, we obtain

$$F(x_1,x_2,x_3)F(\infty,x_2,\infty) = F(x_1,x_2,\infty)F(\infty,x_2,x_3). \tag{1}$$

Thus, if the conditional inequality independence constraint $X_1 \perp\!\!\!\perp X_3|\omega(x_2)$ is also implied by the covariance graph model for the joint Gaussian CDF $F(x_1, x_2, x_3)$, then the above equality should hold for all $(x_1, x_2, x_3) \in \mathbb{R}^3$ and for any positive-definite covariance matrix $\mathbf{\Sigma}$ for which $\sigma_{13} = \sigma_{31} = 0$. Let $x_1 = x_2 = x_3 = 0$ and let $\mathbf{\Sigma}$ be given by

$$\mathbf{\Sigma} = \begin{bmatrix} 1 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 1 & -\frac{1}{2} \\ 0 & -\frac{1}{2} & 1 \end{bmatrix},$$

so that $\rho_{12} = \frac{\sqrt{2}}{2}, \rho_{23} = -\frac{1}{2}$ are the pairwise correlations between X_1, X_2 and X_2, X_3. From Stuart and Ord (1994), we can analytically evaluate joint Gaussian CDFs at the origin as a function of *correlation parameters, so that*

$$
\begin{aligned}
F(\infty,0,\infty) &= \frac{1}{2}, \\
F(0,0,\infty) &= \Phi\left(\begin{bmatrix}0\\0\end{bmatrix};\mathbf{0},\mathbf{\Sigma}_{12}\right) = \frac{1}{4}+\frac{1}{2\pi}\sin^{-1}\rho_{12} = \frac{3}{8}, \\
F(\infty,0,0) &= \Phi\left(\begin{bmatrix}0\\0\end{bmatrix};\mathbf{0},\mathbf{\Sigma}_{23}\right) = \frac{1}{4}+\frac{1}{2\pi}\sin^{-1}\rho_{23} = \frac{1}{6}, \\
F(0,0,0) &= \Phi\left(\begin{bmatrix}0\\0\\0\end{bmatrix};\mathbf{0},\mathbf{\Sigma}\right) = \frac{1}{8}+\frac{1}{4\pi}(\sin^{-1}\rho_{12}+\sin^{-1}\rho_{23}+\sin^{-1}\rho_{13}) \\
&= \frac{1}{8}+\frac{1}{4\pi}(\sin^{-1}\rho_{12}+\sin^{-1}\rho_{23}) = \frac{7}{48},
\end{aligned}
$$

where $\mathbf{\Sigma}_{ij}$ is the sub-matrix consisting of rows and columns (i,j) in $\mathbf{\Sigma}$, ρ_{ij} is the correlation coefficient between variables i,j, and $\rho_{13}=0$ is implied by the covariance graph. From Equation (1)*, we must have*

$$F(0,0,0)F(\infty,0,\infty) = F(0,0,\infty)F(\infty,0,0) \Leftrightarrow \frac{7\cdot 1}{48\cdot 2} = \frac{3\cdot 1}{8\cdot 6},$$

so that the equality does not hold. Thus, the conditional inequality independence constraint $X_1 \perp\!\!\!\perp X_3|\omega(x_2)$ is not implied by the covariance graph model. It can also be verified that the expression for $F(x_1,x_2,x_3)$ given in Equation (1) *does not in general correspond to a proper PDF when $F(x_1,x_2),F(x_2,x_3),F(x_2)$ are Gaussians, as $\partial_{x_1,x_2,x_3}\Big[F(x_1,x_2,x_3)\Big]$ is not non-negative for all $(x_1,x_2,x_3)\in\mathbb{R}^3$.*

The previous example shows that while graph separation of variable node sets A,B with respect to both bi-directed graphical models and CDNs of the same connectivity implies the same set of marginal independence constraints, in CDNs we have the *additional* constraint of $A \perp\!\!\!\perp B|\omega(\mathbf{x}_C)$, a constraint that is not implied by the corresponding bi-directed graphical model. The above example shows how such additional constraints can then impose constraints on the joint probabilities that can be modeled by CDNs. However, for probabilities that can be modeled by any of CDN, bi-directed graph or corresponding canonical DAG models, CDNs can provide closed-form parameterizations where other types of probability models might not.

In the case of CDNs defined over discrete variables taking values in an ordered set $\mathcal{X} = \{r_1,\cdots,r_K\}$, the conditional independence property $A \perp\!\!\!\perp B|\omega(\mathbf{x}_W)$ for $W \subseteq V\setminus(A\cup B)$ (Theorem 8) implies that conditioning on the event $\mathbf{X}_C = r_1\mathbf{1}$ yields conditional independence between disjoint sets $A,B,C\subseteq V$ in which C separates A,B with respect to $\mathcal{G}$. We define the corresponding *min-independence* property below.

Definition 14 (Min-independence) *Let $\mathbf{X}_A,\mathbf{X}_B,\mathbf{X}_C$ be sets of ordinal discrete variables that take on values in the totally ordered alphabet $\mathcal{X}$ with minimum element $r_1\in\mathcal{X}$ defined as $r_1 \prec \alpha\,\forall\alpha\neq r_1,\alpha\in\mathcal{X}$. $\mathbf{X}_A$ and $\mathbf{X}_B$ are said to be min-independent given $\mathbf{X}_C$ if*

$$\mathbf{X}_A \perp\!\!\!\perp \mathbf{X}_B|\mathbf{X}_C = r_1\mathbf{1},$$

where $r_1\mathbf{1} = [r_1\; r_1\;\cdots\; r_1]^T$. □

Theorem 15 (Min-independence property of CDNs) *Let $\mathcal{G} = (V,S,E)$ be a CDN defined over ordinal discrete variables that take on values in the totally ordered alphabet $\mathcal{X}$ with minimum element $r_1 \in \mathcal{X}$ defined as $r_1 \prec \alpha \,\forall \alpha \neq r_1, \alpha \in \mathcal{X}$. Let $A,B,C \subseteq V$ be arbitrary disjoint subsets of V, with C separating A,B with respect to $\mathcal{G}$. Then $\mathbf{X}_A$ and $\mathbf{X}_B$ are min-independent given $\mathbf{X}_C$.* □

Proof This follows directly from Theorem 8 with $\mathbf{x}_c = r_1\mathbf{1}$. ■

Thus, in the case of a CDN defined over discrete variables where each variable can have values in the totally ordered alphabet $\mathcal{X}$, a finite difference with respect to variables $\mathbf{X}_C$, when evaluated at the vector of minimum elements $\mathbf{X}_C = r_1\mathbf{1}$ is equivalent to directly evaluating the CDF at $\mathbf{X}_C = r_1\mathbf{1}$. This means that in the case of models defined over ordinal discrete variables, the particular set of conditional independence relationships amongst variables in the model is determined as a function of the ordering over possible labels for each variable in the model, so that one must exercise care in how such variables are labeled and what ordering is satisfied by such labels.

2.3 Stochastic Orderings in a Cumulative Distribution Network

The CDN, as a graphical model for the joint CDF over many random variables, also allows one to easily specify *stochastic ordering* constraints between subsets of variables in the model. Informally, a stochastic ordering relationship $X \preceq Y$ holds between two random variables X,Y if samples of Y tend to be larger than samples of X. We will focus here on first-order stochastic ordering constraints (Lehmann, 1955; Shaked and Shanthikumar, 1994) of the form $X \preceq Y$ and how one can specify such constraints in terms of the CDN functions in the model. We note that such constraints are not a necessary part of the definition for a CDN or for a multivariate CDF, so that the graph for the CDN alone does not allow one to inspect stochastic ordering constraints based on graph separation of variables. However, the introduction of stochastic ordering constraints, in combination with separation of variables with respect to the graph, do impose constraints on the products of CDN functions, as we will now show. We will define below the concept of first-order stochastic orderings among random variables, as this is the primary definition for a stochastic ordering that we will use. We refer the reader to Lehmann (1955) and Shaked and Shanthikumar (1994) for additional definitions.

Definition 16 *Consider two scalar random variables X and Y with marginal CDFs $F_X(x)$ and $F_Y(y)$. Then X and Y are said to satisfy the first-order stochastic ordering constraint $X \preceq Y$ if $F_X(t) \geq F_Y(t)$ for all $t \in \mathbb{R}$.* □

The above definition of stochastic ordering is stronger than the constraint $\mathbb{E}[X] \leq \mathbb{E}[Y]$ which is often used and one can show that $X \preceq Y$ implies the former constraint. Note that the converse is not true: $\mathbb{E}[X] \leq \mathbb{E}[Y]$ does not necessarily imply $X \preceq Y$. For example, consider two Gaussian random variables X and Y for which $\mathbb{E}[X] \leq \mathbb{E}[Y]$ but $Var[X] \gg Var[Y]$. The definition of a stochastic ordering can also be extended to disjoint sets of variables $\mathbf{X}_A$ and $\mathbf{X}_B$.

Definition 17 *Let $\mathbf{X}_A$ and $\mathbf{X}_B$ be disjoint sets of variables so that $\mathbf{X}_A = \{X_{\alpha_1}, \cdots, X_{\alpha_K}\}$ and $\mathbf{X}_B = \{X_{\beta_1}, \cdots, X_{\beta_K}\}$ for some strictly positive integer K. Let $F_{\mathbf{X}_A}(\mathbf{t})$ and $F_{\mathbf{X}_B}(\mathbf{t})$ be the CDFs of $\mathbf{X}_A$ and $\mathbf{X}_B$. Then $\mathbf{X}_A, \mathbf{X}_B$ are said to satisfy the stochastic ordering relationship $\mathbf{X}_A \preceq \mathbf{X}_B$ if*

$$F_{\mathbf{X}_A}(\mathbf{t}) \geq F_{\mathbf{X}_B}(\mathbf{t})$$

for all $\mathbf{t} \in \mathbb{R}^K$. □

Having defined stochastic orderings, we will now present the corresponding constraints on CDN functions which are implied by the above definitions.

Proposition 18 *Let $\mathcal{G} = (V,S,E)$ be a CDN, with $A,B \subset V$ so that $A = \{\alpha_1,\cdots,\alpha_K\}$ and $B = \{\beta_1,\cdots,\beta_K\}$ for some strictly positive integer K. Let $\mathbf{t} \in \mathbb{R}^K$. Then A,B satisfy the stochastic ordering relationship $\mathbf{X}_A \preceq \mathbf{X}_B$ if and only if*

$$\prod_{s\in\mathcal{N}(A)} \lim_{\mathbf{u}_{\mathcal{N}(s)\setminus A}\to\infty} \phi_s(\mathbf{u}_{\mathcal{N}(s)\setminus A},\mathbf{t}_{\mathcal{N}(s)\bigcap A}) \geq \prod_{s\in\mathcal{N}(B)} \lim_{\mathbf{u}_{\mathcal{N}(s)\setminus B}\to\infty} \phi_s(\mathbf{u}_{\mathcal{N}(s)\setminus B},\mathbf{t}_{\mathcal{N}(s)\bigcap B})$$

for all $\mathbf{t} \in \mathbb{R}^K$. □

The above can be readily obtained by marginalizing over variables in $V\setminus A, V\setminus B$ respectively to obtain expressions for $F(\mathbf{x}_A), F(\mathbf{x}_B)$ as products of CDN functions. The corresponding ordering then holds from Definition 17 if and only if $F_{\mathbf{X}_A}(\mathbf{t}) \geq F_{\mathbf{X}_B}(\mathbf{t})$ for all $\mathbf{t} \in \mathbb{R}^K$.

2.4 Discussion

We have presented the CDN and sufficient conditions on the functions in the CDN in order for the CDN to model to a CDF. We have shown that the conditional independence relationships that follow from graph separation in CDNs are different from the relationships implied by graph separation in Bayesian networks, Markov random fields and factor graph models. We have shown that the conditional independence properties of CDNs include, but are not limited to, the marginal independence properties of bi-directed graphs, such that CDNs model a subset of all probability distributions that could be modeled by bi-directed graphs.

As we have shown, performing marginalization in a CDN consists of computing limits, unlike marginalization in models for probability densities. Furthermore, conditioning on observations in a CDN consists of computing derivatives. In the next section, we show how these two operations can be performed efficiently for tree-structured CDNs using message-passing, where messages being passed in the graph for the CDN correspond to mixed derivatives of the joint CDF with respect to variables in subtrees of the graph.

3. The Derivative-sum-product Algorithm

In the previous section, we showed that for a joint CDF, we could compute conditional probabilities of the forms $F(\mathbf{x}_A|\omega(\mathbf{x}_B)), F(\mathbf{x}_A|\mathbf{x}_B), P(\mathbf{x}_A|\omega(\mathbf{x}_B))$ and $P(\mathbf{x}_A|\mathbf{x}_B)$, in addition to probabilities of the type $P(\mathbf{x}_A), F(\mathbf{x}_A)$. In directed, undirected or factor graphs, computing and evaluating such conditional CDFs/PDFs would generally require us to integrate over several variables. In a CDN, computing and evaluating such conditionals corresponds to *differentiating* the joint CDF and then evaluating the total mixed derivative for any given vector of observations $\mathbf{x}$. In this section we will show that if we model the joint CDF using a CDN with a tree-structured graph, then we can derive a class of message-passing algorithms called *derivative-sum-product* (DSP) for efficiently computing and evaluating derivatives in CDNs. Since that the CDF factorizes for a CDN, the global mixed derivative can then be decomposed into a series of local mixed derivative computations, where each function $s \in S$ and its derivatives is evaluated for observations $\mathbf{x}_s$. Throughout this section, we will assume that the sufficient conditions for the CDN functions $\phi_s(\mathbf{x}_s)$ hold in order for the CDN to model a valid joint CDF (Lemma 6). We will further assume that the derivatives/ finite differences of CDN functions $\phi_s(\mathbf{x}_s)$ with respect to all subsets of argument variables exist and that the order of differentiation does not affect the computation of any mixed derivatives. In the case where we are differentiating with respect to a set of variables $\mathbf{X}_C$ that are observed with values $\mathbf{x}_C$, we assume that the resulting derivative/finite difference is evaluated at the observed values $\mathbf{x}_C$. In the case where we are given a function $G(x)$ defined over a single ordinal discrete variable $x \in \mathcal{X}$ where $\mathcal{X} = \{r_0, r_1, \cdots, r_{N-1}\}$ and $r_0 < r_1 \cdots < r_{N-1}, r_i \in \mathbb{R}$ are N real-valued scalars, we define the finite difference of G with respect to x, evaluated at x as

$$\partial_x \Big[G(x) \Big] = \begin{cases} G(r_0) & \text{if } x = r_0, \\ G(r_i) - G(r_{i-1}) & \text{if } x = r_i,\ i = 1, \cdots, N-1. \end{cases}$$

3.1 Differentiation in Cumulative Distribution Networks

We first consider the problem of computing the marginal CDF $F(x_\alpha)$ for particular variable X_α. We note that in the CDN, marginalization corresponds to taking limits with respect to the variables in the model, so if we let

$$F(\mathbf{x}) = F(x_\alpha, \mathbf{x}_{V\setminus\alpha}) = \prod_{s\in\mathcal{N}(\alpha)} \phi_s(x_\alpha, \mathbf{x}_{\mathcal{N}(s)\setminus\alpha}) \prod_{s\notin\mathcal{N}(\alpha)} \phi_s(\mathbf{x}_s),$$

then the marginal CDF for X_α is given by

$$F(x_\alpha) = \lim_{\mathbf{x}_{V\setminus\alpha}\to\infty} F(x_\alpha, \mathbf{x}_{V\setminus\alpha}) = \prod_{s\in\mathcal{N}(\alpha)} \phi_s(x_\alpha, \infty) \prod_{s\notin\mathcal{N}(\alpha)} \phi_s(\infty) = \prod_{s\in\mathcal{N}(\alpha)} \phi_s(x_\alpha, \infty).$$

Thus for any x_α, we can obtain any distribution of the type $F(\mathbf{x}_A)$ in time $O(|S||V|)$ by taking the product of limits of functions $\lim_{\mathbf{x}_{\mathcal{N}(s)\setminus\alpha}\to\infty} \phi_s(x_\alpha, \mathbf{x}_{\mathcal{N}(s)\setminus\alpha}) = \phi_s(x_\alpha, \infty)$. Furthermore, we can compute any conditional cumulative distribution of the type $F(\mathbf{x}_A|\omega(\mathbf{x}_B))$ in the same fashion by marginalizing the joint CDF over variables in $V \setminus (A \cup B)$ and computing

$$F(\mathbf{x}_A|\omega(\mathbf{x}_B)) = \frac{F(\mathbf{x}_A, \mathbf{x}_B)}{F(\mathbf{x}_B)} = \frac{\lim_{\mathbf{x}_{V\setminus(A\cup B)}\to\infty} F(\mathbf{x})}{\lim_{\mathbf{x}_{V\setminus B}\to\infty} F(\mathbf{x})}.$$

Note that the above marginalization contrasts with the problem of exact inference in density models, where local marginalization corresponds to computing integrals or sums of the joint PDF/PMF over variable states.

Although obtaining marginals in the CDN is relatively simple, computing and evaluating probability distributions of the form $F(\mathbf{x}_A|\mathbf{x}_B), P(\mathbf{x}_A|\omega(\mathbf{x}_B)), P(\mathbf{x}_A|\mathbf{x}_B)$ and $P(\mathbf{x}_A)$ is more involved. We have seen previously that in order to compute conditional CDFs, we must compute corresponding higher-order derivatives with respect to these observed variables. In particular, given observed data we may wish to numerically evaluate probabilities under the model, such that computing derivatives for each function ϕ_s requires that we store only the numerical value for the derivatives. Provided that the CDN functions are chosen to be themselves tractable to evaluate and differentiate, computing derivatives of these functions will consist of tractable function evaluations.

Since the factorization of the joint CDF modeled by a CDN consists of a product of functions $\phi_s(\mathbf{x}_s)$, the intuition here is that we can distribute the differentiation operation such that at each function node in the CDN, we compute the derivatives with respect to local variables and pass the result to its neighbors. The resulting algorithm consists of passing messages $\mu_{\alpha\to s}(\mathbf{x}), \mu_{s\to\alpha}(\mathbf{x})$ from variable nodes to function nodes and from function nodes to variable nodes, analogous to the operation of the sum-product algorithm in factor graphs. In the Appendix, we present the derivation of the algorithm in the setting where we wish to compute the mixed derivative of the CDF $F(\mathbf{x})$ modeled by a tree-structured CDN: the derivation is analogous to the derivation for the sum-product algorithm, but with the summation operator replaced by the differentiation operator. To illustrate the corresponding message-passing algorithm, consider the following toy example.

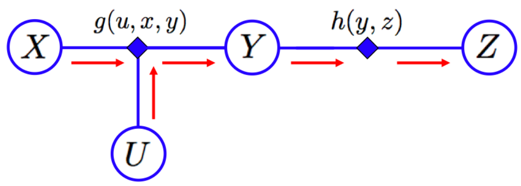


Figure 11: Flow of messages in the toy example of CDN defined over variables X,Y,Z,U.

Example 5 *Consider the CDN over four random variables U,X,Y,Z from Figure 11. The joint CDF is given by $F(u,x,y,z) = g(u,x,y)h(y,z)$. Let Z be the root node so that X and U are leaf nodes. Then the messages from leaf variable nodes to the root are given by*

$$\begin{aligned}
&\mu_{X\to g}(x) = 1,\\
&\mu_{U\to g}(u) = 1,\\
&\mu_{g\to Y}(y;u,x) = \partial_{u,x}\Big[g(u,x,y)\mu_{X\to g}(x)\mu_{U\to g}(u)\Big],\\
&\mu_{Y\to h}(y;u,x) = \mu_{g\to Y}(y;u,x),\\
&\mu_{h\to Z}(z;u,x,y) = \partial_y\Big[h(y,z)\mu_{Y\to h}(y;u,x)\Big].
\end{aligned}$$

Figure 11 shows the flow of the above messages.

Once we have propagated messages from the leaf nodes to the root node, we can evaluate the joint probability $P(u,x,y,z) = \partial_z\Big[\mu_{h\to Z}(z;u,x,y)\Big]$ at the root node as

$$\begin{aligned}
P(u,x,y,z) = \partial_z\Big[\mu_{h\to Z}(z;u,x,y)\Big] &= \partial_z\Big[\partial_y\Big[h(y,z)\mu_{Y\to h}(y;u,x)\Big]\Big]\\
&= \partial_z\Big[\partial_y\Big[h(y,z)\mu_{g\to Y}(y;u,x)\Big]\Big]\\
&= \partial_z\Big[\partial_y\Big[h(y,z)\partial_{u,x}\Big[g(u,x,y)\mu_{X\to g}(x)\mu_{U\to g}(u)\Big]\Big]\Big]\\
&= \partial_{x,y,z,u}\Big[g(u,x,y)h(y,z)\Big]\\
&= \partial_{x,y,z,u}\Big[F(u,x,y,z)\Big].
\end{aligned}$$

The above example illustrates the fact that if the graph topology is a tree, then the message-passing algorithm yields the correct mixed derivatives with respect to each variable in the CDN so that we obtain the joint probability $P(\mathbf{x}) = \partial_{\mathbf{x}}\Big[F(\mathbf{x})\Big]$ at the root node of the tree by multiplying all incoming messages to the root.

The above example also illustrates a potential source for complexity: each message consists of a symbolic expression that is a sum of products of derivatives of CDN functions. For larger graphs, it is easy to see that such a message-passing scheme would grow in complexity as the symbolic expression for each message would grow in size as we pass from leaf nodes to the root. However, for practical purposes in which we wish to obtain numerical values for probabilities at the observed data, we are interested in *evaluating* derivatives corresponding to marginal/conditional probabilities for observed data $\mathbf{x}$, with unobserved variables marginalized out by taking limits. As the message-passing algorithm allows us to decompose the total mixed derivative computation into a series of local computations, each term in this decomposition consists of a derivative that can be ”clamped” to the observed values for its arguments. Moreover, this ”clamping” need only be performed locally for each CDN function as we evaluate each outgoing message. In the above example, given observed values u^*, x^* the message $\mu_{g\to Y}(y;u,x)$ consists of computing a derivative with respect to u, x, *followed by evaluation* of the derivative at u^*, x^*. Thus by ”clamping” to observed values, messages in the above scheme will not increase in size, regardless of the functional forms chosen for the CDN functions. By evaluating each derivative in the example for u^*, x^*, y^*, z^*, we can obtain a numerical value for the probability $P(u^*, x^*, y^*, z^*)$ by multiplying messages at the root node.

3.2 Inference in Cumulative Distribution Networks

Thus far we have presented a message-passing scheme for computing derivatives of the joint CDF in order to obtain the joint PDF/PMF $P(\mathbf{x})$. Here we will demonstrate the correspondence between computing higher-order derivatives and the problem of inference in a CDN. The relation between differentiation and inference in CDNs is analogous to the relation between marginalization and inference in factor graphs. Thus, in analogy to how the sum-product algorithm allows one to compute distributions of the type $P(\mathbf{x}_A|\mathbf{x}_B)$, message-passing in a CDN allows us to compute conditional distributions of the form $F(\mathbf{x}_A|\mathbf{x}_B)$ and $P(\mathbf{x}_A|\mathbf{x}_B)$ for disjoint sets $A, B \subset V$. In order to compute conditional distributions of the above types, we will assume that when computing a conditional distribution such as $F(\mathbf{x}_A|\mathbf{x}_B)$ or $P(\mathbf{x}_A|\mathbf{x}_B)$, we have $P(\mathbf{x}_B) = \partial_{\mathbf{x}_B}\Big[F(\mathbf{x}_B)\Big] > 0$. Now consider the problem of computing the quantity $F(\mathbf{x}_A|\mathbf{x}_B)$. We can write this as

$$F(\mathbf{x}_A|\mathbf{x}_B) = \frac{\partial_{\mathbf{x}_B}\Big[F(\mathbf{x}_A,\mathbf{x}_B)\Big]}{\partial_{\mathbf{x}_B}\Big[F(\mathbf{x}_B)\Big]} = \frac{\lim_{\mathbf{x}_{V\setminus(A\cup B)}\to\infty}\partial_{\mathbf{x}_B}\Big[F(\mathbf{x})\Big]}{\lim_{\mathbf{x}_{V\setminus B}\to\infty}\partial_{\mathbf{x}_B}\Big[F(\mathbf{x})\Big]} = \frac{\partial_{\mathbf{x}_B}\left[\lim_{\mathbf{x}_{V\setminus(A\cup B)}\to\infty}F(\mathbf{x})\right]}{\partial_{\mathbf{x}_B}\left[\lim_{\mathbf{x}_{V\setminus B}\to\infty}F(\mathbf{x})\right]}$$
$$\propto \partial_{\mathbf{x}_B}\left[\lim_{\mathbf{x}_{V\setminus(A\cup B)}\to\infty}F(\mathbf{x})\right],$$

so that by combining the operations of taking limits and computing derivatives/finite differences, we can compute any conditional probability of the form $F(\mathbf{x}_A|\mathbf{x}_B)$. To compute the conditional CDF for any variable node in the network, we can pass messages from leaf nodes to root and then from the root node back to the leaves. For any given variable node, we can then multiply all incoming messages to obtain the conditional CDF for that variable, up to a scaling factor. We will now demonstrate this principle using the previous toy example CDN.

Example 6 *Consider the toy example of a CDN over four random variables U,X,Y,Z from Figure 11. Suppose we wish to compute $F(y|x,z) = \lim_{u\to\infty} F(u,y|x,z)$. This is equivalent to message-passing in a CDN defined over variables X,Y,Z with U marginalized out (Figure 12) so that $\tilde{g}(x,y) = \lim_{u\to\infty} g(u,x,y)$. Thus the message updates are given by*

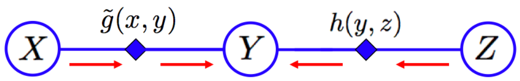


Figure 12: Flow of messages in the toy example CDN of Figure 11 with variable U marginalized out in order to compute the conditional CDF $F(y|x,z)$. Messages are here passed from all observed variable nodes to the root node.

$$\mu_{X\to\tilde{g}}(x) = 1,\ \mu_{\tilde{g}\to Y}(y;x) = \partial_x\Big[\tilde{g}(x,y)\mu_{X\to\tilde{g}}(x)\Big] = \partial_x\Big[\tilde{g}(x,y)\Big],$$
$$\mu_{Z\to h}(z) = 1,\ \mu_{h\to Y}(y;z) = \partial_z\Big[h(y,z)\mu_{Z\to h}(z)\Big] = \partial_z\Big[h(y,z)\Big].$$

Once we have computed the above messages, we can evaluate the conditional CDF $F(y|x,z)$ at node Y as

$$F(y|x,z) = \frac{\mu_{\tilde{g}\to Y}(y;x)\mu_{h\to Y}(y;z)}{\mathcal{Z}} = \frac{\partial_z\Big[h(y,z)\Big]\partial_x\Big[\tilde{g}(x,y)\Big]}{\mathcal{Z}}.$$

Note that the normalizing constant $\mathcal{Z}$ can be readily obtained by computing

$$\mathcal{Z} = \lim_{y\to\infty}\partial_z\Big[h(y,z)\Big]\partial_x\Big[\tilde{g}(x,y)\Big] = \partial_{x,z}\Big[\lim_{y\to\infty} h(y,z)\tilde{g}(x,y)\Big],$$

so that

$$F(y|x,z) = \frac{\mu_{\tilde{g}\to Y}(y;x)\mu_{h\to Y}(y;z)}{\mathcal{Z}} = \frac{\partial_z\Big[h(y,z)\Big]\partial_x\Big[\tilde{g}(x,y)\Big]}{\partial_{x,z}\Big[\lim_{y\to\infty} h(y,z)\tilde{g}(x,y)\Big]} = \frac{\lim_{u\to\infty}\partial_z\Big[h(y,z)\Big]\partial_x\Big[\tilde{g}(u,x,y)\Big]}{\partial_{x,z}\Big[\lim_{u,y\to\infty} h(y,z)\tilde{g}(u,x,y)\Big]}$$
$$= \frac{\partial_{x,z}\Big[\lim_{u\to\infty} F(u,x,y,z)\Big]}{\partial_{x,z}\Big[\lim_{u,y\to\infty} F(u,x,y,z)\Big]}.$$

Note that in the above, if we were to observe $X = x^*, Z = z^*$, we could then evaluate $F(y|x^*,z^*)$ given any candidate value y for variable Y.

The above example shows that the message-passing algorithm can be used to compute conditional CDFs of the form $F(\mathbf{x}_A|\mathbf{x}_B)$, up to a normalizing constant $\mathcal{Z}$. Messages are passed once from all variable nodes on which we are conditioning to the root node: in the example, messages are passed from variable nodes X, Z to variable node Y in order to compute $F(y|x,z)$. If we wished to compute, say, $F(x|y,z)$, then messages would be passed from variable nodes Y, Z to variable node X.

To obtain distributions of the type $P(\mathbf{x}_A|\mathbf{x}_B)$ from $F(\mathbf{x}_A|\mathbf{x}_B)$, we first compute $\partial_{\mathbf{x}_A}\Big[F(\mathbf{x}_A|\mathbf{x}_B)\Big]$ using the above message-passing scheme and then multiply messages together to obtain conditional PDFs. We note that computing the normalizing constant $\mathcal{Z}$ can be viewed as the result of message-passing in a CDN in which the variables $\mathbf{X}_A$ have been marginalized out in addition to variables $\mathbf{X}_{V\setminus(A\cup B)}$ and then evaluating the resulting messages at the observed values $\mathbf{x}_B$. Equivalently, one can compute $\mathcal{Z} = \lim_{\mathbf{x}_A\to\infty} \partial_{\mathbf{x}_B}\Big[F(\mathbf{x}_A,\mathbf{x}_B)\Big]$ after message-passing with only variables in $V\setminus(A\cup B)$ marginalized out.

3.3 Derivative-sum-product: A Message-passing Algorithm for Inference in Cumulative Distribution Networks

- **Input: A tree-structured CDN $\mathcal{G} = (V,S,E)$, root node $\alpha \in V$ and a vector x of observations**
- **Output: The probability mass function (PMF) $P(\mathbf{x})$**
- For each leaf variable node α' and for all function nodes $s \in \mathcal{N}(\alpha')$, propagate $\mu_{\alpha'\to s}(\mathbf{x}) = 1$. For each leaf function node with function $\phi_s(x_{\alpha'})$, send the messages $\mu_{s\to\alpha'}(\mathbf{x}) = \phi_s(x_{\alpha'})$.
- For each non-leaf variable node α and neighboring function nodes $s \in \mathcal{N}(\alpha)$,

$$\mu_{\alpha\to s}(\mathbf{x}) = \prod_{s'\in\mathcal{N}(\alpha)\setminus s} \mu_{s'\to\alpha}(\mathbf{x}).$$

- For each non-leaf function node s and neighboring variable nodes $\alpha \in \mathcal{N}(s)$,

$$\mu_{s\to\alpha}(\mathbf{x}) = \partial_{\mathbf{x}_{\mathcal{N}(s)\setminus\alpha}}\left[\phi_s(\mathbf{x}_s) \prod_{\beta\in\mathcal{N}(s)\setminus\alpha} \mu_{\beta\to s}(\mathbf{x})\right].$$

- Repeat the 2^{nd} and 3^{rd} steps towards the root node α.

Table 1: The derivative-sum-product (DSP) algorithm for computing the probability mass function $P(\mathbf{x})$ in a CDN defined over discrete variables.

Given that the fundamental operations required for message-passing consist of differentiation/finite differences, sums and products, we will refer to the above class of message-passing algorithms as the derivative-sum-product (DSP) algorithm. For CDNs defined over discrete ordinal variables, the DSP algorithm is shown in Table 1. As can be seen, for graphs defined over discrete variables, the DSP algorithm is analogous to the sum-product algorithm with the summation operation replaced by a finite difference operation. For graphs defined over discrete ordinal variables that take on one of K values, for an observed $\mathbf{x}$, each message $\mu_{\alpha\to s}, \mu_{s\to\alpha}$ consists of a K-vector, analogous to messages in the sum-product algorithm. To see this, we note that each time we compute a finite difference with respect to variables in $\mathcal{N}(s)\setminus\alpha$, we also evaluate the result at $\mathbf{x}_{\mathcal{N}(s)\setminus\alpha}$, ensuring that each message is a K-vector.

In contrast to the DSP algorithm for discrete variables, the required complexity increases for CDNs defined over continuous variables. For such models, we are required to invoke the product rule of differential calculus in order to express these messages in terms of the derivatives of CDN functions and combinations thereof. To this end, we need to define two additional sets of messages $\lambda_{\alpha\to s}(\mathbf{x})$ and $\lambda_{s\to\alpha}(\mathbf{x})$ which correspond to $\partial_{x_\alpha}\Big[\mu_{\alpha\to s}(\mathbf{x})\Big]$ and $\partial_{x_\alpha}\Big[\mu_{s\to\alpha}(\mathbf{x})\Big]$ respectively. We first derive the expression for $\lambda_{\alpha\to s}(\mathbf{x})$ by applying the product rule of differential calculus to the message $\mu_{\alpha\to s}(\mathbf{x})$, bearing in mind that each of the messages $\mu_{s\to\alpha}(\mathbf{x})$ depends on variable X_α. This yields

$$\lambda_{\alpha\to s}(\mathbf{x}) = \partial_{x_\alpha}\Big[\mu_{\alpha\to s}(\mathbf{x})\Big] = \partial_{x_\alpha}\left[\prod_{s'\in\mathcal{N}(\alpha)\setminus s}\mu_{s'\to\alpha}(\mathbf{x})\right] = \mu_{\alpha\to s}(\mathbf{x})\sum_{s'\in\mathcal{N}(\alpha)\setminus s}\frac{\lambda_{s'\to\alpha}(\mathbf{x})}{\mu_{s'\to\alpha}(\mathbf{x})}.$$

In order to derive the general expressions for $\mu_{s\to\alpha}(\mathbf{x})$, $\lambda_{s\to\alpha}(\mathbf{x})$, we first note that for any two differentiable multivariate functions $f(\mathbf{x}), g(\mathbf{x})$, the product rule for computing the higher-order derivative of a product of functions is given by

$$\partial_{\mathbf{y}}\Big[f(\mathbf{y})g(\mathbf{y})\Big] = \sum_{\mathbf{y}_A\subseteq\mathbf{y}}\partial_{\mathbf{y}_A}\Big[f(\mathbf{y})\Big]\partial_{\mathbf{y}\setminus\mathbf{y}_A}\Big[g(\mathbf{y})\Big].$$

The key observation we make here is that to evaluate the above derivative for observed $\mathbf{y}$, we can evaluate each term in the summation for the observed $\mathbf{y}$ such that the above is merely a sum of products of scalars. Thus, given a vector of observed variable values $\mathbf{x}$, the messages in the DSP algorithm for continuous variables will all consist of scalars, allowing us to obtain numerical values for probabilities under the model.

To compute messages $\mu_{s\to\alpha}(\mathbf{x}), \lambda_{s\to\alpha}(\mathbf{x})$ from $\mu_{s\to\alpha}(\mathbf{x})$, applying the above product rule yields

$$\begin{aligned}
\mu_{s\to\alpha}(\mathbf{x}) &= \partial_{\mathbf{x}_{\mathcal{N}(s)\setminus\alpha}}\left[\phi_s(x_\alpha,\mathbf{x}_{\mathcal{N}(s)\setminus\alpha})\prod_{\beta\in\mathcal{N}(s)\setminus\alpha}\mu_{\beta\to s}(\mathbf{x})\right] \\
&= \sum_{B\subseteq\mathcal{N}(s)\setminus\alpha}\partial_{\mathbf{x}_B}\Big[\phi_s(\mathbf{x}_s)\Big]\prod_{\beta\in B}\mu_{\beta\to s}(\mathbf{x})\prod_{\beta\in\mathcal{N}(s)\setminus(\alpha\cup B)}\lambda_{\beta\to s}(\mathbf{x}), \\
\lambda_{s\to\alpha}(\mathbf{x}) &= \partial_{x_\alpha}\Big[\mu_{s\to\alpha}(\mathbf{x})\Big] \\
&= \sum_{B\subseteq\mathcal{N}(s)\setminus\alpha}\partial_{\mathbf{x}_B,x_\alpha}\Big[\phi_s(\mathbf{x}_s)\Big]\prod_{\beta\in B}\mu_{\beta\to s}(\mathbf{x})\prod_{\beta\in\mathcal{N}(s)\setminus(\alpha\cup B)}\lambda_{\beta\to s}(\mathbf{x}),
\end{aligned}$$

where we have made use of the tree-structure of the CDN to write the derivative of a product of messages as a product of derivatives of the messages. The above updates then define the DSP algorithm for CDNs defined over continuous variables, with a total of four sets of messages defined solely in terms of the CDN functions, their derivatives and linear combinations thereof. The message-passing algorithm for continuous CDNs is summarized in Table 2 and is illustrated in Figure 13.

We see from Table 2 that the DSP algorithm grows exponentially in complexity as the number of neighboring variable nodes for any given function increases, as the updates at function nodes

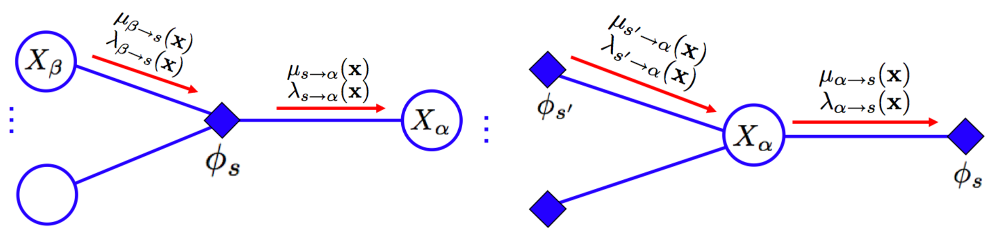


Figure 13: The DSP algorithm. a) Computation of the message from a function node s to a variable node α; b) Computation of the message from a variable node α to a function node s.

- **Input: A tree-structured CDN $\mathcal{G} = (V, S, E)$, root node $\alpha \in V$ and a vector x of observations**
- **Output: The probability density function (PDF) $P(\mathbf{x})$**
- For each leaf variable node α' and for all function nodes $s \in \mathcal{N}(\alpha')$, propagate $\mu_{\alpha'\to s}(\mathbf{x}) = 1, \lambda_{\alpha'\to s}(\mathbf{x}) = 0$. For each leaf function node with function $\phi_s(x_{\alpha'})$, send the messages $\mu_{s\to\alpha'}(\mathbf{x}) = \phi_s(x_{\alpha'}), \lambda_{s\to\alpha'}(\mathbf{x}) = \partial_{x_{\alpha'}}\left[\phi_s(x_{\alpha'})\right]$.
- For each non-leaf variable node α and neighboring function nodes $s \in \mathcal{N}(\alpha)$,

$$\mu_{\alpha\to s}(\mathbf{x}) = \prod_{s'\in\mathcal{N}(\alpha)\setminus s} \mu_{s'\to\alpha}(\mathbf{x}),$$

$$\lambda_{\alpha\to s}(\mathbf{x}) = \partial_{x_\alpha}\left[\mu_{\alpha\to s}(\mathbf{x})\right] = \mu_{\alpha\to s}(\mathbf{x}) \sum_{s'\in\mathcal{N}(\alpha)\setminus s} \frac{\lambda_{s'\to\alpha}(\mathbf{x})}{\mu_{s'\to\alpha}(\mathbf{x})}.$$

- For each non-leaf function node s and neighboring variable nodes $\alpha \in \mathcal{N}(s)$,

$$\mu_{s\to\alpha}(\mathbf{x}) = \sum_{B\subseteq\mathcal{N}(s)\setminus\alpha} \partial_{\mathbf{x}_B}\left[\phi_s(\mathbf{x}_s)\right] \prod_{\beta\in B} \mu_{\beta\to s}(\mathbf{x}) \prod_{\beta\in\mathcal{N}(s)\setminus\{\alpha\cup B\}} \lambda_{\beta\to s}(\mathbf{x}),$$

$$\lambda_{s\to\alpha}(\mathbf{x}) = \partial_{x_\alpha}\left[\mu_{s\to\alpha}(\mathbf{x})\right]$$

$$= \sum_{B\subseteq\mathcal{N}(s)\setminus\alpha} \partial_{\mathbf{x}_B, x_\alpha}\left[\phi_s(\mathbf{x}_s)\right] \prod_{\beta\in B} \mu_{\beta\to s}(\mathbf{x}) \prod_{\beta\in\mathcal{N}(s)\setminus\{\alpha\cup B\}} \lambda_{\beta\to s}(\mathbf{x}).$$

- Repeat the 2^{nd} and 3^{rd} steps towards root node α.

Table 2: The derivative-sum-product (DSP) algorithm for computing the joint probability density function $P(\mathbf{x})$ in a CDN defined over continuous variables.

require one to perform a sum over all subsets of neighboring variables. However, in many cases the computational complexity will be tractable for sparser graphs, as demonstrated by the following example.

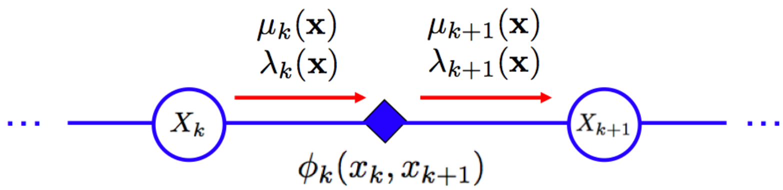


Figure 14: The DSP algorithm for a chain-structured CDN.

Example 7 (Derivative-sum-product on a linear first-order chain CDN) *Consider the CDN defined over K variables such that the joint CDF over these variables is given by*

$$F(\mathbf{x}) = \prod_{k=1}^{K-1} \phi_k(x_k, x_{k+1}),$$

so that the variable nodes are connected in the chain-structured graph shown in Figure 14. In this case, the DSP messages can be written as

$$\begin{aligned}
\mu_{k+1}(\mathbf{x}) &\equiv \mu_{\phi_k \to X_{k+1}}(\mathbf{x}) \\
&= \partial_{x_k}\Big[\phi_k(x_k, x_{k+1})\Big]\mu_k(\mathbf{x}) + \phi_k(x_k, x_{k+1})\lambda_k(\mathbf{x}), \\
\lambda_{k+1}(\mathbf{x}) &\equiv \lambda_{\phi_k \to X_{k+1}}(\mathbf{x}) \\
&= \partial_{x_k, x_{k+1}}\Big[\phi_k(x_k, x_{k+1})\Big]\mu_k(\mathbf{x}) + \partial_{x_{k+1}}\Big[\phi_k(x_k, x_{k+1})\Big]\lambda_k(\mathbf{x}), \quad k = 1, \cdots, K-1.
\end{aligned}$$

Example 8 (Sampling from a cumulative distribution network) *We can further take advantage of the DSP algorithm for generating samples from the CDF modeled by a CDN. We can proceed as follows: arbitrarily select a variable in the model, say X_1. Then, generate a sample x_1^* from its marginal CDF $F(x_1)$ (which we obtain by marginalizing over all other variables). Given x_1^*, we can then proceed to generate samples for its children by marginalizing out all other unobserved variables and then sampling from the conditional distribution $F(x_2|x_1^*)$. We can continue this way until we have sampled a complete configuration $\mathbf{x}^* = [x_1^*, \cdots, x_K^*]$. The algorithm for sampling from the joint CDF modeled by a CDN is then given by*

- *Pick a sampling ordering $X_1, X_2, \cdots, X_K$,*
- *For variable $X_k, k = 1, \cdots, K$, compute*

$$F(x_1, \cdots, x_k) = \lim_{x_{k+1}, \cdots, x_K \to \infty} F(x_1, \cdots, x_k, x_{k+1} \cdots, x_K).$$

- *Sample x_i^* from*

$$F(x_k|x_1, \cdots, x_{k-1}) = \frac{\partial_{x_1, \cdots, x_{k-1}}\Big[F(x_1, \cdots, x_k)\Big]}{\lim_{x_k \to \infty} \partial_{x_1, \cdots, x_{k-1}}\Big[F(x_1, \cdots, x_k)\Big]}.$$

From the above we see that if the CDN has a tree structure, then we can compute the conditional CDFs $F(x_k|x_1,\cdots,x_{k-1})$ exactly via DSP. In the case of a CDN with cycles, we can always convert it to one with a tree structure by clustering variables and corresponding function nodes (Lauritzen and Spiegelhalter, 1988). This generally incurs an increase in function node complexity, but with the benefit of being able to sample from the joint CDF modeled by the CDN.

3.4 Discussion

We have presented the derivative-sum-product (DSP) algorithm for computing derivatives in tree-structured CDNs. For graphs defined over continuous variables, the DSP algorithm can be implemented through two sets of messages in order to compute the higher-order derivatives of the joint CDF. While we have presented the DSP algorithm for computing derivatives given a set of CDN functions, we have not addressed here the issue of how to learn these CDN functions from data. A possible method would be to run DSP to obtain the joint PDF and then maximize this with respect to model parameters for a particular $\mathbf{x}$. Another issue we have not addressed is how to perform inference in graphs with cycles: an interesting future direction would be to investigate exact or approximate methods for doing so and connections to methods in the literature (Minka, 2001; Neal, 1993) for doing this in traditional graphical models. We will further discuss these issues in the concluding section.

Having defined the CDN and having described the DSP algorithm, we will now proceed to apply both of these to the general problem of learning to rank from examples. As we will see, the ability to model a joint CDF using a graphical framework will yield advantages in both representation and computation for this class of problems.

4. Learning to Rank in Multiplayer Team-based Games with Cumulative Distribution Networks

In this section, we will apply CDNs and the DSP algorithm to the problem of structured ranking learning in which the goal is to learn a model for ranking players in a multiplayer game. For this problem, we observe the scores achieved by several players over many games $t = 1\cdots,T$ in which players interactively compete in groups, or teams, which change with each game. For any given game, players compete in teams so that at the end of each game, each player will have achieved a score as a result of actions taken by all players during the game. For example, these player scores could correspond to the number of targets destroyed or the number of flags stolen, so that a higher player score reflects a better performance for that player. Here we will define a game Γ_t as a triplet $(\mathcal{P}_t, \mathcal{T}_t, \mathcal{O}_t)$, where $\mathcal{P}_t \subset \mathcal{P}$ is a subset of the set $\mathcal{P}$ of all players and $\mathcal{T}_t$ is a partition of $\mathcal{P}_t$ into sets corresponding to teams for game Γ_t, so that if $\mathcal{T}_t = \{\mathcal{T}_t^1,\cdots,\mathcal{T}_t^N\}$ then there are N teams for game Γ_t and player $k \in \mathcal{P}_t$ is assigned to team n for game Γ_t if and only if $k \in \mathcal{T}_t^n$. For example, a game involving six players labeled $1,2,3,4,5,6$ organized into three teams of two players each could correspond to $\mathcal{P}_t = \{1,2,3,4,5,6\}$ and $\mathcal{T}_t = \{\{1,2\},\{3,4\},\{5,6\}\}$. Without loss of generality we will label the teams in a game by $n = 1,\cdots,N$ where each team corresponds to a set in the partition $\mathcal{T}_t$.

In addition to the above, we will denote by $\mathcal{O}_t$ the *outcome* of a game that consists of the pair $(\mathbf{x}_{\mathcal{P}_t}, \mathbf{r}_{\mathcal{T}_t})$, where $\mathbf{x}_{\mathcal{P}_t} \in \mathbb{R}^{|\mathcal{P}_t|}$ is a vector of player scores for game Γ_t and the set $\mathbf{r}_{\mathcal{T}_t}$ is defined as a partially ordered set of team performances, or set of ranks for each team. Such ranks are obtained by first computing the sum of the player scores for each team $n = 1,\cdots,N$, and then ranking the teams by sorting the resulting sums. We will refer to these sums in the sequel as the team scores t_n. An example of this for the previous example is $\mathbf{x}_{\mathcal{P}_t} = [30\ 12\ 15\ 25\ 100\ 23]^T$, so that $\mathbf{r}_{\mathcal{T}_t} = \{2,\ 1,\ 3\}$ is the corresponding partially ordered set of team rankings. We will also denote by $\mathbf{x}_n \in \mathbb{R}^{|\mathcal{T}_t^n|}$ the vector of player scores for team n in game Γ_t. Games can also be classified into various types, such that the sizes and/or number of teams are constrained in different ways for different game types. For example, a "SmallTeam" game type would consist of two teams with at most two players per team, whereas a "FreeForAll" game type would constrain the number of teams to be at most eight, with one player per team. Furthermore, the team rankings are a function of unweighed sums of player scores: although there is no reason *a priori* to weigh the scores of players differently for determining the rank of a team, one could extend the above scheme for determining team rankings to weigh player scores according to player type or player-specific features.

Given the above, the goal is to construct a model that will allow us to predict the outcome $\mathcal{O}_t$ of the new game before it begins, given $\mathcal{P}_t$ and previous game outcomes $\mathcal{O}_1, \cdots, \mathcal{O}_{t-1}$. In particular, we wish to construct a model that will minimize the number of mis-ordered teams based on the set of team performances $\mathbf{r}_{\mathcal{T}_t}$ for game Γ_t. Here, the probability model for the given game should account for the team-based structure of games, such that team performances are determined by individual player scores and a game outcome is determined by the ordering of team scores. We will demonstrate here that the graphical framework of CDNs makes it straightforward to model both stochastic orderings of variables in the model as well as statistical independence relationships among these variables. In particular, the model we will construct here will be amenable to exact inference via the DSP algorithm.

Our model will be similar in design to the TrueSkill$^{\text{TM}}$ model of Herbrich et al. (2007) for skill rating in Halo 2$^{\text{TM}}$, whereby each player $k \in \mathcal{P}_t$ is assigned a probability distribution over latent skill variables S_k, which is then inferred from individual player scores over multiple games using the expectation propagation algorithm for approximate inference (Minka, 2001). Inference in the TrueSkill$^{\text{TM}}$ model thus consists of applying expectation propagation to a factor graph for a given game in order to update probabilities over player skills. An example of such a factor graph is shown in Figure 15. In TrueSkill$^{\text{TM}}$, the factors connecting team-specific nodes to one another dictate a constraint on relative differences in the total player scores between teams, while factors connecting player nodes to their team-specific nodes enforce the constraint that the team score is determined by the sum of player scores. Finally, for teams $n, n+1$, there is a difference variable $H_{n,n+1}$ and a corresponding factor which declares a tied rank between two teams if the difference between the two team scores is below some threshold parameter.

4.1 A Cumulative Distribution Network for Modeling Multiplayer Game Outcomes

Here we will examine a model for multiplayer game outcomes that will be modeled using a CDN. The model will be designed on a game-by-game basis where the team assignments of players for a given game determines the connectivity of the graph $\mathcal{G}$ for the CDN. In our model the team variables will correspond to the ranks of teams: we will call such variables *team performances* and denote these as R_n for team n in order to contrast these with the team score variables T_n in the TrueSkill model. Our model will account for player scores X_k for each player $k \in \mathcal{P}_t$ in the game, the team performances R_n for each team $n = 1, \cdots, N$ in the game and each player's skill function $s_k(x_k)$, which is a CDF specific to each player. For any given game, R_n will be determined as the sum of the player scores for team n, and then sorting the resulting sums so that R_n corresponds to the rank of

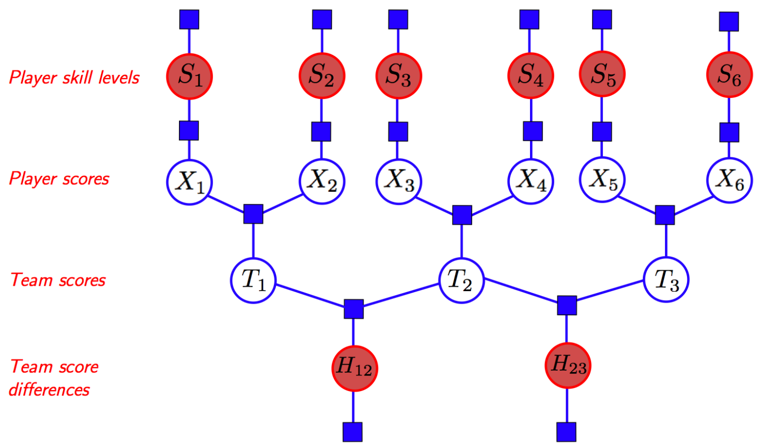


Figure 15: The TrueSkill™ factor graph for a particular Halo 2™ game involving three teams with two players each with the team scores $T_1 = t_1, T_2 = t_2, T_3 = t_3$ with $t_1 < t_2 < t_3$ so that team 3 here achieved the highest total of player scores. The variables H_{12}, H_{23} correspond to differences in team scores which determine the ranking of teams, so that teams n and $n+1$ are tied in their rankings if the difference in their team scores is below a threshold parameter. Here, $\mathcal{P}_t = \{1,2,3,4,5,6\}$ and $\mathcal{T}_t = \{\{1,2\},\{3,4\},\{5,6\}\}$. Unobserved variables correspond to nodes shaded in red and observed variables correspond to unshaded variable nodes. Each player $k = 1,2,3,4,5,6$ is assigned a skill function that reflects the distribution of that player's skill level S_k given past game outcomes. Each player then achieves score X_k in any given game and team scores $T_n, n = 1,2,3$ are then determined as the sum of player scores for each team.

team n. The set of observed team performances $\mathbf{r}_{\mathcal{T}_t}$ will be given by the joint configuration of the R_n variables for that game. The goal will then be to adapt player skill functions $s_k(x_k)$ for each game as a function of game outcome. We will design our model according to two principles. First, the relationship between player scores and team performances is modeled as being stochastic, as both player scores and team assignments vary from one game to the next, so that given knowledge of the players in that game and their team assignments, there is some uncertainty in how a team will rank once the game is over. Second, team performance variables depend on those of other teams in the game, so that each team's performance should be linked to that of other teams in a game.

The CDN framework allows us to satisfy both desiderata in the form of modeling constraints on the marginal CDFs for variables in the model. To address the first point, we will require a set of CDN functions that connect player scores to team performances. Here we will make use of the cumulative model for ordinal regression (see Appendix) that relates a linear function $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ on inputs $\mathbf{x}$ to a single output ordinal variable $y \in \{r_1, \cdots, r_L\}$ so that $\mathbb{P}[y = r_l] = \mathbb{P}[\theta(r_{l-1}) < f(\mathbf{x}) + \varepsilon \leq \theta(r_l)] = F_\varepsilon(\theta(r_l) - f(\mathbf{x})) - F_\varepsilon(\theta(r_{l-1}) - f(\mathbf{x}))$, where ε is an additive noise variable and $\theta(r_0), \cdots, \theta(r_L)$ are the cutpoint parameters of the model with $\theta(r_0) = -\infty, \theta(r_L) = \infty$. Equivalently, we can write $\mathbb{P}[y \leq r_l] = \mathbb{P}[\varepsilon \leq \theta(r_l) - f(\mathbf{x})]$. In the context of multiplayer games, we perform separate ordinal regressions for different game types, as the cutpoints that are learned for a given game type may vary between different game types due to differing team sizes between game types. For a given game type, we treat the set of all games as a bag of pairs of player score vectors $\mathbf{x}_n$ and team performances r_n from which cutpoints in an ordinal regression model can be learned. Thus, we learn a set of cutpoints $\theta(r_0) < \cdots < \theta(r_L)$ once using all of the games in the training data set for a given game type. Team performances are treated as being independent: thus, we can use the CDN framework to augment the above parametric model in order to account for statistical dependencies between multiple team performances in any given game.

We will model multiplayer games using a CDN in which players are grouped into teams and teams compete with one another. To model dependence between player scores and team performance, we will combine the above cumulative model for ordinal regression with prior player score distributions under the assumptions that players contribute equally to team performance and that players perform equally well on average. To do this, we will use functions g_n where if there are N teams for any given game, then we can assign a CDN function g_n for each team such that

$$g_n(\mathbf{x}_n, r_n) = \int_{-\infty}^{\mathbf{x}_n} F\big(\theta(r_n); \mathbf{1}^T\mathbf{u}, \sigma^2\big) P\big(\mathbf{u}\big)\, d\mathbf{u}, \tag{2}$$

where $F\big(\theta(r_n); \mathbf{1}^T\mathbf{u}, \sigma^2\big)$ is a cumulative model relating input player scores to output team performance and $\mathbf{x}_n, r_n$ are the player scores and team performance for team n. The regression function in the cumulative model is given by $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ with $\mathbf{w}$ set to the vector of ones $\mathbf{1}$, as we weigh the contributions of players on a team equally. Furthermore, $\theta(r_n)$ are the cutpoints that define contiguous intervals in which r_n is the ranking for team n based on that team's performance and $P(\mathbf{u})$ is a probability density over a vector of latent player scores $\mathbf{u}$. Once the cutpoints have been estimated by ordinal regression, we will model the distributions $F\big(\theta(r_n); \mathbf{1}^T\mathbf{u}, \sigma^2\big), P\big(\mathbf{u}\big)$ in Equation (2) as

$$\begin{aligned} F\big(\theta(r_n); \mathbf{1}^T\mathbf{u}, \sigma^2\big) &= \Phi\big(\theta(r_n); \mathbf{1}^T\mathbf{u}, \sigma^2\big), \\ P(\mathbf{u}) &= Gaussian(\mathbf{u}; \mu\mathbf{1}, \sigma^2\mathbf{I}). \end{aligned}$$

By combining functions g_n (which assume equal player skills on average) with individual player skills whilst accounting for the dependence between players' skills and team performances, we can update each player's skill function s_k conditioned on the outcome of a game.

To address the fact that teams compete in any given game, we model ordinal relationships between team performance using the notion of stochastic orderings (Section 2.3), so that for two teams with team performances R_X, R_Y, $R_X \preceq R_Y$ if $F_{R_X}(t) \geq F_{R_Y}(t) \,\forall\, t \in \mathbb{R}$, where $F_{R_X}(\cdot), F_{R_Y}(\cdot)$ are the marginal CDFs of R_X, R_Y. This then allows us to design models in which we can express differences in team performances in the form of pairwise constraints on their marginal CDFs. We note at this juncture that while it is possible to model such stochastic ordering constraints between variables using directed, undirected or factor graphs, doing so introduces additional constraints that are likely to increase the difficulty of performing inference under such models. In contrast, the CDN framework here allows us to explicitly specify such stochastic ordering constraints, in addition to allowing for tractable computations in the resulting model. Thus, although each of the R_n variables is a deterministic function of the sum of player scores, we can nevertheless model them as being stochastic using the framework of CDNs to specify orderings among the R_n variables. By contrast, it will generally be more difficult in terms of computation and representation to enforce constraints of the type $\big[R_n \preceq R_{n+1}\big]$ in a directed/undirected/factor graph model.

For the proposed CDN model, given N ranked teams, we can thus define $N-1$ functions $h_{n,n+1}$ so that

$$h_{n,n+1}(r_n, r_{n+1}) = \Phi\left(\begin{bmatrix} r_n \\ r_{n+1} \end{bmatrix}; \begin{bmatrix} \tilde{r}_n \\ \tilde{r}_{n+1} \end{bmatrix}, \mathbf{\Sigma}\right),$$

where

$$\mathbf{\Sigma} = \begin{bmatrix} \sigma^2 & \rho\sigma^2 \\ \rho\sigma^2 & \sigma^2 \end{bmatrix},$$

and $\tilde{r}_n \leq \tilde{r}_{n+1}$ are chosen without loss of generality such that $\tilde{r}_n = n$ so as to enforce $R_n \preceq R_{n+1}$ in the overall model. Finally, we will use a *skill function* $s_k(x_k)$ for each player k to model that player's distribution over game scores given previous game outcomes. The player performance nodes in the CDN will then be connected to the team performance nodes via the above CDN functions g_n and team performance variable nodes R_n are linked to one another via the above CDN functions $h_{n,n+1}$. The joint CDF for a given game Γ_t with N teams is then given by

$$F(\mathbf{x}_{\mathcal{P}_t}, \mathbf{r}_{\mathcal{T}_t}) = \prod_{n=1}^{N} g(\mathbf{x}_n, r_n) \prod_{n=1}^{N-1} h_{n,n+1}(r_n, r_{n+1}) \prod_{k \in \mathcal{P}_t} s_k(x_k).$$

The above functions and model variables jointly define the CDN for modeling multiplayer games. An example is given in Figure 16 for a game with three teams and six players. One can readily verify from the CDN of Figure 16 using Proposition 18 that for the above model and for any given game, the stochastic ordering relationship $R_1 \preceq R_2 \preceq \cdots \preceq R_N$ as defined above can be enforced by marginalizing over all player scores in the CDN and having selected appropriate cutpoints that satisfy $\theta(r_1) < \theta(r_2) < \theta(r_3)$ and parameters $\tilde{r}_1 < \tilde{r}_2 < \tilde{r}_3$, so that we have $F(r_1) \geq F(r_2) \geq F(r_3)$.

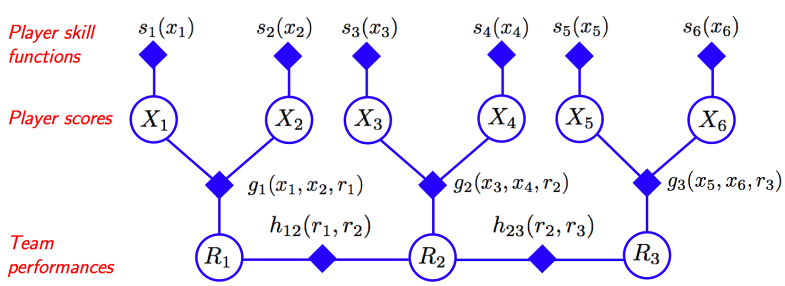


Figure 16: The CDN for the player scores and team performances in a game of Halo 2™ for a game with three teams with two players each. Each player $k = 1,2,3,4,5,6$ achieves score X_k in a match and team performances $R_n, n = 1,2,3$ are determined based on the sum of player scores for each team.

Having presented the CDN for modeling multiplayer games, we will now proceed to describe a method for predicting game outcomes in which we update player skill functions after each game using message-passing.

4.2 Ranking Players in Multiplayer Games Using the Derivative-sum-product Algorithm

Here we will apply the DSP algorithm in the context of ranking players in multiplayer games with a team structure, where the problem consists of jointly predicting multiple ordinal output variables. It should be noted that while it may be possible to construct similar models using a directed, undirected or factor graph, the CDN allows us to simultaneously specify both ordinal and statistical independence relationships among model variables while allowing for a tractable inference algorithm.

In order to compute the DSP messages using the above CDN functions, we must compute the derivatives of all CDN functions. Since all of our functions are themselves Gaussian CDFs, the derivatives $\partial_{\mathbf{x}_A}\Big[\phi_s(\mathbf{x}_s)\Big]$ can be easily evaluated with respect to variables $\mathbf{X}_A$ as

$$\partial_{\mathbf{x}_A}\Big[\Phi\big(\mathbf{x};\boldsymbol{\mu},\boldsymbol{\Sigma}\big)\Big] = Gaussian\Big(\mathbf{x}_A;\boldsymbol{\mu}_A,\boldsymbol{\Sigma}_A\Big)\Phi\Big(\mathbf{x}_B;\tilde{\boldsymbol{\mu}}_B,\tilde{\boldsymbol{\Sigma}}_B\Big),$$

where

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_A \\ \mathbf{x}_B \end{bmatrix}, \quad \boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_A \\ \boldsymbol{\mu}_B \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_A & \boldsymbol{\Sigma}_{A,B} \\ \boldsymbol{\Sigma}_{A,B}^T & \boldsymbol{\Sigma}_B \end{bmatrix},$$

$$\tilde{\boldsymbol{\mu}}_B = \boldsymbol{\mu}_B + \boldsymbol{\Sigma}_{A,B}^T\boldsymbol{\Sigma}_A^{-1}(\mathbf{x}_A - \boldsymbol{\mu}_A),$$
$$\tilde{\boldsymbol{\Sigma}}_B = \boldsymbol{\Sigma}_B - \boldsymbol{\Sigma}_{A,B}^T\boldsymbol{\Sigma}_A^{-1}\boldsymbol{\Sigma}_{A,B}.$$

The message computations in the CDN are given in the Appendix. We ensure that each message is properly normalized by locally computing the constant $\mathcal{Z}$ as described in Section 3.2 for each message and multiplying each message pair μ,λ by $\mathcal{Z}^{-1}$.

Given the above CDN model for multiplayer games, we would like to then estimate the player skill functions $s_k(x_k)$ for each player k from previous games played by that player. Let $T_k \subseteq \{1,\cdots,T\}$ be the set of games in which player k participated. We then seek to estimate $s_k(x_k)$ for player k given previous team performances $\mathbf{r}_{\mathcal{T}_t}, t \in T_k$ and player scores for *all other* players $\mathbf{x}_{\mathcal{P}_t\setminus k}$ for all games $t \in T_k$ in which player k participated. Denote by O_t^{-k} the outcome of a game with the player score for player k removed from $\mathbf{x}_{\mathcal{P}_t}$. We will define the skill function $s_k(x_k)$ for a player to be given by

$$s_k(x_k) = F\left(x_k|\{O_t^{-k}\}_{t\in T_k}\right) = \prod_{t\in T_k} F(x_k|O_t^{-k}).$$

The above expression for the skill function $s_k(x_k)$ for player k corresponds to the conditional distribution $F\left(x_k|\{O_t^{-k}\}_{t\in T_k}\right)$ given all past games played by player k with the assumption that team performances and player scores are independently drawn from CDFs $F(\mathbf{r}_{\mathcal{T}_t},\mathbf{x}_{\mathcal{P}_t})$ for $t = 1,\cdots,T$. The skill function s_k can then be readily estimated by the DSP algorithm, since each game outcome is modeled by a tree-structured CDN. More precisely, we first initialize $s_k(x_k)$ to the Gaussian CDF $\Phi(x_k;\mu,\beta^2)$ evaluated at many values for x_k. For each game Γ_t we can perform message-passing to obtain the conditional CDF $F(x_k|O_t^{-k}) = \mu_{g_n\to X_k}(\mathbf{r}_{\mathcal{T}_t},\mathbf{x}_{\mathcal{P}_t\setminus k})$ for player k (assuming the message $\mu_{g_n\to X_k}$ has been properly normalized as described above) and then perform a multiplicative update $s_k(x_k) \leftarrow s_k(x_k)\mu_{g_n\to X_k}(\mathbf{r}_{\mathcal{T}_t},\mathbf{x}_{\mathcal{P}_t\setminus k})$. The updates consist of pointwise multiplications of $s_k(x_k)$ and $\mu_{g_n\to X_k}$ for different values of x_k. The skill function $s_k(x_k)$ can then be used to make predictions for player k's scores in future games. We will proceed in the next section to apply the model and the above inference procedure to the problem of modeling Halo 2$^{\text{TM}}$ games.

4.3 The Halo 2™ Beta Data Set

The Halo 2™ Beta data set (v1.1)[2] consists of player scores for four game types ("HeadToHead", "FreeForAll", "SmallTeams" and "LargeTeams") over a total of 6,465 players. The descriptions for each of the four game modes are given below.

- HeadToHead: 6227 games/1672 players, one player competing against another player
- FreeForAll: 60022 games/5943 players, up to eight players playing against each other
- SmallTeams: 27539 games/4992 players, up to four players per team, two competing teams
- LargeTeams: 1199 games/2576 players, up to eight players per team, two competing teams

To construct the above CDN model, we set the cutpoints $\theta(r_n)$ in the above cumulative model using ordinal regression of team ranks on team performances for all games in the training set. We initialized all player skill functions to $s_k(x_k) = \Phi(x_k; \mu, \beta^2)$. The set of parameters $\{\mu, \rho, \beta, \sigma\}$ in the CDN model was set to $\{25, -0.95, 20, 0.25\}$ for "HeadToHead", $\{50, -0.2, 10, 0.2\}$ for "FreeForAll", $\{20, -0.1, 10, 0.027\}$ for "SmallTeams" and $\{1, -0.9, 1, 0.01\}$ for "LargeTeams" game modes.[3] For each of these game modes, we applied the DSP algorithm as described above in order to obtain updates for the player skill functions $s_k(x_k)$. An example of such an update at the end of a game with four competing players is shown in Figure 17.

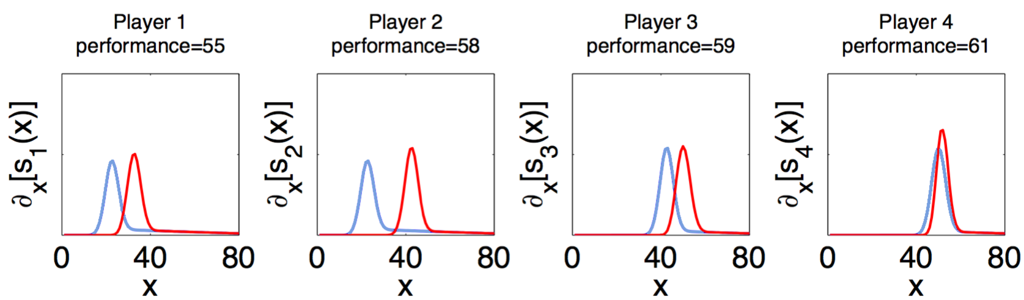


Figure 17: An example of derivative-sum-product updates for a four-player free-for-all game, with the derivative of the skill functions before the updates (light blue) and afterwards (red).

Before each game, we can predict the team performances using the player skills learned thus far via the rule $x_k^* = \arg\max_{x_k} \partial_{x_k}\left[s_k(x_k)\right]$. For each game, the set of team performances is then defined by the ordering of teams once the game is over, where we add the predicted player scores x_k^* together for each team and sorting the resulting sums in ascending order. For any predicted set of team performances, an error is incurred for that game if two teams for that game were mis-ranked such that the number of errors for a given game is $\sum_{n=1}^{N-1} \sum_{m>n}^{N} [R_n \leq R_m] \wedge [R_n^{true} > R_m^{true}]$. One can then compute an error rate over the entire set of games for which we make predictions about team performances.

2. Credits for the use of the Halo 2™ Beta Data Set are given to Microsoft Research Ltd. and Bungie.
3. These parameter settings were selected using a validation set and differ from those of Huang and Frey (2008).

A plot showing the average prediction error rate obtained for the above CDN models over five runs of DSP is shown in Figure 18. It is worth noting that our choice of multivariate Gaussian CDFs as CDN functions in the above model requires that we use a rejection sampling method in order to evaluate the CDN functions, so that the error bars over the five runs are shown. In addition, Figure 18 also shows the error rates reported by Herbrich et al. (2007) for TrueSkill™ and ELO (Elo, 1978), which is a statistical rating system used in chess. Here, we see that the ability to specify both ordinal relationships and statistical dependence relationships between model variables using a CDN allows us to achieve higher predictive accuracy than either TrueSkill™or the ELO method.

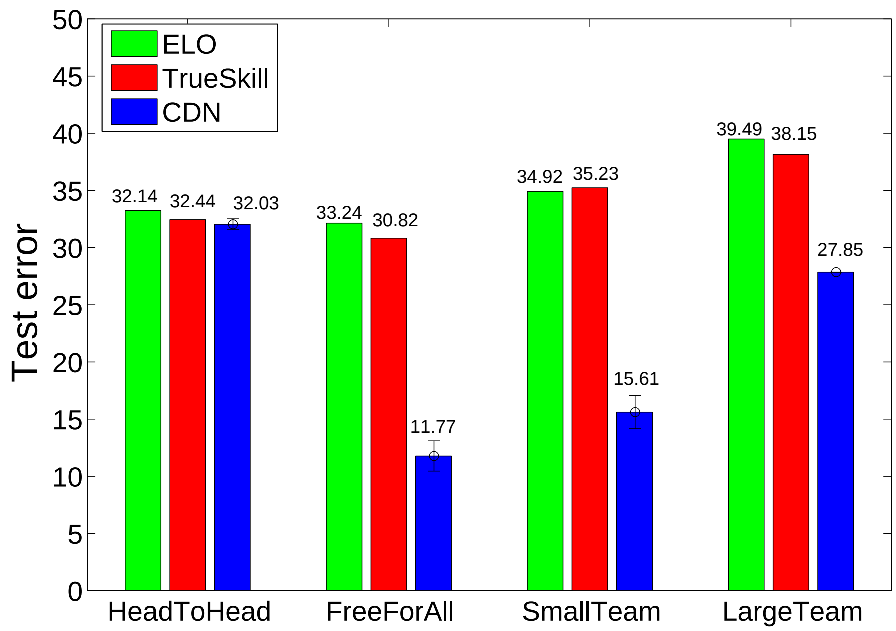


Figure 18: Prediction error on the Halo 2™ Beta data set (computed as the fraction of team predicted incorrectly before each game) for DSP, ELO (Elo, 1978) and TrueSkill™ (Herbrich, Minka and Graepel, 2007) methods. Error bars over five runs of DSP are shown.

4.4 Discussion

In this section we presented a model and method for learning to rank in the context of multiplayer team-based games such as Halo 2™. Our model represent both statistical dependence relationships and stochastic orderings of variables in the model such as team performances and individual player scores. We then used the DSP algorithm to compute conditional CDFs for each player's score. Comparisons to the TrueSkill™ and ELO methods for factor graph models show that our model and method allows both for fast estimation and improved test error on the Halo 2™ Beta data set.

While the above method has the advantage of providing a flexible probabilistic model and allowing for tractable inference, the choice of multivariate Gaussian CDFs for CDN functions requires the use of sampling methods in order to evaluate DSP messages. Future work could focus on finding closed-form parameterizations of CDN functions for which computing derivatives is tractable.

5. Conclusion

We have proposed the CDN as a graphical model for joint CDFs over many variables. We have shown that the conditional independence properties of a CDN are distinct from the independence properties of directed, undirected and factor graphs. However, these properties include, but are not limited to, those for bi-directed graphs. We have then demonstrated that inference in a CDN corresponds to computing derivatives/finite differences. We described the DSP algorithm for computing such derivatives/finite differences by passing messages in the CDN where each message corresponds to local derivatives of the joint CDF.

We used the graphical framework provided by CDNs to formulate models and methods for learning to rank in a structured setting in which we must account for statistical dependence relationships between model variables. We first applied the DSP algorithm to the problem of ranking in multiplayer gaming where players compete in teams. The DSP algorithm allowed us to compute distributions over player scores given previous game outcomes while accounting for the team-based structure of the games, whereby we were able to show improved results over previous methods. The CDN framework was then used to construct loss functionals for structured ranking learning where we wish to account for statistical dependence relationships which arise in ranking a set of objects. We showed that many probability models for rank data can be viewed as particular CDNs with different connectivities between pairwise object preferences. Based on the work and results presented, we can recommend future directions of research pertaining to the methods presented in this manuscript.

5.1 Future Work

While we presented a framework for constructing a graphical model for a joint CDF, there may be applications in which one may wish to instead optimize the log-probability density $\log P(\mathbf{x}|\boldsymbol{\theta})$. We presented the DSP algorithm for both discrete and continuous-variable networks and we showed how DSP could be used to compute the probability density $P(\mathbf{x}|\boldsymbol{\theta})$ from the joint CDF $F(\mathbf{x}|\boldsymbol{\theta})$ modeled by the CDN. In order to perform maximum likelihood learning in which we wish to maximize the log-likelihood $\mathcal{L}(\mathbf{x};\boldsymbol{\theta}) = \log P(\mathbf{x}|\boldsymbol{\theta})$ with respect to a parameter vector $\boldsymbol{\theta}$ for a given set of observed variables $\mathbf{x}$, one can use modified versions of DSP messages in order to compute the gradient $\nabla_{\boldsymbol{\theta}}\mathcal{L}(\mathbf{x};\boldsymbol{\theta})$ of the log-likelihood. The guiding principle here is that the gradient operator can be distributed amongst local functions in the CDF, much like the differentiation operation in DSP, so that by modifying DSP messages appropriately we can obtain the gradient $\nabla_{\boldsymbol{\theta}}\mathcal{L}(\mathbf{x};\boldsymbol{\theta})$. Once computed, the gradient vector can then be used in a gradient-descent algorithm to optimize the log-likelihood. Future research in this direction could be directed at establishing what class of graphs can yield tractable gradient computations, as well as the complexity/accuracy tradeoffs involved in computing gradients in graphs with cycles.

We have shown that our message-passing algorithm leads to the correct set of derivatives of the joint CDF provided that the underlying graph is a tree. As with the sum-product algorithm for factor graphs, if the graph contains cycles, then the derivative-sum-product is no longer guaranteed to yield the correct mixed derivatives of the joint CDF, so that messages may begin to 'oscillate' as they propagate around cycles in the graph. One important direction to pursue is to establish conditions under which the presence of cycles will not lead to oscillations in messages: one could resort to a similar methodology as that employed by Weiss and Freeman (2001), where a graph with cycles is “unwrapped” and the resulting messages are analyzed.

We showed that for graphs defined over continuous variables, the complexity of computing DSP message updates at a given function node increased exponentially with the number of neighboring variable nodes, as one has to sum over products of messages incoming from all subsets of variables connected to the function node. However, it may be possible to approximate messages using simpler, tractable forms such as conditional univariate Gaussian CDFs. Future work here would be to establish tractable methods for performing such approximations and gauge the performance of such an approximate scheme for inference in CDNs on both synthetic and real-world data.

As we have demonstrated, the graph separation criterion for assessing conditional independence in CDNs includes those of bi-directed graphs (Richardson and Spirtes, 2002). As such graphs are a special case of mixed graphs containing undirected, directed and bi-directed edges, a future avenue of research would be to investigate whether one can tractably approximate such mixed graphical models using a hybrid graphical formulation combining the CDN model with that of factor graphs for joint probability density/mass functions. The Bayesian learning approach adopted by Silva and Ghahramani (2009b) could provide a framework with which to qualitatively and quantitatively compare the use of CDNs for constructing such mixed graphical models.

Acknowledgments

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Appendix A.

Lemma 19 *Let* $M = \{\mathbf{x}_C < \mathbf{X}_C \leq \mathbf{x}_C + \boldsymbol{\epsilon}\} \equiv \bigcap_{\gamma \in C} \{x_\gamma < X_\gamma \leq x_\gamma + \varepsilon\}$ *with* $\varepsilon > 0$ *for* $\mathbf{X}_C \subset \mathbf{X}$ *and* $\boldsymbol{\epsilon} = [\varepsilon \cdots \varepsilon]^T \in \mathbb{R}^{|\mathbf{X}_C|}$. *Consider the set of random variables* $\mathbf{X}_A \subset \mathbf{X}$ *with* $\mathbf{X}_C \cap \mathbf{X}_A = \emptyset$. *If both* $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x}_C)\Big]$ *and* $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x}_A, \mathbf{x}_C)\Big]$ *exist for all* $\mathbf{x}_C$ *with* $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x}_C)\Big] > 0$, *then the conditional CDF* $F(\mathbf{x}_A|\mathbf{x}_C) \equiv \lim_{\boldsymbol{\epsilon} \to \mathbf{0}^+} F(\mathbf{x}_A|\mathbf{x}_C < \mathbf{X}_C \leq \mathbf{x}_C + \boldsymbol{\epsilon}) = \lim_{\boldsymbol{\epsilon} \to \mathbf{0}^+} \frac{\mathbb{P}\Big[\{\mathbf{X}_A \leq \mathbf{x}_A\} \cap \{\mathbf{x}_C < \mathbf{X}_C \leq \mathbf{x}_C + \boldsymbol{\epsilon}\}\Big]}{\mathbb{P}\Big[\mathbf{x}_C < \mathbf{X}_C \leq \mathbf{x}_C + \boldsymbol{\epsilon}\Big]}$ *is given by*

$$F(\mathbf{x}_A|\mathbf{x}_C) = \frac{\partial_{\mathbf{x}_C}\Big[F(\mathbf{x}_A, \mathbf{x}_C)\Big]}{\partial_{\mathbf{x}_C}\Big[F(\mathbf{x}_C)\Big]} \propto \partial_{\mathbf{x}_C}\Big[F(\mathbf{x}_A, \mathbf{x}_C)\Big],$$

where $\partial_{\mathbf{x}_C}\Big[\cdot\Big]$ *is a mixed derivative operator with respect to* $\{x_\gamma, \gamma \in C\}$.

Proof We can proceed by induction on variable set $\mathbf{X}_C$ with the base case given by Lemma 3. Let $\mathbf{X}_C = \mathbf{X}_{C'} \cup X_\beta$ with $X_\beta \notin \mathbf{X}_{C'} \cup \mathbf{X}_A$. Let $M' \equiv M'(\boldsymbol{\xi}) = \{\mathbf{x}_{C'} \le \mathbf{X}_{C'} \le \mathbf{x}_{C'} + \boldsymbol{\xi}\} = \bigcap_{\gamma \in C'} \{x_\gamma < X_\gamma \le x_\gamma + \xi\}$ and $M \equiv M(\boldsymbol{\xi}, \varepsilon) = M' \cap \{x_\beta < X_\beta \le x_\beta + \varepsilon\}$ with $\boldsymbol{\epsilon} = [\boldsymbol{\xi}^T\ \varepsilon]^{\mathrm{T}}$. Suppose that $\partial_{\mathbf{x}_{C'}}\Big[F(\mathbf{x}_{C'})\Big] > 0$ and we have computed

$$F(\mathbf{x}_A, x_\beta | \mathbf{x}_{C'}) \equiv \lim_{\boldsymbol{\xi} \to 0^+} F\big(\mathbf{x}_A, x_\beta | M'(\boldsymbol{\xi})\big) = \frac{\partial_{\mathbf{x}_{C'}}\Big[F(\mathbf{x}_A, x_\beta, \mathbf{x}_{C'})\Big]}{\partial_{\mathbf{x}_{C'}}\Big[F(\mathbf{x}_{C'})\Big]},$$

and

$$F(x_\beta | \mathbf{x}_{C'}) \equiv \lim_{\boldsymbol{\xi} \to 0^+} F\big(x_\beta | M'(\boldsymbol{\xi})\big) = \frac{\partial_{\mathbf{x}_{C'}}\Big[F(x_\beta, \mathbf{x}_{C'})\Big]}{\partial_{\mathbf{x}_{C'}}\Big[F(\mathbf{x}_{C'})\Big]}.$$

Then we can write

$$F(\mathbf{x}_A \mid M) = \frac{\mathbb{P}\Big[\{\mathbf{X}_A \le \mathbf{x}_A\} \cap \{x_\beta < X_\beta \le x_\beta + \varepsilon\} \mid M'\Big]}{\mathbb{P}\Big[x_\beta < X_\beta \le x_\beta + \varepsilon \mid M'\Big]} = \frac{\frac{F(\mathbf{x}_A, x_\beta + \varepsilon | M') - F(\mathbf{x}_A, x_\beta | M')}{\varepsilon}}{\frac{F(x_\beta + \varepsilon | M') - F(x_\beta | M')}{\varepsilon}}.$$

Thus, since $\partial_{\mathbf{x}_C}\Big[F(\mathbf{x}_C)\Big] > 0$ by hypothesis, we obtain

$$\begin{aligned} F(\mathbf{x}_A | \mathbf{x}_C) &= \lim_{\varepsilon \to 0^+, \boldsymbol{\xi} \to 0^+} \frac{\frac{F(\mathbf{x}_A, x_\beta + \varepsilon | M') - F(\mathbf{x}_A, x_\beta | M')}{\varepsilon}}{\frac{F(x_\beta + \varepsilon | M') - F(x_\beta | M')}{\varepsilon}} = \frac{\lim_{\varepsilon \to 0^+} \dfrac{F(\mathbf{x}_A, x_\beta + \varepsilon | \mathbf{x}_{C'}) - F(\mathbf{x}_A, x_\beta | \mathbf{x}_{C'})}{\varepsilon}}{\lim_{\varepsilon \to 0^+} \dfrac{F(x_\beta + \varepsilon | \mathbf{x}_{C'}) - F(x_\beta | \mathbf{x}_{C'})}{\varepsilon}} \\ &= \frac{\partial_{x_\beta, \mathbf{x}_{C'}}\Big[F(\mathbf{x}_A, x_\beta, \mathbf{x}_{C'})\Big]}{\partial_{x_\beta, \mathbf{x}_{C'}}\Big[F(x_\beta, \mathbf{x}_{C'})\Big]} = \frac{\partial_{\mathbf{x}_C}\Big[F(\mathbf{x}_A, \mathbf{x}_C)\Big]}{\partial_{\mathbf{x}_C}\Big[F(\mathbf{x}_C)\Big]}. \end{aligned}$$

■

Thus a conditional CDF of the form $F(\mathbf{x}_A | \mathbf{x}_C)$ can be obtained by differentiation of the joint CDF. By Schwarz's Theorem this differentiation is invariant to the order in which variables are processed provided that the derivatives required to compute $F(\mathbf{x}_A | \mathbf{x}_C)$ exist and are continuous.

A.1 Derivation of the Derivative-sum-product Algorithm

To begin, let $\mathcal{G} = (V, S, E)$ be a tree-structured CDN and suppose we wish to compute the joint probability $P(\mathbf{x})$ and evaluate it at observation $\mathbf{x}$. We note that we can root the graph at some node α and we can write the joint CDF as

$$F(\mathbf{x}) = \prod_{s \in \mathcal{N}(\alpha)} T_s\big(\mathbf{x}_{\tau_s^\alpha}\big),$$

where $\mathbf{x}_{\tau_s^\alpha}$ denotes the vector of configurations for all variables in the subtree τ_s^α rooted at variable node α and containing function node s (Figure 19), and $T_s\big(\mathbf{x}_{\tau_s^\alpha}\big)$ corresponds to the product of all functions located in the subtree τ_s^α.

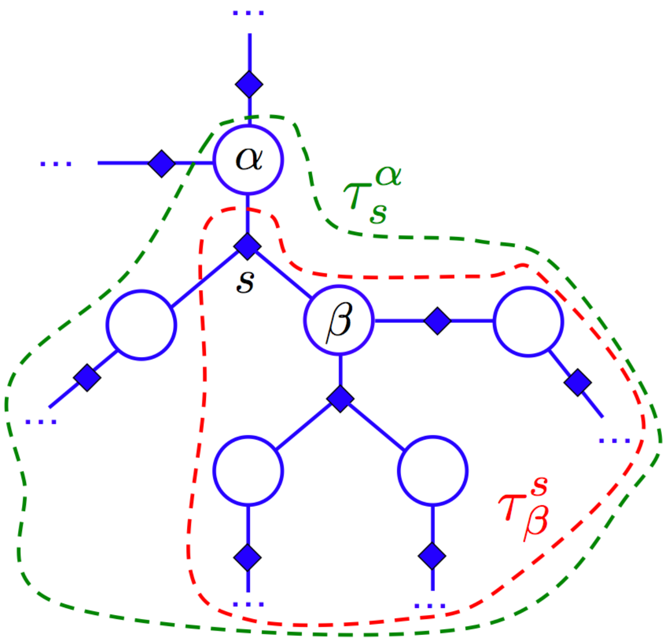

Figure 19: Example of the subtrees $\tau_s^\alpha, \tau_\beta^s$ for a tree-structured CDN given by the graph $\mathcal{G}$.

Now suppose we are interested in computing the probability

$$P(\mathbf{x}) = \partial_{\mathbf{x}}\Big[F(\mathbf{x})\Big] = \partial_{\mathbf{x}}\left[\prod_{s\in\mathcal{N}(\alpha)} T_s\big(\mathbf{x}_{\tau_s^\alpha}\big)\right].$$

Here, we take advantage of the fact that the graph has a tree structure, so that

$$\partial_{\mathbf{x}}\left[\prod_{s\in\mathcal{N}(\alpha)} T_s\big(\mathbf{x}_{\tau_s^\alpha}\big)\right] = \partial_{x_\alpha}\left[\prod_{s\in\mathcal{N}(\alpha)} \partial_{\mathbf{x}_{\tau_s^\alpha\setminus\alpha}}\Big[T_s\big(\mathbf{x}_{\tau_s^\alpha}\big)\Big]\right] = \partial_{x_\alpha}\left[\prod_{s\in\mathcal{N}(\alpha)} \mu_{s\to\alpha}\big(\mathbf{x}_{\tau_s^\alpha}\big)\right].$$

We have introduced the set of functions $\mu_{s\to\alpha}(\mathbf{x}) \equiv \mu_{s\to\alpha}\big(\mathbf{x}_{\tau_s^\alpha}\big)$ defined by

$$\mu_{s\to\alpha}(\mathbf{x}) \equiv \mu_{s\to\alpha}\big(\mathbf{x}_{\tau_s^\alpha}\big) = \partial_{\mathbf{x}_{\tau_s^\alpha\setminus\alpha}}\Big[T_s\big(\mathbf{x}_{\tau_s^\alpha}\big)\Big], \tag{3}$$

where we have assumed that each of the derivatives/finite differences have been evaluated at the desired values $\mathbf{x}_{\tau_s^\alpha\setminus\alpha}$. By its definition, $\mu_{s\to\alpha}(\mathbf{x})$ only depends on variables in the subtree τ_s^α and corresponds to the higher-order derivative of the joint CDF with respect to variables in the subtree $\tau_s^\alpha\setminus\alpha$. We can thus view the functions $\mu_{s\to\alpha}(\mathbf{x})$ as messages being passed from each function node $s\in\mathcal{N}(\alpha)$ in the CDN to a neighboring variable node α.

We can now write $T_s\big(\mathbf{x}_{\tau_s^\alpha}\big)$ as a product of functions owing to the tree structure of the graph $\mathcal{G}$, so that

$$T_s\big(\mathbf{x}_{\tau_s^\alpha}\big) = \phi_s(x_\alpha, \mathbf{x}_{\mathcal{N}(s)\setminus\alpha}) \prod_{\beta\in\mathcal{N}(s)\setminus\alpha} T_\beta\Big(\mathbf{x}_{\tau_\beta^s}\Big), \tag{4}$$

where $\mathbf{x}_{\tau_\beta^s}$ denotes the vector of configurations for all variables in the subtree τ_β^s which is rooted at function node s and contains node β (Figure 19), and T_β is the product of all functions in the subtree τ_β^s. Substituting Equation (4) into Equation (3), we obtain

$$\begin{aligned}\mu_{s\to\alpha}(\mathbf{x}) \equiv \mu_{s\to\alpha}\left(\mathbf{x}_{\tau_s^\alpha}\right) &= \partial_{\mathbf{x}_{\tau_s^\alpha\setminus\alpha}}\left[\phi_s(x_\alpha, \mathbf{x}_{\mathcal{N}(s)\setminus\alpha}) \prod_{\beta\in\mathcal{N}(s)\setminus\alpha} T_\beta\left(\mathbf{x}_{\tau_\beta^s}\right)\right] \\ &= \partial_{\mathbf{x}_{\mathcal{N}(s)\setminus\alpha}}\left[\phi_s(x_\alpha, \mathbf{x}_{\mathcal{N}(s)\setminus\alpha}) \prod_{\beta\in\mathcal{N}(s)\setminus\alpha} \partial_{\mathbf{x}_{\tau_\beta^s\setminus\beta}}\left[T_\beta\left(\mathbf{x}_{\tau_\beta^s}\right)\right]\right] \\ &= \partial_{\mathbf{x}_{\mathcal{N}(s)\setminus\alpha}}\left[\phi_s(x_\alpha, \mathbf{x}_{\mathcal{N}(s)\setminus\alpha}) \prod_{\beta\in\mathcal{N}(s)\setminus\alpha} \mu_{\beta\to s}\left(\mathbf{x}_{\tau_\beta^s}\right)\right]. \end{aligned} \quad (5)$$

Here we have defined messages $\mu_{\beta\to s}(\mathbf{x}) \equiv \mu_{\beta\to s}\left(\mathbf{x}_{\tau_\beta^s}\right)$ from variable nodes to function nodes. Similar to the definition for $\mu_{s\to\alpha}(\mathbf{x})$, the message $\mu_{\beta\to s}(\mathbf{x})$ only depends on variables in the subtree τ_β^s and corresponds to the higher-order derivative of the joint CDF with respect to variables in the subtree $\tau_\beta^s \setminus \beta$.

Finally, to compute the messages $\mu_{\beta\to s}(\mathbf{x})$ from variables to functions, we can write each of the functions $T_\beta\left(\mathbf{x}_{\tau_\beta^s}\right)$ as a product such that

$$T_\beta\left(\mathbf{x}_{\tau_\beta^s}\right) = \prod_{s'\in\mathcal{N}(\beta)\setminus s} T_{s'}\left(\mathbf{x}_{\tau_{s'}^\beta}\right),$$

where $T_{s'}$ is defined identically to T_s above but for function node s'. Substituting this into the expression for $\mu_{\beta\to s}(\mathbf{x})$ in Equation (5) yields

$$\begin{aligned}\mu_{\beta\to s}(\mathbf{x}) = \partial_{\mathbf{x}_{\tau_\beta^s\setminus\beta}}\left[T_\beta\left(\mathbf{x}_{\tau_\beta^s}\right)\right] &= \prod_{s'\in\mathcal{N}(\beta)\setminus s} \partial_{\mathbf{x}_{\tau_{s'}^\beta\setminus\beta}}\left[T_{s'}\left(\mathbf{x}_{\tau_{s'}^\beta}\right)\right] \\ &= \prod_{s'\in\mathcal{N}(\beta)\setminus s} \mu_{s'\to\beta}(\mathbf{x}).\end{aligned}$$

Thus, to compute messages from variables to functions, we simply take the product of all incoming messages except for the message coming from the destination function node. As in the sum-product algorithm, variables with only two neighboring functions simply pass messages through unchanged. We see here that the process of differentiation in a CDN can be implemented as an algorithm in which we pass messages $\mu_{\alpha\to s}$ from variables to neighboring function nodes and messages $\mu_{s\to\alpha}$ from functions to neighboring variable nodes. Messages can be computed recursively from one another as described above: we start from an arbitrary root variable node α and propagate messages up from leaf nodes to the root node. As in the sum-product algorithm, leaf variable nodes α' send the message $\mu_{\alpha'\to s}(\mathbf{x}) = 1$ while leaf function nodes $\phi_s(x_{\alpha'})$ send the message $\mu_{s\to\alpha'}(\mathbf{x}) = \phi_s(x_{\alpha'})$.

The message-passing algorithm proceeds until messages have been propagated along every edge in the network and the root variable node has received all incoming messages from the remainder of the network. Once all messages have been sent, we can obtain the probability density of the variables in the graph from differentiating the product of incoming messages at the root node α, so that

$$P(\mathbf{x}) = \partial_{x_\alpha}\left[\prod_{s\in\mathcal{N}(\alpha)} \mu_{s\to\alpha}(\mathbf{x})\right].$$

A.2 Ordinal Regression

In many domains, one is faced with the problem of predicting multinomial variables that can each take one of a finite number of values in some discrete set $\mathcal{X} = \{r_1, \cdots, r_K\}$ for some integer K. Such multinomial variables can then be distinguished as being of the type

- *Nominal*, or *categorical*, so that the set $\mathcal{X}$ does not admit an ordering of variable values.
- *Ordinal*, so that the set $\mathcal{X}$ admits a total ordering over variable values of the type $r_1 \prec \cdots \prec r_K$.

An example of a nominal variable is gender, such as $\mathcal{X} = \{Male, Female\}$ and an example of an ordinal variable is a grading scheme $\mathcal{X} = \{A,B,C,D\}$ so that the possible variable values satisfy the total ordering $D \prec C \prec B \prec A$.

In ordinal regression, the goal is to predict a discrete variable $y \in \{r_1, \cdots, r_K\}$ given a set of features $\mathbf{x}$, where $r_1 \prec \cdots \prec r_K$ are an ordered set of labels. Unlike the general problem of multiclass classification in which variables to be predicted are nominal, output labels in the setting of ordinal regression are not permutation-invariant and so any model for the problem should account for the orderings of the output variable values.

One model for performing ordinal regression is the *cumulative model* (McCullagh, 1980), which relates an input vector $\mathbf{x}$ to an ordinal output y via a function f and a set of *cutpoints* $\theta(r_1) < \cdots < \theta(r_K)$ along the real line $\mathbb{R}$ so that $y = r_k$ if $\theta(r_{k-1}) < f(\mathbf{x}) + \varepsilon \leq \theta(r_k)$, where ε is additive noise and we define $\theta(r_0) = -\infty, \theta(r_K) = \infty$ (Figure 20). If $P(\varepsilon)$ is the probability density function from which the noise variable ε is drawn, then we can write

$$\begin{aligned}\mathbb{P}\big[y = r_k\big] &= \mathbb{P}\big[\theta(r_{k-1}) < f(\mathbf{x}) + \varepsilon \leq \theta(r_k)\big] \\ &= \mathbb{P}\big[\{\theta(r_{k-1}) - f(\mathbf{x}) < \varepsilon\} \bigcap \{\varepsilon \leq \theta(r_k) - f(\mathbf{x})\}\big] \\ &= F_\varepsilon(\theta(r_{k-1}) - f(\mathbf{x})) - F_\varepsilon(\theta(r_k) - f(\mathbf{x})),\end{aligned}$$

where $F_\varepsilon \equiv F(\varepsilon)$ is the corresponding cumulative distribution function for $P(\varepsilon)$. The above equation defines a likelihood function for a given observed pair $(\mathbf{x}, y)$, so that the cutpoints $\theta(r_k)$ and the regression function $f(\mathbf{x})$ can subsequently be estimated from training data by maximizing the likelihood function with respect to the cutpoints $\theta(r_k)$ and the regression function $f(\mathbf{x})$.

A.3 Derivative-sum-product Message Updates for Learning to Rank in Multiplayer Games

Here we present the DSP algorithm for updating player ranks. Messages are ensured to be properly normalized locally by computing the constant $\mathcal{Z} = \lim_{z\to\infty} \mu(z)$ for each message and multiplying the message pair μ, λ by $\mathcal{Z}^{-1}$.

- Initialize for each player score node X_k:

$$\begin{aligned}\mu_{X_k\to g_n}(x_k) &= s_k(x_k), \\ \lambda_{X_k\to g_n}(x_k) &= \partial_{x_k}\Big[s_k(x_k)\Big].\end{aligned}$$

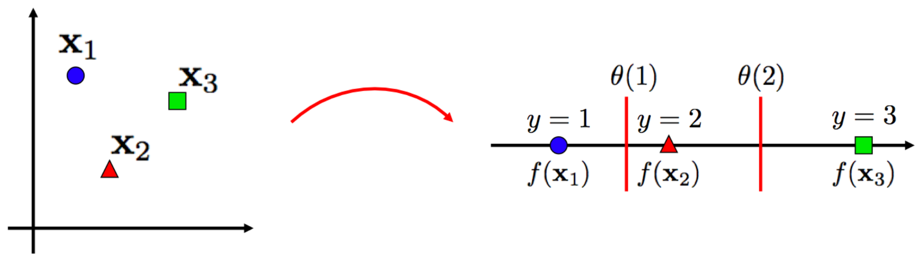

Figure 20: An illustration of the ordinal regression model. A given point has label $y = r_k$ if $\theta(r_{k-1}) < f(\mathbf{x}) + \varepsilon \leq \theta(r_k)$, where ε is a noise variable.

- Pass messages from function node g_n to team performance node R_n for neighboring player nodes $\mathbf{X}_n$, $n = 1, \cdots, N$:

$$\mu_{g_n \to R_n}(\mathbf{r}, \mathbf{x}) = \sum_{\substack{s,t | \mathbf{X}_s \cup \mathbf{X}_t = \mathbf{X}_n \\ \mathbf{X}_s \bigcap \mathbf{X}_t = \emptyset}} \partial_{\mathbf{x}_s} \Big[g_n(\mathbf{x}_n, r_n) \Big] \prod_{j | X_j \in \mathbf{X}_s} \mu_{X_j \to g_n}(x_j) \prod_{j | X_j \in \mathbf{X}_t} \lambda_{X_j \to g_n}(x_j),$$

$$\lambda_{g_n \to R_n}(\mathbf{r}, \mathbf{x}) = \sum_{\substack{s,t | \mathbf{X}_s \cup \mathbf{X}_t = \mathbf{X}_n \\ \mathbf{X}_s \bigcap \mathbf{X}_t = \emptyset}} \partial_{\mathbf{x}_s, r_n} \Big[g_n(\mathbf{x}_n, r_n) \Big] \prod_{j | X_j \in \mathbf{X}_s} \mu_{X_j \to g_n}(x_j) \prod_{j | X_j \in \mathbf{X}_t} \lambda_{X_j \to g_n}(x_j).$$

- Set $\mu_{h_{n-1,n} \to R_n}(\mathbf{r}, \mathbf{x}) = \lambda_{h_{n-1,n} \to R_n}(\mathbf{r}, \mathbf{x}) = 1$ for $n = 1$. Pass messages from team performance node R_n to neighboring team performance nodes R_{n+1} and function nodes $h_{n,n+1}$ for $n = 1, \cdots, N$:

$$\begin{aligned}
\mu_{R_n \to h_{n,n+1}}(\mathbf{r}, \mathbf{x}) &= \mu_{h_{n-1,n} \to R_n}(\mathbf{r}, \mathbf{x}) \mu_{g_n \to R_n}(\mathbf{r}, \mathbf{x}), \\
\lambda_{R_n \to h_{n,n+1}}(\mathbf{r}, \mathbf{x}) &= \lambda_{h_{n-1,n} \to R_n}(\mathbf{r}, \mathbf{x}) \mu_{g_n \to R_n}(\mathbf{r}, \mathbf{x}) \\
&\quad + \mu_{h_{n-1,n} \to R_n}(\mathbf{r}, \mathbf{x}) \lambda_{g_n \to R_n}(\mathbf{r}, \mathbf{x}), \\
\mu_{h_{n,n+1} \to R_{n+1}}(\mathbf{r}, \mathbf{x}) &= \mu_{R_n \to h_{n,n+1}}(\mathbf{r}, \mathbf{x}) \partial_{r_n} \Big[h_{n,n+1}(r_n, r_{n+1}) \Big] \\
&\quad + \lambda_{R_n \to h_{n,n+1}}(\mathbf{r}, \mathbf{x}) h_{n,n+1}(r_n, r_{n+1}), \\
\lambda_{h_{n,n+1} \to R_{n+1}}(\mathbf{r}, \mathbf{x}) &= \mu_{R_n \to h_{n,n+1}}(\mathbf{r}, \mathbf{x}) \partial_{r_n, r_{n+1}} \Big[h_{n,n+1}(r_n, r_{n+1}) \Big] \\
&\quad + \lambda_{R_n \to h_{n,n+1}}(\mathbf{r}, \mathbf{x}) \partial_{r_{n+1}} \Big[h_{n,n+1}(r_n, r_{n+1}) \Big].
\end{aligned}$$

- Set $\mu_{h_{n,n+1} \to R_n}(\mathbf{r}, \mathbf{x}) = \lambda_{h_{n,n+1} \to R_n}(\mathbf{r}, \mathbf{x}) = 1$ for $n = N$. Pass messages from team performance node R_n to neighboring team performance nodes R_{n-1} and function nodes $h_{n-1,n}$ for $n =$

$1,\cdots,N$:

$$\begin{aligned}
\mu_{R_n\to h_{n-1,n}}(\mathbf{r},\mathbf{x}) &= \mu_{h_{n,n+1}\to R_n}(\mathbf{r},\mathbf{x})\mu_{g_n\to R_n}(\mathbf{r},\mathbf{x}),\\
\lambda_{R_n\to h_{n-1,n}}(\mathbf{r},\mathbf{x}) &= \lambda_{h_{n,n+1}\to R_n}(\mathbf{r},\mathbf{x})\mu_{g_n\to R_n}(\mathbf{r},\mathbf{x})\\
&\quad + \mu_{h_{n,n+1}\to R_n}(\mathbf{r},\mathbf{x})\lambda_{g_n\to R_n}(\mathbf{r},\mathbf{x}),\\
\mu_{h_{n-1,n}\to R_{n-1}}(\mathbf{r},\mathbf{x}) &= \mu_{R_n\to h_{n-1,n}}(\mathbf{r},\mathbf{x})\partial_{r_n}\left[h_{n-1,n}(r_{n-1},r_n)\right]\\
&\quad + \lambda_{R_n\to h_{n-1,n}}(\mathbf{r},\mathbf{x})h_{n-1,n}(r_{n-1},r_n),\\
\lambda_{h_{n-1,n}\to R_{n-1}}(\mathbf{r},\mathbf{x}) &= \mu_{R_n\to h_{n-1,n}}(\mathbf{r},\mathbf{x})\partial_{r_{n-1},r_n}\left[h_{n-1,n}(r_{n-1},r_n)\right]\\
&\quad + \lambda_{R_n\to h_{n-1,n}}(\mathbf{r},\mathbf{x})\partial_{r_{n-1}}\left[h_{n-1,n}(r_{n-1},r_n)\right].
\end{aligned}$$

- Pass messages from each team performance node R_n to neighboring function nodes g_n:

$$\begin{aligned}
\mu_{R_n\to g_n}(\mathbf{r},\mathbf{x}) &= \mu_{h_{n-1,n}\to R_n}(\mathbf{r},\mathbf{x})\mu_{h_{n,n+1}\to R_n}(\mathbf{r},\mathbf{x}),\\
\lambda_{R_n\to g_n}(\mathbf{r},\mathbf{x}) &= \lambda_{h_{n-1,n}\to R_n}(\mathbf{r},\mathbf{x})\mu_{h_{n,n+1}\to R_n}(\mathbf{r},\mathbf{x})\\
&\quad + \mu_{h_{n-1,n}\to R_n}(\mathbf{r},\mathbf{x})\lambda_{h_{n,n+1}\to R_n}(\mathbf{r},\mathbf{x}).
\end{aligned}$$

- Pass messages from function nodes g_n to neighboring player score nodes X_k:

$$\begin{aligned}
\mu_{g_n\to X_k}(\mathbf{r},\mathbf{x}) = &\sum_{\substack{s,t|\mathbf{X}_s\cup\mathbf{X}_t=\mathbf{X}_n\setminus X_k\\ \mathbf{X}_s\bigcap\mathbf{X}_t=\emptyset}} \prod_{j|X_j\in\mathbf{X}_s}\mu_{X_j\to g_n}(x_j)\prod_{j|X_j\in\mathbf{X}_t}\lambda_{X_j\to g_n}(x_j)\\
&\cdot\left(\partial_{\mathbf{x}_s}\left[g_n(\mathbf{x}_n,r_n)\right]\lambda_{R_n\to g_n}(\mathbf{r},\mathbf{x}) + \partial_{\mathbf{x}_s,r_n}\left[g_n(\mathbf{x}_n,r_n)\right]\mu_{R_n\to g_n}(\mathbf{r},\mathbf{x})\right),\\
\lambda_{g_n\to X_k}(\mathbf{r},\mathbf{x}) = &\sum_{\substack{s,t|\mathbf{X}_s\cup\mathbf{X}_t=\mathbf{X}_n\setminus X_k\\ \mathbf{X}_s\bigcap\mathbf{X}_t=\emptyset}} \prod_{j|X_j\in\mathbf{X}_s}\mu_{X_j\to g_n}(x_j)\prod_{j|X_j\in\mathbf{X}_t}\lambda_{X_j\to g_n}(x_j)\\
&\cdot\left(\partial_{\mathbf{x}_s,x_k}\left[g_n(\mathbf{x}_n,r_n)\right]\lambda_{R_n\to g_n}(\mathbf{r},\mathbf{x}) + \partial_{\mathbf{x}_s,x_k,r_n}\left[g_n(\mathbf{x}_n,r_n)\right]\mu_{R_n\to g_n}(\mathbf{r},\mathbf{x})\right).
\end{aligned}$$

- For each player score node X_k,

$$\begin{aligned}
\mu_{X_k\to s_k}(\mathbf{r},\mathbf{x}) &= \mu_{g_n\to X_k}(\mathbf{r},\mathbf{x}),\\
\lambda_{X_k\to s_k}(\mathbf{r},\mathbf{x}) &= \lambda_{g_n\to X_k}(\mathbf{r},\mathbf{x}).
\end{aligned}$$

- Update player skill functions $s_k(x_k)$ using the multiplicative rule

$$s_k(x_k) \leftarrow s_k(x_k)\mu_{g_n\to X_k}(\mathbf{x},\mathbf{r}).$$

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