Bayesian Network with Discrete Random Variables and its Python Implementation

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Contents

2	Bayesia	n Network
	2.1 Mo	tivation
	2.2 Int	roduction to Bayesian Network
	2.3 Im	plementation
	2.3	.1 Distribution
	2.3	.2 onconditional Distriction
	2.3	
	2.3	.4 Vertex
	2.3	5 BayesNetwork
	2.3	6 read_bayes_network_from_txt

1 Preface & Acknowledgements

2 Bayesian Network

2.1 Motivation

Consider a set of random variables $\mathbf{X} = (X_1, \dots, X_n)$ where each $X_i \in \{x_i, \neg x_i\}$ is binary. To specify the joint distribution of \mathbf{X} , we need to list out all the possible combinations:

$$\mathbb{P}(x_1, x_2, \cdots, x_n);
\mathbb{P}(\neg x_1, x_2, \cdots, x_n);
\mathbb{P}(x_1, \neg x_2, \cdots, x_n);
\vdots$$

For n random variables, the number of joint probabilities is $2^n - 1$, which quickly becomes intractable as n grows large, requiring a more efficient framework for modeling joint probabilities. Bayesian Network, or Directed Acyclic Graphical Model (DAGM), is one such framework exploiting *Theorem 1* below.

Theorem 1. (Chain Rule of Probability) Let X_1, \dots, X_n be random variables. Then the joint probability can be expressed as

$$\mathbb{P}(X_{1}, \dots, X_{n}) = \mathbb{P}(X_{1})\mathbb{P}(X_{2}, X_{3}, \dots, X_{n}|X_{1})
= \mathbb{P}(X_{1})\mathbb{P}(X_{2}|X_{1})\mathbb{P}(X_{3}, \dots, X_{n}|X_{1}, X_{2})
= \dots
= \mathbb{P}(X_{1})\mathbb{P}(X_{2}|X_{1})\mathbb{P}(X_{3}|X_{1}, X_{2}) \dots \mathbb{P}(X_{n}|X_{1}, X_{2}, \dots, X_{n-1})
= \prod_{i=1}^{n} \mathbb{P}(X_{i}|X_{1}, X_{2}, \dots, X_{i-1}).$$

Thus, if we have prior knowledge about the conditional independence relationships between the random variables we are modeling, then we can express the joint distribution in a more compact form, which motivates the use of Bayesian Networks.

2.2 Introduction to Bayesian Network

An example of Bayesian Network is shown in Figure 1 below.

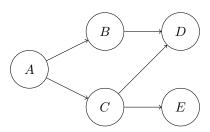


Figure 1: Bayesian Network Example

In this Bayesian Network, each vertex represents a random variable. The arrows denote conditional dependencies between random variables. For example, the edge $A \longrightarrow B$ implies that B is directly conditionally dependent on A. With this structure, we can model the joint distribution of these random variables in the following way:

Definition 1. Let $\mathbf{X} = (X_1, \dots, X_n)$ be a set of random variables modeled by a Bayesian Network. Then the joint probability can be expressed as

$$\mathbb{P}(X_1,\dots,X_n)=\prod_{i=1}^n\mathbb{P}(X_i|\operatorname{Parents}(X_i)).$$

Example 1. For the Bayesian Network shown in *Figure 1*, the joint probability can be expressed as

$$\mathbb{P}(A,B,C,D,E) = \mathbb{P}(A) \cdot \mathbb{P}(B|A) \cdot \mathbb{P}(C|A) \cdot \mathbb{P}(D|B,C) \cdot \mathbb{P}(E|C).$$

Note that *Definition 1* is a special case of *Theorem 1*, given that we have prior knowledge of the conditional independence relationships between the random variables. As a result, we can reduce the number of conditionals in the product and express the joint distribution in a more compact form. To illustrate this concept more clearly, let's define some probabilities for the Bayesian Network shown in *Figure 1*. These probabilities will be used throughout the rest of this document.

Example 2. Let $A, B, C, D, E \in \{0, 1\}$ be binary random variables with the following conditional probabilities:

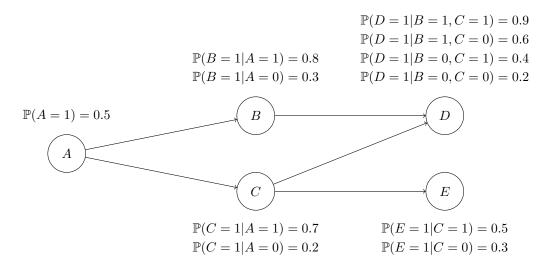


Figure 2: Bayesian Network with Probabilities Example

Note that only 11 conditional probabilities are needed to specify the joint distribution of the 5 random variables in our Bayesian Network, which is a significant improvement compared to the $2^5 - 1 = 31$ joint probabilities in the general case. The exact number of required conditional probabilities depends on the structure of the Bayesian Network, though, but as long as there are some conditional independence relationships between the random variables, we can always expect a reduction in the number of required conditional probabilities.

2.3 Implementation

The implementation of Bayesian Network in this project consists of multiple modules which are discussed separately in the following subsections.

2.3.1 Distribution

The distribution.py file defines an abstract class called Distribution, as well as two inherited classes named UnconditionalDistribution and ConditionalDistribution. The purpose of these classes is to provide a data structure that encodes the probability distribution of a vertex in the Bayesian Network.

The abstract class Distribution has the attribute and method definitions:

```
domain: set
```

This attribute defines the set of possible values for the random variables.

```
__call__(self, *args) -> float
```

This method evaluates the probability of the random variable taking on a specific value in the domain.

2.3.2 UnconditionalDistribution

The UnconditionalDistribution class defines the distribution of a random variable that does not have a parent in the Bayesian Network, as well as the distribution of a random variable conditioned on its parents. Besides the inherited attribute domain, it has the following attribute:

```
distribution: dict[Any, float]
```

This attribute serves as a lookup table for the unconditional distribution of the random variable. The keys of the dictionary are the possible values of the random variable, and the values are the corresponding probabilities.

```
__init__(self, domain: set, distribution: dict[Any, float]) -> None
```

This is the constructor of the class. It takes in the domain and the distribution as arguments. The constructor checks if the provided domain and distribution are valid. If domain does not match the keys of distribution, or the probabilities in distribution do not sum to 1, a ValueError will be raised.

This class also implements the __call__ method. The expected argument is a value in the domain of the random variable, and the method outputs the probability of the random variable taking on that value. If the argument is not in the domain, a ValueError will be raised.

Example 3. For the Bayesian Network shown in Figure 2, the distribution of vertex A would have the following behaviors:

```
>>> dist_A = UnconditionalDistribution(domain={0, 1}, distribution={0: 0.5, 1: 0.5})
>>> dist_A(0)
0.5
>>> dist_A(1)
0.5
```

2.3.3 ConditionalDistribution

This class defines the distribution of a random variable that has parents in the Bayesian Network. It inherits the domain attribute from the Distribution class, and it has the following attributes:

```
distributions[frozenset[str], UnconditionalDistribution]
```

The keys of this dictionary are frozensets of conditionals of the random variable, and the values define the distribution of the random variable conditioned on the values of its parents.

```
distributions: dict[frozenset[str], UnconditionalDistribution]) -> None
```

This constructor takes in the domain and the distributions as arguments. The constructor checks if the provided domain and distributions are valid. If domain does not match the domain of each UnconditionalDistribution object in distribution, a ValueError will be raised.

This class also implements the __call__ method. The expected arguments are a value in the domain of the random variable and a dictionary of the values of its parents. The method outputs the probability of the random variable taking on that value, given the values of its parents. If the value is not in the domain, or if the parents are not in the dictionary, or if the conditioning values are not in the domain of the parents, a ValueError will be raised.

This is slightly confusing, so the following example illustrates this concept.

Example 4. For the Bayesian Network shown in Figure 2, the distribution of vertex D would have the following behaviors:

```
>>> dist_D_B1C1 = UnconditionalDistribution(domain={0, 1}, distribution={0: 0.1, 1: 0.9})
>>> dist_D_B1C0 = UnconditionalDistribution(domain={0, 1}, distribution={0: 0.4, 1: 0.6})
>>> dist_D_B0C1 = UnconditionalDistribution(domain={0, 1}, distribution={0: 0.6, 1: 0.4})
>>> dist_D_B0C0 = UnconditionalDistribution(domain={0, 1}, distribution={0: 0.8, 1: 0.2})
>>> dist_D = ConditionalDistribution(domain={0, 1}, distributions={
    frozenset({'B: 1', 'C: 1'}): dist_D_B1C1,
    frozenset({'B: 1', 'C: 0'}): dist_D_B1C0,
    frozenset({'B: 0', 'C: 1'}): dist_D_B0C1,
    frozenset({'B: 0', 'C: 0'}): dist_D_B0C0
})
>>> dist_D(1, {'B': 1, 'C': 0})
0.6
>>> dist_D(0, {'C': 0, 'B': 0})
0.8
```

The use of a frozenset data structure is a compromise to the need for a hashable data structure. The advantage is that we don't need to memorize the order of the parents when we are looking up the distribution because there is no inherent order for a set object. When looking up probabilities, the order in which we pass in the parents thus does not matter, as long as the values are correct, which ensures the efficiency of the lookup process.

2.3.4 Vertex

The Vertex class represents a vertex in the Bayesian Network. It has the following attributes:

```
name: str
```

This attribute defines the name of the vertex.

```
domain: set
```

This attribute defines the set of possible values for the random variable.

```
parents: dict[str, Self]
```

This attribute holds a list of the vertex's parents in the Bayesian Network. The keys of the dictionary are the names of the parents, and the values are the corresponding Vertex objects.

```
children: dict[str, Self]
```

Similar to the parents attribute, this attribute holds a list of the vertex's children in the Bayesian Network. The keys of the dictionary are the names of the children, and the values are the corresponding Vertex objects.

```
distribution: Optional[Distribution]
```

This attribute holds the distribution of the vertex. Depending on whether the vertex has parents or not, this attribute can be either an UnconditionalDistribution or a ConditionalDistribution object.

The Vertex class also implements the following methods:

```
__init__(self, name: str, domain: set) -> None
```

This constructor takes in the name and domain of the vertex as arguments. It initializes the parents, children, and distribution attributes to empty dictionaries or None.

```
add_parent(self, parent: Self) -> None
add_child(self, child: Self) -> None
```

These two methods add a parent or child to the vertex. If the added vertex is already a parent or child of the vertex, a ValueError will be raised.

```
in_domain(self, value: Any) -> bool
```

This method returns True if the value is in the domain of the vertex, and False otherwise.

```
set_distribution(self, distribution: Distribution) -> None
```

This method sets the distribution of the vertex. This method contains many checks to ensure that distribution is valid. If distribution is not compatible with the vertex, a ValueError will be raised.

```
__call__(self, *args) -> float
```

This method basically calls the __call__ method of the distribution object with the arguments *args. The expected arguments are the same as the __call__ method of the distribution object and outputs a probability. If the distribution attribute for the vertex is None, a ValueError will be raised.

2.3.5 BayesNetwork

This class represents the Bayesian Network. It has the following attribute:

```
vertices: dict[str, Vertex]
```

This attribute holds a list of the vertices in the Bayesian Network. The keys of the dictionary are the names of the vertices, and the values are the corresponding Vertex objects.

The BayesNetwork class implements the following methods:

```
__init__(self) -> None
```

The constructor creates a BayesNetwork object and initializes the vertices attribute to an empty dictionary.

```
__len__(self) -> int
```

This method returns the number of vertices in the Bayesian Network.

```
add_node(self, vertex: Vertex) -> None
```

This method adds a vertex to the Bayesian Network. If the vertex is already in the network, a ValueError will be raised.

```
add_edge(self, parent: Vertex, child: Vertex) -> None
```

This method adds an edge from the parent vertex to the child vertex in the Bayesian Network. If either vertex is not in the network, a ValueError will be raised.

```
find_roots(self) -> list[Vertex]
```

This method returns a list of the root vertices in the Bayesian Network. A root vertex is defined as a vertex that does not have any parents in the network.

```
__call__(self, *args) -> float
```

This method evaluates the joint probability of the random variables in the Bayesian Network. The expected argument is a dictionary with the keys being the names of the random variables and the values being the corresponding values. The method outputs the joint probability of the random variables taking on those values. If values for one or more random variables are not provided, a ValueError will be raised. To compute the probability of a subset of the random variables, use the Variable Elimination algorithm discussed in the next section.

2.3.6 read_bayes_network_from_txt

The above description might be very confusing, so it is not recommended to create a Bayesian Network from scratch. Instead, I provide a function to read in a Bayesian Network from a text file. An example of this text file is provided in this bn_ex.txt file. The text file requires 3 parts, explained using the example file and Figure 2:

```
A: {0, 1}
B: {0, 1}
C: {0, 1}
D: {0, 1}
E: {0, 1}
```

This part defines the vertices in the Bayesian Network. Each line contains the name of the vertex and its domain, enclosed in curly braces. The vertices are separated by new lines.

```
A -> B
A -> C
B -> D
C -> D
C -> E
```

. . .

This part defines the edges in the Bayesian Network. Each line contains the name of the parent vertex and the name of the child vertex, separated by an arrow (->). The edges are separated by new lines.

```
P(A = 1) = 0.5

P(A = 0) = 0.5

P(B = 1 | A = 1) = 0.8

P(B = 0 | A = 1) = 0.2

P(B = 1 | A = 0) = 0.3

P(B = 0 | A = 0) = 0.7

P(D = 1 | B = 1, C = 1) = 0.9

P(D = 0 | B = 1, C = 1) = 0.1

P(D = 1 | B = 1, C = 0) = 0.6

P(D = 0 | B = 1, C = 0) = 0.6

P(D = 0 | B = 1, C = 0) = 0.4

P(D = 1 | B = 0, C = 1) = 0.4

P(D = 1 | B = 0, C = 1) = 0.6

P(D = 1 | B = 0, C = 0) = 0.2

P(D = 0 | B = 0, C = 0) = 0.2
```

This part defines the unconditional and conditional distributions of the vertices in the Bayesian Network. The

conditional distributions are separated by new lines. Note that it is necessary to provide the probabilities for both P(A = 1) and P(A = 0) in the text file, even though the complement can be easily computed.

As long as the format is followed, the order in which the vertices, edges, and distributions are defined does not matter because the function uses regular expression to parse the text file. The function will create a BayesNetwork object and add the vertices, edges, and distributions to the object. The function then returns the BayesNetwork object. It is strongly recommended to use this function to create a Bayesian Network.

To wrap up this section, below is an example of how to use the function to create a Bayesian Network from a text file.

Example 5. Assume that the text file is named bn_ex.txt and is in the same directory as the Python file.

```
>>> bn = read_bayes_network_from_txt('bn_ex.txt')
>>> bn.find_roots()
[A: {0, 1}]
>>> len(bn)
5
```

For some joint probability computations:

```
\mathbb{P}(A=1,B=0,C=1,D=1,E=0) = \mathbb{P}(A=1)\mathbb{P}(B=0|A=1)\mathbb{P}(C=1|A=1)\mathbb{P}(D=1|B=0,C=1)\mathbb{P}(E=0|C=1) \\ = 0.5 \cdot 0.2 \cdot 0.7 \cdot 0.4 \cdot 0.5 \\ = 0.014.
```

The code output confirms this result:

```
>>> bn({'A': 1, 'B': 0, 'C': 1, 'D': 1, 'E': 0})
0.0139999999999999 # Numerical roundoff error
```

3 Variable Elimination