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Geometrical Social Networks

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Abstract

The rise of social networks in the past few years has been remarkable. The main reason behind the tremendous success of the social media is none other than Facebook. Facebook paved the way for other popular social networking applications such as Twitter and Instagram. Facebook is an online social networking application where users can become friends and socialize with anyone throughout the world. To find how two users from various different regions are connected, Facebook came with an idea called the Social Connectedness Index (SCI) to quantitize the strength of the connection. We expected that the relationship between users and their friend, the SCI, and the distance between users and their friends has some characteristic dependence and independence information. Such independence information is nowadays often represented by means of Bayesian networks. A Bayesian network is a type of probabilistic graphical model that captures dependence and independence information as a graph and a joint probability distribution.

In this research, the main emphasis is on finding the right structure of the Bayesian network for predicting the SCI. In particular, we focus on structure learning and parameter learning from data. Tabu search is one of the structure learning algorithms we used to find right structure of the Bayesian network. The resulting network is subsequently validated using K-fold cross-validation, confusion matrices, ROC analysis, and calibration plots to see the difference between observed and predicted probabilities. In addition, the Brier score and the Log-likelihood of the model are calculated. We also compared the results of the model for various different group of countries and also investigated the distribution of SCI and distance between users and friends. The next thing was to find the optimal number of bins when discretizing the data. Finally, we compared the Tabu-search Bayesian network with a naive Bayes network.

We were able to find the right Bayesian network structure using Tabu search. When the network is validated using K-fold cross-validation, the scores we get from that show that the network has performed well. The accuracy obtained is 87 percentage which again shows that the model has performed well and the ROC curve is an other example for showing how well the model has performed. The Brier score obtained is close to 0 which again proves the worth of the model. When the model is compared to the naive Bayes network, the naive Bayes network achieved an accuracy of about 30 percentage and it has performed poorly when we compare it to the Tabu search based model. The calibration plots of scaledsci and distancekm show that the model has calibrated very well. When the model is compared for various different group of countries, the distribution of scaledsci and distancekm changes for every particular group of countries. The optimal number of bins chosen is 4 since for every other bin, the network encountered problems like low accuracy and data imbalancing.

Keywords: Social Connectedness Index, Bayesian networks, machine learning, structure learning, social networks.

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1. Introduction and Related work

1.1 Motivation

Social networks have become so popular that they are involved in almost every person's life. Facebook, Instagram and Twitter are some of the most popular social networking sites. People use social networks to build social relationships with other people who might have similar interests, activities and careers. Social networks make people share their ideas, photos, videos and also inform other people about real-world activities with their friends.

Facebook is one of the major reasons for the success of online social media. It was founded in the year 2004, by Mark Zuckerberg. It is basically a website where every user can register and create a free account. After creating a Facebook profile, each user can introduce themselves by filling in required information, such as updating their profile picture and biography. They can also share their thoughts with others. They can also connect with others by sending a friend request. The person to whom they are sending a friend request can be from any part of the world. Facebook also provides a necessary messaging platform called Facebook Messenger, where every user can chat with their friends. They can also share a variety of information with their Facebook Messenger friends, such as photos, videos, stickers, audios, and files.

Many social networking sites struggle to understand their social connections.So, to overcome this and also to understand how people from different geographical regions are connected, the research group on Facebook, led by Michael Bailey and his fellow colleagues, came with an idea which is known as the 'Social Connectedness Index' (SCI). As a result, in this study, we will build a Bayesian network and see what kinds of effects and insights can be obtained from it.

1.2 Social connectiveness

The **Facebook Social Connectedness Index** (**SCI**) is used for measuring the strength of connectedness among any two regions. The SCI gives variety of information like economic opportunities, social mobility and trade. Using the SCI index, we can measure the connectivity between two people living in two different regions.

SCI is built using the information available from the friendship links between between all Facebook users as of April 2016. It was reported that 58 percentage of United States (US) adult population and 71 percentage of US online population use Facebook [1]. It is also reported that Facebook is common among the age group of 18-29 years old [1].

The Social Connectedness Index (SCI) is a new area of research which is used for computing the frequency and thickness of friendship and companions around the world. It is a type of data which is useful to find out how relationships accepts social outcomes. Since Facebook has more than 2.5 billion active users around the world, SCI delivers the first complete measure of social networks at a global level.

Probabilistic graphical model is a type of a probability model to represent the conditional dependences and independences between variables by means of a graph. They are most commonly used in statistical machine learning. It is possible to learn Bayesian networks from data, i.e. both network structure and probabilistic parameters can be learnt, and if that is done successfully the result offers a lot of insight into the problem domain. It is also possible to do probabilistic inference with a Bayesian network by computing the joint probability distribution of any subset of variables, conditioned on an instantiated other subset of variables.

So, in this thesis, the main intention is to find the right Bayesian network structure and check if it is suitable for this kind of problem. Furthermore, we also evaluate the network using a confusion matrix. We also validate the network using calibration curves, ROC and K-fold cross-validation. We also use log-likelihood to check the goodness of the fit of the model. We also compare the network with a naive Bayes network. We also check how two variables are distributed. We also check the accuracy of the model using Brier score.

The type of Bayesian network which we are going to construct is going to be based on Structure learning. Learning a Bayesian network from the data has two major tasks: learning the structure of the network (structure learning) and learning the parameters (parameter learning). In this research, our will focus is on Structure learning. When we use data to learn the links of our Bayesian networks, then the type of learning is called Structure learning. We will construct a Tabu search-based Bayesian network.

1.3 Research questions

The uncertain relationship between two or more variables can be best represented by a probabilistic graphical model. Bayesian networks which belong to probabilistic graphical models have the advantage of having been investigated extensively. A straightforward Bayesian network is the so-called *naive* Bayes network. It has a fixed structure and makes strong conditional independence assumptions. Nowadays, both network structure and probabilistic parameters of a Bayesian network can also be learnt from data. It is unclear whether this can be done for Facebook data.

This brings us to the following research questions:

- Is it possible to find the right Bayesian network structure from Facebook data such that it can be used to predict the SCI?
- Assuming that we are able to learn a Bayesian network, yields some subsequent research questions:
 - How can such a model be validated?
 - What is the performance compared to a naive Bayes network?
 - Is it possible to obtain any useful information from the model by comparing the models for various groups of countries?
 - What are the optimal number of bins using discretization?

Thus, for answering the research question, we will try to find the right Bayesian network for predicting the SCI between two countries. In particular, we will try to learn a Bayesian network using Tabu search Bayesian network and see if it finds the right structure. We will also evaluate the network by means of a Confusion matrix and ROC curve. We also validate the network using K-Cross validation and by constructing calibration plots. We will also find the Brier score of the model to see if the model has performed well. We will also compare the model with the naive Bayes model and evaluate both the Tabu based search and naive Bayes by means of a confusion matrix and Log-Likelihood. We will also try to find out if any useful information can be extracted from the model by comparing the model for different groups of countries and this will also help us in seeing the probability distribution of scaledsci and distancekm for various group of countries. We will also try to find the optimal number of bins for intervals of discretization.

1.4 Related work

1.4.1 Social networks and Bayesian networks

Koelle et al. discussed the applications of Bayesian networks in social network analysis [2]. In particular, they discussed the limitations of social network analysis and the usage of Bayesian networks in social network analysis. They identified two limitations where the first one is the issues in data collection and the second one is homogeneous node and link types. For the first issue, the authors specified that there have been many sources of uncertainty in the data collection process. Therefore, by using the knowledge of these sources that will make use of the uncertain information, the validity of social network analysis can be improved. Since every person views social network differently, obtaining an objective view is difficult. Furthermore, accumulating a dataset which provides interesting conclusions will require a significant effort. For the second issue, social network does not fully address the various kind of relationships. Many traditional graph-theoretic algorithms used for social network analysis are found to be homogeneous. The three major uses of Bayesian networks in social network analysis are: reasoning about uncertainty, searching the network and inferring links. Reasoning about uncertainty means many graph theoretic algorithms do not consider the role of uncertainty and so, by using a Bayesian network, the graph theoretic algorithms can make use of the uncertainty like considering the certainty of links, the recency of links and any other type of meta information. Searching the network means by using a Bayesian network, an user can find people of similar interest in social networks. Inferring links means using a Bayesian network, new links can be deduced from the information which will be already known with different degrees of freedom.

Farine et al. made use of a Bayesian network for estimating the uncertainty and reliability of social network data [3]. The data which they were dealing with is an animal social network data. One of the main challenges they observed using that data is the limited sample size of the data which in turn gave rise to the uncertainty for estimating the rates of interaction between individuals. So, they made use of the Bayesian network to negate this problem. They found that Bayesian network gave some good information about the uncertainties in the network when the network is well sampled. But, when the sampling is too sparse, the Bayesian inferred networks will be able to come up with realistic uncertainty estimates around edge weights.

Shalforoushan et al. used Bayesian networks for predicting links in social networks [4]. They used Bayesian networks for friend recommendations. For that, the dataset which they used was socpokek obtained from snap.Stanford library. The dataset has 1632803 nodes and 30622564 edges. It also contains personal information about users. The dataset contains two files: relationship files and profile files. Relation files contain information like friendship considerations and the profile file contains profile features and personal attributes for each user. The main attributes that have effect on the friendship have been selected. The selected attributes are user-id, completion percentage, gender, age, region, work, education, marital status and hobbies. So, initially, they determined the attributes and similarities which has the most effect on friendship. After that, the friends who have similar interests will be given has a suggestion to each other. They also used a Friend of Friend algorithm for predicting the link. But, they found that Bayesian network performs much better in predicting an unobserved link between a pair of nodes.

1.4.2 Other techniques for social network analysis

Michael et al. used computationally efficient topological features for link prediction [5]. They found that the link between different users might be missing since they are not found in the online network which means that they don't have an virtual connection. They learnt that in the existing literature that the link prediction techniques are short of scalability. The major problem in link prediction techniques is the problem of extracting structural features. The authors keeping all these in mind presented a very easy way of extracting structural features for finding the missing links. Since they were able to find an easy way to extract structural features and then, they used a machine learning classifier to find the missing links. They concluded that the machine learning classifier which they designed was able to solve this problem even when applied to a complex dataset and they evaluated this model on various different social networking sites like Facebook, Instagram and Twitter.

Nesserine et al. proposed a supervised machine learning technique for link prediction in bipartite graphs [6]. The authors identified the problem of link prediction in two-mode social networks. In their research, the authors focused on two primary topics: predicting links in bipartite graph and

predicting links in uni-modal graph. For doing this, the authors made use of the empirical nature of the bipartite graphs and also how they can increase the prediction of the model which are learnt. This is possible by instigating some changes to the topological features for computing the likelihood of connection of two nodes. They expressed their problem as a two class discrimination one. The authors used classic machine learning models for learning the problem of link prediction. They evaluated the model on two real-time datasets.

David et al. developed approaches for link prediction for solving the proximity of nodes in a network [7]. Their main intention was to understand what measures of proximity will lead to accurate link predictions. They used a network model to solve this problem. Therefore, when they performed experiments on the large co-authorship networks, they deciphered that the information about the future is found from the network topology alone and also some clever methods for identifying node proximity will perform better than various other direct measures.

Elaheh et al. made use of game theory and K-core decomposition for the problem of link prediction in social networks [8]. They recognized that existing link prediction techniques had problems like high time complexity, network size, sparsity and sparsity. They introduced an variation of weighted random walk based on game theory and K-core decomposition. They generated node representations using skipgram. They used Stochastic Gradient Descent (SGD) for optimization process and SGD had linear time complexity with respect to number of vertices. This improved the scalability of their model. For classifying the nodes and edges, they learnt a low dimensional representation which captures the network structure. They compared their model with state of the art techniques and evaluated based on accuracy. They found that their model has performed relatively well when compared to other models.

Yang et al. proposed a distance based model for link prediction. The authors focused on extracting users' relationship based on their mobility information [9]. They proved that for this kind of problem, Distance is going to be the primary metric. In particular, they used the distance metric to find if two people are friends by finding the distance between them. They also made use of the location metric together with distance. When they combined the information of these two metrics, they found that the distance between a user and stranger gets even larger. They proved that distance is an useful metric to solve the link prediction problem and they also used a machine learning classifier to improve the performance. They performed experiments on Twitter dataset and found that their model performs better.

1.4.3 Learning Bayesian networks from the data

Dimitris Margaritis focused on the problem of determining the structure of directed models for which she used Bayesian networks [10]. The author mentioned that by learning the structure of a Bayesian network, the network will give insights into causal structure. The author also mentioned that Bayesian network is used for predicting quantities which are tough, difficult and expensive. The author proposed an algorithm for obtaining a structure of Bayesian network using statistical independent statements, a statistical test for continuous variables and an application of structure learning to a decision support where the model is learned from the data (structure).

Agnieszka et al. used the parameters of Bayesian network for learning it from small datasets [11]. This turned to be an application of Noisy-OR gates. They found that the datasets which existed now can reduce the knowledge engineering effort which is required to parameterize Bayesian network. However, they found that when the dataset is small, a lot of conditioning cases are represented by few or no data. So, they used the concept of Noisy-OR to negate this problem and by reducing the requirements of data for learning conditional probabilities. They tested their model for diagnosing liver disorders and found out that their model performs well.

Cohen et al. focused on learning Bayesian networks for facial expression recognition for both labeled and unlabeled data [12]. In particular, they used a Bayesian network classifier [12]. They

found that understanding the emotions of human is a important skill since it can be used for the computer to interact intelligently with them. They created a Bayesian classifier for classifying the expressions from a video. They found out that Bayesian networks can handle missing data better for both training and testing. Their main focus however was on labeled and unlabeled data. They showed when they used unlabeled data for learning classifiers, the performance of the classifier was improved. They then introduced an stochastic structured based algorithm for learning the structure of Bayesian network. They found that the model makes use of the unlabeled data to improve the performance of classifier.

Nir et al. concentrated on learning Bayesian networks for massive datasets [13]. They labeled their algorithm has an sparse candidate one. They decoded that the standard heuristic techniques doesn't work quite well for large datasets since the search procedures spend a lot of time finding the candidates that are irrelevant. To overcome this problem. the authors designed an algorithm that achieves faster learning process by restricting the search space. This iterative algorithm limits the parameters of each variables to belong to a small subset of candidates. After this, they will search the network which will match these candidates. They evaluated the network on real time data and found that their model performs really well.

Tommi et al. negated the problem of combinatorial by finding the highest scoring Bayesian network which is learnt from the data [14]. The authors viewed this structured learning problem as an inference problem since the variables mention the choise of parents for each node in a graph. There is a global constraint that a graph has to be an acyclic one and this was the core combinatorial problem. Thus, they casted this structured learning problem as linear over a polytope. For modifying this problem, they maintained an outer bound approximation to the polytope and for searching the valid constraints, they iteratively tightened it. This will find the right Bayesian network and the results suggested that the model performed well.

Pedro et al. used structured learning of Bayesian networks for analyzing the performance of control parameters [15]. In particular, they addressed the problem of search for the Bayesian network which is best when a database of cases are given. By also using the genetic algorithm, they found the method of searching among alternative structures. For constructing the network, they started by ordering the nodes of network structures. This is needed since the networks which are chosen by genetic algorithm should be a legal one. Next using a repair operator, they convert illegal structures to legal structures. They show that the best results are obtained with an elitist genetic algorithm.

Cassio et al. tackled the problem of structured learning of Bayesian networks using constraints [16]. In particular, they addressed the exact learning of Bayesian network structure from data and also experts knowledge which is based on score functions. This will describe the properties that will lessen the time and memory costs of algorithms like hill-climbing and dynamic programming. After that, they presented a Branch and bound algorithm which will integrate both the parameters and structural constraints and these wil in turn ensure global optimality. These have the properties of being applied to large datasets and the existing methods cannot do this.

Lobna et al. found that they can improve the algorithms for structured learning in Bayesian networks using the concept of implicit score [17]. The authors investigated that in the existing research, the most commonly used heuristic search for graph is by defining a score metric and employing a search strategy to find the network which will have the maximum score. Therefore, the authors proposed a new metric called the implicit score and implemented this with the help of K2 and MWST algorithms for network structure learning. They evaluated this on a benchmark database and found that this new metric performs well.

Mikko et al. presented an algorithm which finds the most accurate posterior probability of a sub network [18]. This is actually an modified version of the algorithm which finds the most probable network structure. They found out that this exact computation will be helpful in solving complex cases where the existing methods like Monte Carlo and local search procedures fail. They also show that when a domain contains large number of variables, exact computation will be feasible given certain restrictions like priori and when both exact and inexact methods are possible.

1.4.4 Comparison of my work to the literature

When I compare my work to the literature, it has to be said that there have been no papers which even gives a small insight about my work. This is because my research involves finding a Bayesian network for a social network problem and even though there are lot of papers focused on Bayesian networks, none of those papers are concerned with the problem of social networks. So, my work is a novel idea since we are using Bayesian network to solve the problem of social networks and also since we try to find the right Bayesian network structure for the same problem. The other difference is also we focus on structured learning part of Bayesian network for finding a solution for social networks and in the existing literature, there have been no papers centered upon this.

Therefore, my work is completely new due to these reasons:

- Using a Bayesian network for a social network problem
- Using structured learning in Bayesian networks for social networks
- Finding the right Bayesian network structure for social networks

1.5 Structure of the report

The report is structured as follows: Chapter 2 gives background on SCI and also on Bayesian networks. Chapter 3 provides the methodology for constructing the Bayesian network and Chapter 4 gives the results and discussion. Chapter 5 is the conclusion.

2. Background

2.1 Social connectedness index

The **Social Connectedness Index**, abbreviated to $SCI_{i,j}$, calculates the relative probability of a Facebook friendship link between a user in the location i and user in the location j. The SCI is defined as follows:

$$SCI_{i,j} = \frac{C_{i,j}}{U_i \cdot U_j} \tag{2.1}$$

In Equation (2.1), U_i and U_j depicts the total number of connections among number of users between two different locations i and j. $C_{i,j}$ depicts the total number of Facebook friendship connections between people in two different locations, i and j. If the measure is twice as large the original measure, then the person in the location i is more likely to connected to the person in the location j.

The product $U_i \cdot U_j$ gives the maximum number of connections between people at location *i* and *j*. On the other hand, $C_{i,j}$ is the number of actual connections. Hence, the SCI is the ratio between actual and maximal number of connections between people.

The data of Social Connectedness Index contains the SCI measured between two different geographical regions. Each dataset will contain i to j location pairs and vice versa. It also includes links of each location to itself. Every dataset has three columns:

- $user_loc$ First Location
- fr_loc Second location
- $scaled_sci$ Scaled SCI has explained above

The datasets which are included within the folder contain the $SCI_{i,j}$ for the following areas:

- 1. <u>Country-Country</u> Every row is a country-country pair. They are depicted by their ISO2 codes. It excludes countries where Facebook is banned. There are 185 unique countries in total.
- 2. US County-US County Every row is a US county-US county pair. They are depicted by their FIPS code. It does not include counties which has lesser active users.
- 3. <u>US County-US Country</u> Every row is a US county-US country pair. Counties are depicted by their FIPS code whereas countries are depicted by their ISO2 code. It excludes countries with fewer users.
- 4. GADM/NUTS GADM/NUTS There are two more files built on the Database of Global Administrative Areas (GADM) and the European Nomenclature of Territorial Units for Statistics (NUTS) areas. It also excludes regions with fewer users.
 - <u>GADM _ NUTS2</u>: European countries are divided into NUTS2 regions. The countries that are outside Europe are divided into their GADM level 1 regions.
 - <u>GADM1 _ NUTS3 _ Counties</u>: European countries are divided into NUTS3 regions. The United States, Canada and few countries in the Asia are divided into GADM level 2 regions. The rest of the countries are divided into GADM level 1 region.

2.1.1 Social connectedness in the United States

In the United States, Facebook has played a major role for people to interact online with their friends and acquaintances [19]. People usually become friends with people with whom they knew

in real life. SCI is constructed for 3,136 US counties and also between every US county and foreign country. The highest SCI is for the Los Angeles County- Los Angeles County connections. This is the region where people have the largest number of friendship connections.

When considering the San Francisco county, it is found that the people in San Francisco have more social connections with the people in the northeastern United States. When comparing the San Francisco County with the Kern county, it is found that the Kern county have significantly lower social connections with the people in the northeastern United States. The Kern county has more friendship connections to the people in West Coast and Mountain areas. This might be due to past migration patterns since many people migrated from West Coast and Mountain Areas to the Kern county. Kern county has also more friendship links to the oil-producing regions of North Dakota since Ken county is the biggest oil producing region in the United States [19].

The Social Connectedness Index is also affected by physical obstacles such as large rivers and mountain ranges. The counties with a military base have strong connections with the entire United States. Similarly, the counties with native American Reservations are strongly connected with each other. The areas which have some common functions like ski resorts, common languages have strong connections. Similarly, the regions which have African American population have more connections with people in the southern part of the United States [19].

2.1.2 Social connectedness in Europe

Europe consists of many regions and every country in Europe have their language of their own which makes it so unique and relatively different from the United States. The Social Connectedness in Europe is influenced by many factors such as language, migration patterns, political borders, religion, education and age. Two regions which have a common language are expected to have more Social Connectedness Index than two regions which doesn't have a common language [20].

In relation with the migration patterns, people of South-West Oltenia in Romania have more connections with people throughout Europe especially in Italy, Spain, Germany and the United Kingdom. This is due to past migration history. In relation to the language, Limburg, a region in Belgium has more friendship connections with the Netherlands since in Limburg, the official language is Dutch. The regions of Slovenia, Croatia, Serbia, North Macedonia, and Montenegro are made into one community since before the division they were known together as Yugoslavia. This holds for Czech Republic and Slovakia also. Since Belgium has three official languages (Dutch, German and French), the French speaking part of Belgium is expected to have more connections with people in France [20].

2.2 Graph theory

2.2.1 Basic concepts

A graph G is defined as a pairs G = (V(G), E(G)), where V(G) is a finite set of vertices, where a vertex is often denoted by a letter, e.g. $v, u \in V(G)$, and $E(G) \subseteq V(G) \times V(G)$ are called edges. We also use letters with indices, e.g. v_1, v_2 to denote vertices, or sometimes just integers.

Different types of graph can be distinguished. If we have that if $(u, v) \in E(G)$ it follows that $(v, u) \in E(G)$, the graph is called **undirected**. In undirected graphs an edge (u, v) is often denoted by a **line**, or (undirected) edge u - v. On the other hand, if it holds that if $(u, v) \in E(G)$ then $(v, u) \notin E(G)$ the graph is called **directed**. An edge $(u, v) \in E(G)$ in a directed graph G is often indicated by $u \to v$, called an **arc** or directed edge.

Let G be an undirected graph, in that case it is possible to travel through the graph from vertex to vertex, just by following the vertices that are connected to each other by lines, $v_1 - v_2 - \cdots - v_p$, called a **path**. If a path between two vertices v_1 and v_p exist in graph G, they are said to be

connected. A similar situation exists for a directed graph G, but here paths can have different forms, e.g. the form of a **directed path** $v_1 \rightarrow v_2 \rightarrow \cdots \rightarrow v_p$. If for a directed graph G it holds that it does **not** contain a path of the form $v_1 \rightarrow v_2 \rightarrow \cdots \rightarrow v_p = v_1$, called a **directed cycle**, it is called **acyclic**.

In particular in social network analysis, special graphs are used where lines or arcs have an attached weight w; these graphs are called **weighted graphs**, formally denoted as G = (V, E, w), where $w : E(G) \to \mathbb{R}$ acts as a **weight function**.

2.2.2 Some further concepts

For directed acyclic graphs, DAG for short, there is some special terminology used. Let G = (V(G), E(G)) be a DAG, then if $u \to v \in E(G)$, then u is called the **parent** of v, whereas v is known as the **child** of u. If a vertex u can be reached from vertex v by a directed path starting from v, then u is also known as a **descendant** of v. Note that a child is a descendant of its parent; the concept of descendant allows for describing children of children. Furthermore, often when considering paths in a DAG we are not always interested in the direction of the edges connecting the vertices on the paths. In that case, we ignore the direction of edges on the path by considering the **undirected version** of the DAG G, also known as the **underlying graph**.

Some other concepts used in the following are:

- Vertices v, u that are connected by an edge e = (v, u) are called **adjacent** and **incident** to the edge e.
- A vertex u that is not connected to any other vertex by an edge is called **isolated**.
- An **ancestor** u of a vertex v is a vertex on a directed path starting from u and ending at v, $u \neq v$.

2.3 Probabilistic graphical models

We continue with a brief review of some key concepts from probability theory, i.e., we consider events, joint probability distributions, conditional probability distributions, the chain rule, marginalization, and conditional independence, after which we describe probabilistic graphical models.

2.3.1 Basic probability concepts

Let $X = \{X_1, \ldots, X_n\}$ be a set of random variables, where $D(X_i)$ indicates the **domain** of variable $X_i \in X$. The domain of X is the Cartesian product $D(X) = \times_{i=1}^n D(X_i)$. An (elementary) **event** $E \equiv X = x$ is any random variable X with a value x from its domain. The set of all possible Boolean combinations of events, or **Boolean algebra** denoted as $\mathcal{B}(X)$, is defined by using the operators: conjunction $(X = x \land X' = x')$, disjunction $(X = x \lor X' = x')$, and negation $(\overline{X = x})$. This Boolean algebra contains events such as $(X_1 = x_1 \lor X_2 = x_2)$, $(X_3 = x_3 \land X_4 = x_4)$, and $\overline{X_2 = x_2}$. Events are partially ordered by \leq , with the universal lowerbound $\bot \in \mathcal{B}(X)$ and universal upperbound $\top \in \mathcal{B}(X)$, i.e., we have for each $E \in \mathcal{B}(X)$ that $\bot \leq E$ and $E \leq \top$. Usually $(X = x \land X' = x')$ is represented in set notation as $\{X = x, X' = x'\}$. Note that often we do not make a distinction between elementary events, i.e. $X_1 = x_1$ and a conjunction or sets of events, i.e. X = x which might stand for $(X_1, X_2) = (x_1, x_2)$ or $\{X_1 = x_1, X_2 = x_2\}$.

A probability distribution is a function or mapping that assigns probabilities, i.e., values from the closed real interval [0, 1], to any event involving variables in X.

Definition 1 (Probability distribution). A probability distribution for a set of random variables X with **domain** D(X) is defined as a function $P : \mathcal{B}(X) \to [0,1]$, such that the following axioms hold:

- (1) P(E) is a non-negative real value for all $E \in \mathcal{B}(X)$;
- (2) $P(\top) = 1;$
- (3) for any set of disjoint events $E_1, \ldots, E_n \in \mathcal{B}(X)$, with $(E_i \wedge E_j) = \bot$, $1 \le i, j \le n, i \ne j$, we have that:

$$P\left(\bigvee_{k=1}^{n} E_{k}\right) = \sum_{k=1}^{n} P(E_{k}).$$

It is a fundamental property of probability theory that it is sufficient to specify a probability distribution in terms of joint events $\{X_1 = x_1, X_2 = x_2, \ldots, X_n = x_n\}$, i.e., in terms of a **joint probability distribution** $P(X_1, X_2, \ldots, X_n)$ for all values of the domain D(X) (possibly with the exception of one element from D(X), where its probability can be derived from the other probabilities of elements of D(X) according to axioms (2) and (3)).

When the actual value of a random variable in an elementary event does not matter in a given context, we often also write P(X) rather than P(X = x) for the probability of variable X taking the value x.

The **marginal probability distribution** for a set of variables Y given the probability distribution for the random variables X, with $Y \subseteq X$ and $X = Y \cup Z$, where Y and Z are disjoint, is obtained by summing out the other variables (i.e. Z) from the joint probability distribution P(X), and is defined as:

$$P(Y) = \sum_{z \in D(X \setminus Y)} P(Y, Z = z)$$

Let P(X,Y) be a joint probability distribution over a set of random variables X and Y. A **conditional probability distribution** P(X | Y) is defined as:

$$P(X \mid Y) = \frac{P(X,Y)}{P(Y)}$$
(2.2)

with P(Y) > 0.

It is good to realize that P(X | Y) is actually a family of probability distributions, one for every value y of Y. The conditional probability P(X = x | Y = y) is the probability of the event X = x given knowledge about the event Y = y.

The concept of conditional probability is one of the most fundamental and most important concepts in probability theory. In addition, the conditional probability plays an essential role in a wide range of domains, including classification, decision making, prediction and other similar situations, where the results of interest are based on available knowledge.

By moving the denominator on the right of Equation 2.2 to the left, Equation 2.2 can also be written as:

$$P(X,Y) = P(X | Y)P(Y) = P(Y | X)P(X)$$
(2.3)

By applying Equation 2.3 to a set of random variables $\{X_1, X_2, \ldots, X_n\}$, this creates a chain of conditional probabilities, more formally:

Proposition 1 (Chain Rule). Let P be a joint probability distribution over a set of random variables $X = \{X_1, X_2, \ldots, X_n\}$. Then it holds that:

$$P(X_1, X_2, \dots, X_n) = P(X_n \mid X_{n-1}, \dots, X_1) \cdots P(X_2 \mid X_1) P(X_1)$$
(2.4)

The chain rule allows us to compute the joint distribution of a set of any random variables by only making use of conditional probabilities. This rule is particularly useful in Bayesian networks, which we will introduce later in this chapter. Combined with the network structures, the use of the chain rule can facilitate the representation for a joint distribution.

Another immediate result of Equation 2.3 by rearranging terms is **Bayes' rule**, also known as **Bayes' theorem**:

$$P(X \mid Y) = \frac{P(X)P(Y \mid X)}{P(Y)}$$
(2.5)

Bayes' rule tells us how we can calculate a conditional probability given its inverse conditional probability. For example, using Bayes' rule makes it possible for us to derive the conditional probability P(X | Y) from its inverse conditional probability P(Y | X), if we also have information about the prior probability P(X), P(Y) of events X and Y respectively. P(Y) also behaves as a normalizing constant.

A more general conditional version of Bayes' rule, where all probabilities are conditional on the same set of variables Z, also holds:

$$P(X \mid Y, Z) = \frac{P(X \mid Z)P(Y \mid X, Z)}{P(Y \mid Z)}$$

with $P(Y \mid Z) > 0$.

Another fundamental concept in probability theory is **conditional independence**. Two sets of variables X, Y are said to be conditionally independent given a set of variable Z, denoted $X \perp P Y \mid Z$, if

$$P(X | Y, Z) = P(X | Z) \text{ or } P(Y, Z) = 0$$
 (2.6)

Equation 2.6 asserts that given knowledge of a set of variables Z, knowledge of whether Y occurs provides no extra information on the probability of whether X occurs.

2.3.2 Bayesian networks

Bayesian Networks, which are also known as belief networks or Bayes nets, are one of the types of probabilistic graphical models. A Bayesian Network (BN) is used for representing a joint probability distribution, taking into account the conditional independences that hold among the random variables involved in the distribution.

A more formal definition of Bayesian Network is given:

Definition 2. A Bayesian network \mathcal{B} is defined as a pair $\mathcal{B} = (G, \Theta)$ where G is a DAG with vertices $V(G) = \{1, 2, ..., n\}$, corresponding 1–1 to random variables $X = \{X_1, X_2, ..., X_n\}$, and arcs $E(G) \subseteq V(G) \times V(G)$, representing probabilistic independence information; Θ denotes the probabilistic parameters of the network. The following holds: $\Theta_{i|\pi(i)} = P_{\mathcal{B}}(X_i = x_i \mid X_{\pi(i)} = x_{\pi(i)})$ for each realisation $X_i = x_i$, conditioned on the values of the set of parents $X_{\pi}(i) = x_{\pi(i)}$. Correspondingly, \mathcal{B} defines a unique joint probability distribution (JPD) on the random variables X using the chain rule:

$$P_B(X_1 = x_1, X_2 = x_2, \dots, X_n = x_n) = \prod_{i=1}^n P_B(X_i = x_i | X_{\pi(i)} = x_{\pi(i)}) = \prod_{i=1}^n \Theta(i \mid \pi(i))$$
(2.7)

Hence, a Bayesian network is just a factorisation of a JPD, using the chain rule 2.4, taking into account the conditional independences imposed by the graph structure of the network. This is a consequence of the **Markov condition**: any variable is conditionally independence of non-descendants given its parents. The relationship between the structure of the graph of a Bayesian

network and the conditional independences that follow from these is not straightforward and are described by the concept of **d-separation**. In the following we will no longer explicitly distinguish between vertices i and the corresponding variable X_i of a Bayesian network.

When vertex Y has converging arcs (head-to-head) $\cdot \to Y \leftarrow \cdot$, it is called a **collider**. The vertices with other arc connections are called non-colliders and they connect to other vertices as follows:

- tail-to-tail arcs: $\cdot \leftarrow Y \rightarrow \cdot$
- tail-to-head arcs: $\cdot \leftarrow Y \leftarrow \cdot \text{ or } \cdot \rightarrow Y \rightarrow \cdot$
- head-to-head arcs: $\cdot \to Y \leftarrow \cdot$

Later it will appear that head-to-tail is equivalent to tail-to-head, which is why we do not distinguish it. D-separation is defined in terms of blocking.

Notion of Blocking If there are three subsequent variables X_i, X_j , and X_k on an undirected path, the path passing through X_i, X_k , and X_j will be called

- **blocked** by X_k if X_i and X_j are connected by a path in the underlying graph where X_k is the middle vertex and X_k is connected to X_i and X_j as a non-collider, i.e. tail-to-tail or tail-to-head;
- blocked (by nothing) if (X_i, X_k, X_j) form a collider, and unblocked if in the collider $(X_i, X_k, X_j) X_k$ or one of its descendants are given.

D-separation Next, the formal definition of d-separation is given:

Definition 3. Let G = (V(G), E(G)) be a DAG with $X, Y, Z \subseteq V(G)$ sets of vertices. If every path from a vertex in X to every vertex in Y is blocked by a vertex in Z we say that X and Y are *d*-separated given Z written as $X \perp \!\!\! \perp_G^d Y \mid Z$.

If vertices X and Y are not d-separated given Z, we say that they are **d-connected**, written as $X \not\perp _G^d Y \mid Z$.

Figure 2.1 show an example of a DAG.

The tail-to-tail arc in Figure 2.1 is $u \leftarrow v \rightarrow y$. One of the tail-to-head arcs is $\leftarrow u \leftarrow$. Head-to-head arc in the figure is $s \rightarrow t \leftarrow u$.

In Figure 2.1, there is a path between s and v, but since t is a collider, s and v are d-separated. This is also true for the path $x - r \dots - y$, where x and y are d-separated for the same reason. But, if we consider the path but now given t, s and v would be d-connected. x and y are also d-connected since the path is unblocked by t.

Let us assume that Z is a set and contains a set of variables r, v. So, then x and y are d-separated by Z and the same applies for x and s, u and y, s and u. The paths x - r - s, u - v - y and s - t - u is blocked by Z. The only pairs of vertices which remain d-connected conditioned on Z are s and t, u and t. Even though t is not in z, the path is nevertheless blocked by Z since t is a collider.

2.3.3 Independence relation

The notion of d-separation is closely related to the probabilistic notion of conditional independence, which will be described subsequently.

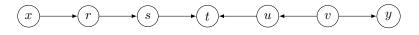


Figure 2.1: D-separation

Definition 4. If $X, Y, Z \subseteq V$ are disjoint sets of random variables and if P is a probability distribution of V then X is said to be **conditional independent** of Y given Z, denoted as

 $X \perp P Y | Z$, if and only if P(X | Y, Z) = P(X | Z)

This relation $\perp\!\!\!\perp_P$ defines a ternary predicate $\perp\!\!\!\perp_P (X, Y, Z)$ for which several properties hold. The most obvious one is called the **symmetry property**:

$$X \perp\!\!\!\perp_P Y \mid Z \Longleftrightarrow Y \perp\!\!\!\perp_P X \mid Z \tag{2.8}$$

Its proof is easy, as it follows from basic probability theory: $P(X \mid Y, Z) = P(X \mid Z)$ according to the left side of the bi-implication. As $P(X \mid Y, Z) = P(Y \mid X, Z)P(X \mid Z)/P(Y \mid Z)$ we have that $P(X \mid Z) = P(Y \mid X, Z)P(X \mid Z)/P(X \mid Z)/P(Y \mid Z) \Rightarrow P(Y \mid X, Z) = P(Y \mid Z)$. There are also some less obvious properties:

• Contraction: If $X, Y, W, Z \subseteq V$ are disjoint sets of random variables, then:

$$X \perp P Y | Z \land X \perp P W | Y \cup Z \implies X \perp P W \cup Y | Z$$

$$(2.9)$$

Note that the d-separation relation \amalg_G^d is defined in terms of paths of a directed graph G, whereas the independence relation \amalg_P is defined in terms of a probability distribution P. These are usually not the same for a Bayesian network. However, because of the way a Bayesian network is defined, any (conditional) dependence between sets of random variables implies that the corresponding sets of vertices are d-connected, which also implies that if sets of vertices are d-separated given a set of other vertices, the corresponding sets of random variables are conditionally independent. It is also said that a Bayesian network is an **I-map** (Independence map): a DAG G is called an directed I-map if the following holds: $X \coprod_G^d Y \mid Z \implies X \coprod_P Y \mid Z$, which is always the case for a Bayesian network by definition.

Markov Network A Markov network is a set of random networks having a Markov property which is described by an undirected graph. A Markov network is similar to a Bayesian network in the representation of its dependencies. The difference between a Bayesian network and a Markov network is that Bayesian networks are directed and acyclic whereas Markov networks are undirected and might be cyclic. Due to this, Markov networks can represent certain dependencies which Bayesian networks cannot.

2.3.4 Example of a Bayesian network

Figure 2.2 shows an example of a Bayesian network model which describes the relationship between the season whether rain falls during the cloudy season, whether the sprinkler is on during the cloudy season and whether the grass would get wet. Every node is specified by a Conditional Probability Distribution (CPD). If the variables are discrete, the distribution can be represented in the form of a table called the Conditional Probability Table (CPT) which will contain the combination of values of a vertex parents the probability that the node takes on each of its different values [21].

Rain: When the season is cloudy, the probability of rain is 0.8 otherwise the probability of rain is 0.2.

Sprinkler: When the season is dry, the probability that the sprinkler is on is 0.4 and the probability that the sprinkler is off is 0.6. When there is rain, the probability of sprinkler being on is 0.01 and the probability of sprinkler being off is 0.99.

Grass Wet: For the Grass Wet node, there are two possible causes: the probability that the sprinkler is on or it is raining.

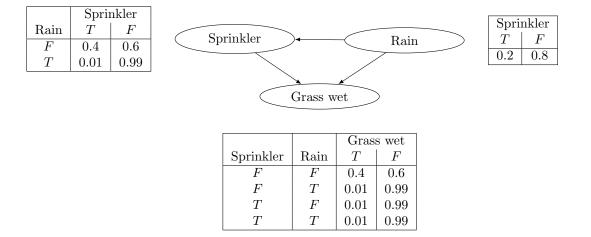


Figure 2.2: Example of Bayesian Network

2.3.5 Special form Bayesian Networks

The two special kind of Bayesian networks are:

- naive (independent) form Bayesian networks
- Tree-Augmented Bayesian networks

naive form Bayesian network

Definition 5. If C is a class variable and if E_i are the evidence variables and $\mathcal{E} \subseteq \{E_1, \ldots, E_m\}$. It is assumed that $E_i \perp \!\!\perp E_j \mid C$. So, by Bayes' rule:

$$P(C|\mathcal{E}) = \frac{P(\mathcal{E}|\mathcal{C})P(C)}{P(\mathcal{E})}$$

with:

$$P(\mathcal{E}|\mathcal{C}) = \prod_{E \in \mathcal{E}} P(E|C)$$

by conditional independence

$$P(\mathcal{E}) = \sum_{C} P(\mathcal{E}|\mathcal{C}) P(C)$$

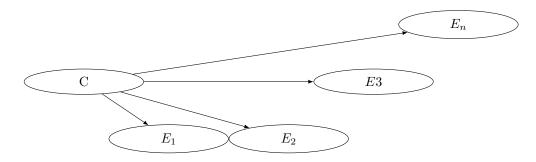


Figure 2.3: naive form Bayesian network

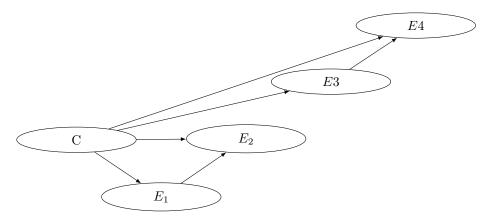


Figure 2.4: Tree-Augmented Bayesian Network

Tree-Augmented Bayesian Network (TAN) TAN is the extension of Bayesian network which is used for reducing the number of independent assumptions. As with naive Bayes you have a class variable and evidence variables, and an evidence variable has two parents: the class variable and another evidence variable. Together the evidence variable form a tree. This does indeed allow representing dependence's between evidence variable (not always via the class variable as holds for naive Bayes).

2.3.6 Description about probability distributions

Continuous probability distributions A continuous probability distribution is a distribution where the random variable X can take on any value that is continuous. Since X can assume infinite values, the probability of X taking on one specific value is 0. The continuous random variable is infinite and uncountable.

Discrete probability distributions A discrete probability distribution is a distribution which describes the set of possible outcomes in a discrete way (eg:coin toss, roll of a die). In a discrete probability distribution, the probabilities are encoded by a discrete list of probabilities of outcomes which is called as the Probability Mass Function. A discrete probability distribution is countable.

Mixed Random Variables If a random variable is neither continuous nor discrete, then that random variable is called as a mixed random variable. The mixed random variable has both the continuous and discrete part.

Multivariate Gaussian distribution A Gaussian distribution $X \sim \mathcal{N}(\mu, \sigma^2)$ is also called as Normal distribution. It is kind of continuous probability distribution for real valued random variable. The probability density function of Gaussian distribution is:

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}$$
(2.10)

The parameter μ is called the mean or expectation of the distribution. The parameter σ is called the standard deviation and the variance of the distribution is σ^2 . A random variable with a Gaussian distribution is said to be normally distributed and is called a normal deviate.

A multivariate Gaussian distribution is a generalization of the univariate Gaussian distribution to higher dimensions. It is often used to describe a set of correlated real values random values clustered around a mean.

$$f(y_{i}|\mu,\Sigma) = f((y_{i1}, y_{i2}, ..., y_{in})' | \mu = (\mu_{1}, ..., \mu_{n})', \Sigma = \begin{bmatrix} \sigma_{1}^{2} & \sigma_{1n} \\ & \ddots & \\ \sigma_{n1} & \sigma_{n}^{2} \end{bmatrix})$$
$$= \frac{1}{\sqrt{(2\pi)^{n}|\Sigma|}} exp(-\frac{1}{2}(y_{i} - \mu)'\Sigma^{-1}(y_{i} - \mu))$$
(2.11)

The symbol $|\Sigma|$ refers to the determinant of the matrix Σ . The determinant is a single real number. The symbol Σ^{-1} is the inverse of Σ , a matrix for which $\Sigma\Sigma^{-1} = I$. This equation assumes that Σ can be inverted, and one sufficient condition for the existence of an inverse is that the determinant is not 0.

The matrix Σ must be positive semi-definite in order to assure that the most likely point is $\mu = (\mu_1, \mu_2, \dots, \mu_n)$ and that, as y_i moves away from μ in any direction, then the probability of observing y_i declines.

The denominator in the formula for the multivariate normal distribution is a normalizing constant, one which assures us that the distribution integrates to 1.0.

Multinomial distribution The Binomial is actually the Bernoulli distribution. The Binomial is Bernoulli applied to a sequence of tests. The Binomial distribution with parameters n and p is a discrete type probability distribution where it is used for sequence of n independent experiments where each experiment should answer a yes or no question and each of the experiments will have a Boolean valued outcome with probability p for success and probability p - 1 for failure. A single experiments will be called a Bernoulli experiment where the sequence of the experiments is called a Bernoulli process for a single trial. Therefore, the Binomial distribution is a Bernoulli distribution. The notation, expectation, variance, Probability Mass Function (PMF) of Binomial distribution is given below:

 $\begin{array}{lll} \text{Notation:} & X \sim \text{Bin}(n,\theta) \\ & \text{where } n > 0 \text{ and } 0 \leq \theta \leq 1 \\ \text{Support:} & \{0,1,\ldots,n\} \\ & \text{PMF:} & \binom{n}{x} \theta^x (1-\theta)^{n-x} \\ \text{Expectation:} & n\theta \\ & \text{Variance:} & n\theta(1-\theta) \end{array}$

The Multinomial distribution is a generalization of binomial distribution.

Structures	Observability	Learning Method
Known	Fully known	Maximum-Likelihood estimation
Known	Partially known	Expectation-Maximization (EM) and Markov Chain Monte Carlo (MCMC)
Unknown	Fully known	Search model space
Unknown	Partially known	EM and Search model space

 Table 2.1: Different cases in learning BN

The notation, expectation, variance, Probability Mass Function (PMF) of Multinomial distribution is given below:

Notation:
$$X \sim \mathsf{Mult}(n, \theta)$$

where $n > 0, \theta = [\theta_1, \dots, \theta_k]$ and $\sum \theta_j = 1$
Support: $\{x_1, \dots, x_k \mid \sum x_j = n, x_j \ge 0\}$
PMF: $\binom{n}{x_1, \dots, x_k} \prod \theta_j^{x_j}$
 $\mathbb{E}[X] = n\theta$
 $\mathsf{Var}[X_j] = n\theta_j(1 - \theta_j)$
 $\mathsf{Cov}[X_i, X_j] = -n\theta_i\theta_j$

Example: Let X denote the vector of the number of times each side of a *i* sided die has landed face up in *n* tosses of the die, and let θ_j be the probability that the number *j* is rolled on each toss of the die. For example, x_1 represents the number of times a '1' was rolled, x_2 represents the number of times a '2' was rolled, etc.

In this example the categories are $1, \ldots, k$, but in general they can be completely arbitrary. There is no need to make them ordered, or even numeric.

2.3.7 Learning Bayesian networks from data

In various different applications, the resulted Bayesian network needs to be determined by the use of the dataset. This will require construction of graph representation, such that someone already has knowledge and data at their disposal. After this, parameter estimation of the joint probability distribution in the Bayesian network takes place. This is called fitting Bayesian network to the data. The construction of graph in the absence of expert knowledge is done using appropriate structured learning algorithms.

So, the task of learning a Bayesian networks can be divided into two types:

- Structural learning
- Parameter learning

2.3.8 Structured learning

Structural learning identifies the topology of Bayesian network. The idea behind structured learning to find the best network structure is to score all the possible DAGs by a scoring function and choose the DAG that has the best score. Structured learning problem is NP-hard.

As seen in the Table 2.2, it will become impossible for searching the space of DAGs exhaustively in a sensible time for values of $n \ge 6$ and so, heuristic methods are needed to find the optimal network structures. The problem of structured learning can be divided into two types. They are:

- Constraint based methods
- Search and score methods

2.3.9 Search and score method

Search and score is used for finding the quality measures of the Bayesian networks. As the name implies, this method has two types:

- Scoring metric: Used for computing the quality of Bayesian networks
- Searching procedure: Used for determining which network is the best.

2.3.10 Scoring function

Scoring function is used for measuring how well a network structure fits a data. So, it calculates the probability of network graph G given dataset D, P(G|D). This scoring function should be similar which means it should return the same score for Markov equivalent DAGs. So, if D is a dataset, and if B = (G, P) and B' = (G', P') are two Bayesian networks,

$$q = \frac{P(G|D)}{P(G'|D)} \tag{2.12}$$

Where q is a Bayesian measure and Pr is the probability distribution used for ranking the Bayesian network structures. It has to be noted that,

$$q = \frac{P(G|D)/P(D)}{P(G'|D)/P(D)} = \frac{P(G,D)}{P(G',D)}$$
(2.13)

and

$$P(G,D) = P(D|G)P(G)$$
(2.14)

So,

$$\log P(G, D) = \log P(D|G) + \log P(G)$$
(2.15)

which must be found for every Bayesian network B. For determining P(D|G), three assumptions must be made: no values should be missed in D, the case $v \in D$, where v signifies vertices, should have occurred independently and there should be discrete network parameters. So, the quality measure of a Bayesian network is:

$$P(D|G) = \prod_{i=1}^{N} \prod_{j=1}^{q_i} \prod_{k=1}^{r_i} \theta_{ijk} n_{ijk}$$

where N is the number of variables, q_i represents the number of states over the parents X_i , r_i represents the number of states of X_i , θ is the estimate of the model and n_{ijk} represents the number of cases in the database with X_i in its *kth* state and the parent of X_i in its *jth* state. This measure is used for determining the maximum likelihood parameters of the model.

2.3.11 Search algorithms

The main idea behind search algorithm is to find the most probable network structure given the dataset. The algorithms which are described in this section have various different ways of searching for this structure.

Number of variables	Number of possible DAGs
n	
1	1
2	3
3	25
4	543
5	29,281
6	3,781,503
7	1,138,779,265
8	78,370,2329,343
9	1,213,442,454,842,881
10	4,175,098,976,430,598,100

 Table 2.2:
 Number of possible DAGs for different number of variables

Exhaustive search

Exhaustive search is also known as brute force search. It does not reduce the search space of possible DAGs instead it generates all possible DAGs and chooses the one with highest score. The DAG whose score is the highest is the global optimum, so this structure is the best possible structure.

Greedy search

Greedy search is a simple search algorithm. The algorithm will start with a initial network structure G. For each step, the algorithm defines a set of neighbourhood graph and calculates the score of each graph in this neighbour set. The neighbour graph which has the highest score is selected and used for the next iteration. The search is stopped where there is no neighbourhood network graph with a score higher than the current structure.

Tabu search is a form of greedy search with some extras. Local search methods grasps a likely solution and checks its immediate neighbours in order to find a better solution. But, local search methods gets stuck in suboptimal regions where there are lot of solutions which are equally better.

By using Tabu search, we can rectify this. Tabu search improves this by modifying the first rule. So, initially, if none of the better solutions are found, worsening moves will be preferred. Furthermore, 'prohibitions' are initiated so that the search method doesn't again search the previously visited solutions.

2.3.12 Constraint based structured learning

Constraint based structured learning is used for determining conditional independencies. They approach the problem by various statistical conditional independence tests in order to produce the dependencies between the variables. DAG is used for illustrating the dependencies and independencies. The algorithms is used for calculating the conditional independencies between the variables. After that, the constraints of conditional independencies are then spread across the DAG. The next step is to eliminate the incompatible ones. These algorithms produce only I-equivalent graphs that are the ones with which specify identical independence relations. The main basis of Constraint based algorithm is the Pearl's Inductive Causation algorithm. The most commonly used constraint based algorithms is the PC algorithm.

PC algorithm

The PC algorithm involves the following steps:

- Initially, the conditional independencies of variables are tested to derive the conditional dependencies and independencies of variables.
- The graph skeleton (=undirected graph) is identified induced by those relations.
- The convergent $(X \to Z \leftarrow Y \text{ structures})$ and divergent connections are identified.

2.3.13 Parameter learning

Parameter learning is a method where the model is fit to the data by producing an estimation of the parameters of the global parameter distribution. If a given structure is known to the user, either through proper structure learning algorithm or prior knowledge, we calculate the estimation of parameters of local distribution. So, every node will have a corresponding CPT. This will reflect the node's CPD, according to the values of the parent nodes.

2.4 Evaluation metrics

Here we will introduce the 5 metrics which will be used for evaluating Bayesian networks.

2.4.1 Confusion matrix

The **confusion matrix** is a table which describes the performance of classification model. The confusion matrix reports number of False Positives (FP), False Negatives (FN), True Positives (TP) and True Negatives (TN). True Positive is a case where the model will exactly predict the positive class. True Negative is an outcome where the model will accurately predict the negative class. False Positive is a case where the model won't predict the positive class correctly. False Negative is an outcome where the model won't predict the negative class correctly. Accuracy is the ratio of observations which we correctly predict to total number of observations.

$$Accuracy = (TP + TN)/(TP + TN + FP + FN)$$
(2.16)

2.4.2 Receiver Operating Characteristic (ROC) curve

To evaluate a classification model at all the thresholds of classification, a ROC curve is used. An **ROC curve** is useful for plotting two parameters: True Positive Rate (TPR) and False Positive Rate (FPR).

TPR is otherwise known as recall. The formula for TPR is

$$TPR = \frac{TP}{TP + FN} \tag{2.17}$$

The formula for FPR is

$$FPR = \frac{FP}{FP + TN} \tag{2.18}$$

So, the ROC is curve will plot FPR vs TPR for all classification thresholds. If any curve is close to the top left corner, then it will indicate that the model has performed well.

2.4.3 Brier score

Brier Score (BS) is an another way of verifying if a probabilistic model has performed well. Brier score is quite similar to the Mean Squared Error.

The formula of **Brier score** is

$$BS = \frac{1}{N} \sum_{t=1}^{N} (f_t - o_t)^2$$
(2.19)

where f_t is the predicted probability and o_t is the actual outcome of the event and N is the number of total observations.

2.4.4 Log-likelihood

To find the goodness of fit of a probabilistic model, the likelihood can used. The **likelihood** l is just the probability of the data given the model: P(D:M), where D are the data and M the model and P is obtained from the probabilistic model M. Usually it is assumed that the records in the data D are independent and identically distributed (iid, for short) (using M) and this allows to compute

$$l(D:M) = P(D:M) = \prod_{r \in D} P(r:M)$$

However, as it is usually easier to compute a sum, rather than a product, usually the **log-likelihood** L is computed:

$$L(D:M) = \log P(D|M) = \sum_{r \in D} \log P(r:M)$$

A disadvantage of the log-likelihood is that when the probability $\downarrow 0$, the log-likelihood $\rightarrow -\infty$.

2.4.5 Bayesian Information Criterion (BIC) and Bayesian Dirichlet equivalence (BDe) score

BIC, also known as Schwarz Information Criterion, is used for scoring and choosing a model. The BIC is defined as follows:

$$BIC = k \log n - 2\hat{L}(D:M) \tag{2.20}$$

where

- \hat{L} is the largest value of the log-likelihood function of the model
- n are the number of observations
- k are the number of parameters estimated by the model M

BDe is an another scoring metric used for computing the score of a Bayesian network. Dirichlet process belong to a family of stochastic process who realizations are expressed in probability distributions. They are very common in Bayesian networks where they are used for describing the prior knowledge about how the random variables are distributed which means finding out how likely the random variables are distributed according to one or more distributions.

3. Methodology

In this Section, a description is provided of the Facebook social network data used in the research.

3.1 Description of the dataset

	UserLocation	FriendsLocation	scaledsci	Distancekm	Population2017userloc	Popiulation2017frloc
0	NO05	SE12	2362.0	6591.963399	896503.0	1664145.0
1	NO05	UKH3	342.0	1275.061542	896503.0	1813609.0
2	NO05	PT11	242.0	6356.241875	896503.0	3584575.0
3	NO05	RO41	339.0	8650.538077	896503.0	1972979.0
4	NO05	SE22	2411.0	3655.564450	896503.0	1483018.0

 Table 3.1: Description of the dataset

A description of the dataset is provided in Table 3.1. The dataset contains information about a person and the person's friend living in two different locations, represented in the dataset by Userlocation and Friendslocation. The scaled SCI represents the strength between people living in two different locations. The distance represents the distance between the two regions (userlocation and friendslocation). The population reflects upon the number of people living in the regions. Furthermore, every country are divided into many regions and all those regions are uniquely identified by their codes. If one ignores the numeric code attached to the location, a specific country is obtained (e.g. NO05 without '05' yields 'Norway'). There were about 112600 records in the dataset, with varying amounts of missing values, in particular for countries with small social networks.

3.2 Description of the features

3.2.1 Input variables

User Location and Friends Location

The user location specifies the place where the user is residing and the friends location signifies the place where the friend of the user lives.

Population

The population feature represents the number of people living in both the pop_user and pop_fr location. This feature is continuous.

$dist_km$

The distance feature represents the distance between the location of i and j. This feature is also continuous.

3.2.2 Target variable

$\mathbf{scaled_sci}$

This feature is used for calculating the strength of social connectedness between two regions. This feature is continuous.

3.3 Aim

The main thing which we are going to do is to find the right Bayesian network structure for this problem. We will also see the probability distribution of the features. Therefore, we will use a naive Bayes network and also a search based network in the form of Tabu search and also compare these two networks.

So, the input and the output variables which we will be using are described above. Regarding the input variables, as mentioned above, we will use the population feature for calculating the prior probabilities of user location and friends location and it will also help us in obtaining the total population of every country. instead it is divided into many regions and those regions are indexed by a code.

3.4 Construction of the naive Bayes network

We construct naive Bayes network and predict scaled sci based on distance and population features. Thus, to achieve this, we convert continuous variables to discrete variables using quantiles.

3.4.1 Quantiles

Quantiles are cut points that are used to determine how many values are above or below a given threshold. It's used to divide a distribution into subgroups of equal size and proximity. It is utilized to divide the distribution into four equal portions in our scenario.

We use Quantiles for in naive Bayes where we converted continuous to categorical variables.

3.5 Problems with the data

The data is the reason why the naive Bayes network failed. As a result, each user location in the data had 332 or 0 records. The reason for the 0 records is that these records have missing values. As a result, determining whether two sites are dependent or not is challenging. As a result, obtaining prior probability for the countries is similarly problematic.

For example, if we return to the basics of probability theory, so, if there are two variables X and Y the idea is that X tells something about Y. So, if X = 1, it is almost certain that Y = 1 and this is expressed as P(Y = 1|X = 1) > P(Y = 1). Therefore, this means that both X and Y are dependent. But, when we convert this to frequencies of occurrences and take a note of all the cases occurring for X = 1, there will obviously be more cases for Y = 1 even though it is relative to the number of cases with X = 1 versus Y = 1 and total number of cases. So, in our case, P(Y = 1) is always uniform (0.5 in the binary case, 1/3 with 3 values, etc). This is due to the way the data is collected. This means that we won't have the prior probabilities for P(Y) and also P(X).

Due to the problem with the data and also for obtaining prior probabilities, we will reconstruct the data. This is explained in the next section.

3.6 Finding the right Bayesian network structure

Next, we aim to determine the best Bayesian network structure by utilizing the Tabu network to train the network.

So, the algorithm for this is as follows:

• Initially, we consider only a small subset of countries.

- Thus, all regional codes are changed to nation codes. For instance, NL1 is changed to NL.
- As a result, all regional codes are changed to nation codes. For instance, NL1 is changed to NL.
- This association list will help us to compute the total population per country.
- The next stage is to use Tabu search to learn a Bayesian network, which determines the correct structure. Because we only utilized one variable to calculate both attributes, the odds of both user and friend location will be uniform.

3.7 Package for constructing Bayesian networks

For our research, the bnlearn package from R was used to build Bayesian networks. Bnlearn supports structured learning of Bayesian networks various algorithms to compute probability distributions given evidence and evaluation. Algorithms for structure learning, such as constraint-based learning, score-based learning, and Bayesian network classifiers are included in the package.

4. Results

4.1 Analysis

In this Section, the results of our analysis are provided and subsequently discussed.

4.1.1 naive Bayes

A naive Bayesian network was created for predicting the social connectedness index based on the distance and population features. Note that such a network graph is not learnt from data; only the probabilistic parameters are learnt from the data.

Quantiles

Initially, quantiles were used to turn continuous variables into categorical variables for each input and output characteristic. In this scenario, the accuracy is found to be 30 percentage after constructing the naive Bayes network. Table 6.1 displays the confusion matrix. The confusion matrix shows that there is equal prediction for every level. Based on these outcomes, we can conclude

Table 4.1. Confusion matrix when using quantities							
nb.pred	0	1	2	3			
0	1030	707	610	633			
1	638	730	706	659			
2	384	497	552	453			
3	577	681	715	837			

 Table 4.1: Confusion matrix when using quantiles

that naive Bayes is not the right fit due to the problem of accuracy; in the next section we will try to find the right Bayesian network structure using structure learning.

4.1.2 Trying to find the structure of the Bayesian network

In all the previous experiments, all the regions in the countries were identified by their codes but to answer the second research question, we have removed all the numeric codes and consider every country as one. Although countries are represented in the dataset in terms of locations, originally the dataset did not contain prior information of population size. However, later information of population size of particular location was added for some of the locations, which allowed us to compute the population size from these numbers in our program. These numbers were subsequently used to compute prior probabilities of countries.

In addition, only a small set of the countries were considered in the analysis as the general structure of the Bayesian networks obtained will not change by including many different countries and this restriction allowed us to focus on the relationship between particular countries. After that, we have learnt a Bayesian network using the score-based learning algorithm tabu search.

The obtained graph of the Bayesian network is presented in Figure 4.1 and the Bayesian network with its marginal probability distributions is shown in Figure 4.2. There are four vertices in total, as shown in the diagram: UserLocation, FriendsLocation, scaledsci, and distance. We selected a portion of the data by restricting to certain regions in order to render interpretation of the results obtained feasible for us. After structure learning, the probabilistic parameters were estimated based on the data. Note that the prior probability distribution of both vertices UserLocation and FriendsLocation are identical, as a user also acts as friend.

We used discretization in intervals to discretize the distance and scaledsci characteristics. After that, we used structure learning with Tabu search to build a Bayesian network.

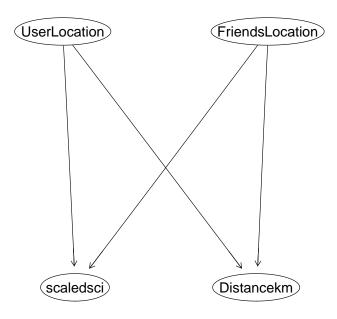


Figure 4.1: Bayesian network graph obtained by structure learning.

4.1.3 Obtaining prior probabilities for countries

As both UserLocation and FriendLocation only need prior probabilistic information for their assessment, due to the fact that both vertices do not have parents, the parameter learning algorithm from bnlearn simply estimates these parameters based on the data. However, we discovered that for each of the locations (UserLocation and FriendLocation) in the data only included were a fixed number of instances: 332 to be exact. Although it was not clear to us where this number came from or where it was based on, it is clear that by using a fixed number of instances per location it is not possible to assess the prior probabilities of locations. When doing this, we would have assumed that every location has a fixed number of Facebook users. What we did instead is to use information of the number of inhabitants of locations, and use this information to compute the prior probabilities.

The following is how the prior probabilities were calculated: If we have five countries, for example, we obtained the total population of each country separately by summing the totals for each location. So, to get the prior probability, we'll divide the population of each country by the total population of all the countries. The prior probability will be calculated as a result of this.

Labie 1.1 The probabilities				
Country name	Prior probability			
Austria	0.047			
Belgium	0.061			
France	0.360			
Germany	0.439			
Netherlands	0.092			

 Table 4.2:
 Prior probabilities

Table 4.2 shows the prior probabilities computed for each country. Germany has a higher prior probability than other countries, as expected, because of its huge population and larger size in

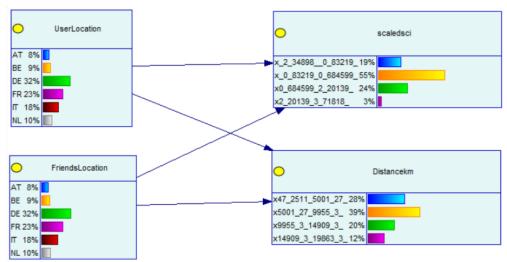
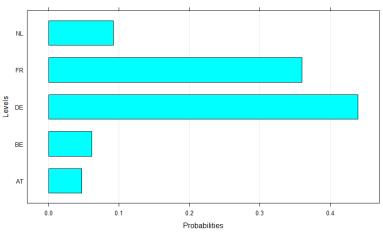


Figure 4.2: Bayesian network with marginal probability distributions

comparison to other countries. Austria has the lowest prior probability since its population is small and the country's size is similarly small.



Conditional Probabilities for Node UserLocation

Figure 4.3: Marginal probability distribution for country (UserLocation)

This can be verified by looking into the conditional probability plot in Figure 4.3. As expected, the probability level of Germany (DE) and France (FR) is high when we compare it to other countries.

4.2 Validation

4.2.1 Cross-validation

For cross-validation, we use 10 folds and the structure learning algorithm which we use is the 'hill climbing' and we evaluate the network using 2 score functions namely : Bayesian Information Criterion (BIC) and Bayesian Likelihood Equivalence (BDe). The plot for the same is shown in Figure 4.4. The Log-Likelihood loss for both BIC and BDe is found to be 5.19. The comparison between both the score function is almost similar.

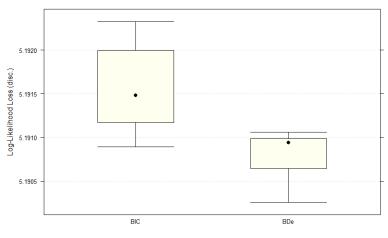
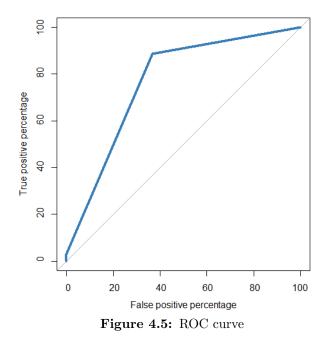


Figure 4.4: K-fold cross-validation

According to [22], if a score is below 6, it is given that the model is good. So, we can conclude that since we obtained for a score of 5.19, we can safely conclude that the model has performed well.

4.2.2 Classification performance

We evaluate the model using these basic evaluation methods: ROC and confusion matrix. The



Receiver Operating Characteristic (ROC) curve can be seen in Figure 4.5. We have obtained 76.5 of the AUC (area under the ROC curce). As an AUC of 50 indicates a non-discriminative model and the curve in the figure is closer to the top left corner, the model has performed reasonably well.

The confusion matrix plot can be seen in Table 4.3. According to the table, the accuracy of the

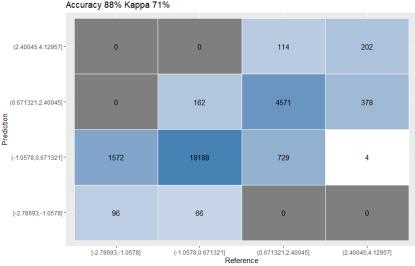


 Table 4.3: Confusion matrix (4 bins)

 Accuracy 88% Kappa 71%

model is found to 88 percentage and as seen in the figure, there are four classes and all the data points are distributed for the four classes.

4.2.3 Brier score

The Brier score of the model is found to be 0.1164788. According to [23], a brier score of 0 means perfect accuracy and a score of 1 means imperfect accuracy. Therefore, since the score which we obtained is so close to 0, this means that our model performed well.

4.2.4 Comparison to the naive Bayes model

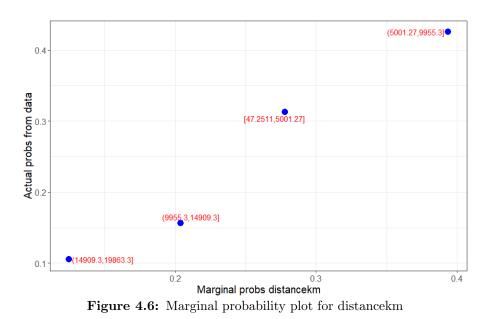
When comparing the present model to the naive Bayes model, the naive Bayes model has a 30 percent accuracy and also has a data imbalance problem. The current model, on the other hand, did not face the issue of data imbalance. There is also a significant difference in accuracy, with the present model achieving an accuracy rate of 87 percent.

The present model's log-likelihood is -189082.8, while naive Bayes' is -205864.2. According to [24], the higher the model's likelihood, the better the model's fit. As evidenced by the accuracy and the problem of data imbalance, this is yet another parameter demonstrating that the present model fits the data better than the naive Bayes model.

4.2.5 Calibration plots

We have utilized the Graphical Independence Network software, or gRain, to generate the calibration graphs. With the fitted Bayesian network as input, the marginal probability for the required feature were calculated using the query method. This yielded the marginal probability for the predicted feature, and by dividing the sum of each individual class of each feature by the overall sum of all the classes for that feature, the real marginals were obtained.

The calibration plots for the features distancekm, scaledsci are shown from 4.6, and 4.7 respectively. In these plots, we compare the marginals of every feature with with the actual probabilities. From the figures 4.6 and 4.7 it can be concluded that the calibration of both distancekm and scaledsci are good.



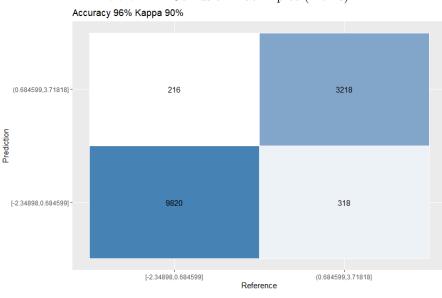
Information obtained from the model 4.2.6

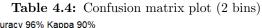
The distribution of SCI and distance is shown in figures 4.8 - 4.10 by using two different countries as user location and friends location every time.

As it is clearly visible from the figures, the distribution varies for all the different combination of countries.

4.2.7Number of bins

The confusion matrix plots obtained for bins 2, 3, 5, 6 are shown from the tables 4.4 - 4.7, respectively. The accuracy decreases for every bin and also there is a problem of data imbalance for bins 3, 5, 6.





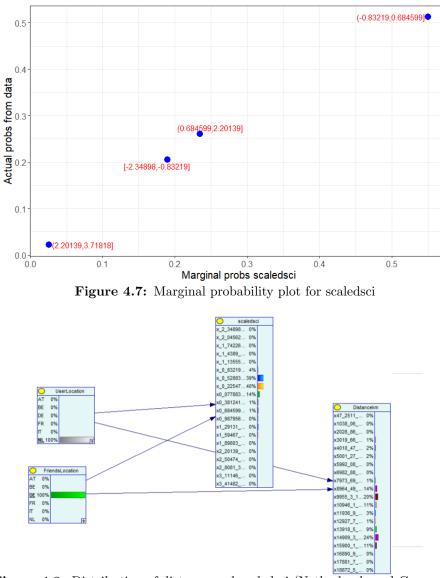


Figure 4.8: Distribution of distance and scaledsci (Netherlands and Germany)

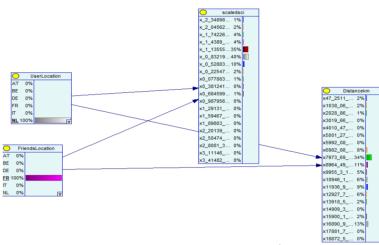
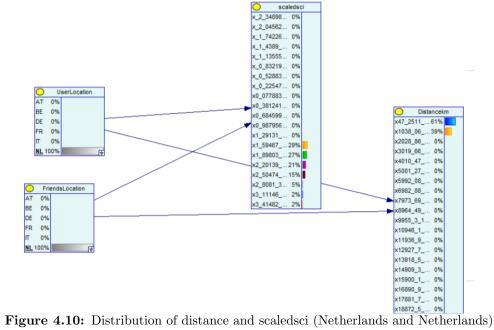


Figure 4.9: Distribution of distance and scaledsci (Netherlands and France)



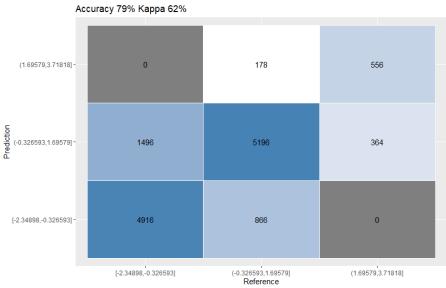
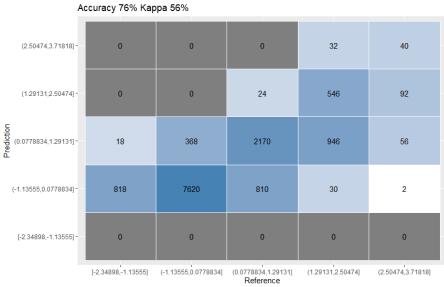


Table 4.5: Confusion matrix plot (3 bins)



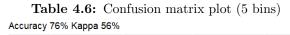


Table 4.7: Confusion matrix plot (6 bins)Accuracy 71% Kappa 57%

(2	2.70698,3.71818] -	0	0	0	0	0	0		
(1	.69579,2.70698] -	0	0	0	140	434	50		
Prediction	684599,1.69579]-	0	0	216	2182	348	64		
рел (-0.3	26593,0.684599] -	6	1490	2566	270	20	4		
(-1.3	3779,-0.326593] -	520	4396	842	24	0	0		
[-2.	34898,-1.33779] -	0	0	0	0	0	0		

[-2.34898,-1.33779] (-1.33779,-0.326593]-0.326593].0.684599](0.684599,1.69579] (1.69579,2.70698] (2.70698,3.71818] Reference

4.3 Discussion

4.3.1 Problems with the naive Bayesian network and TAN

We built both naive Bayesian networks and TAN first, before moving on to a strucure learning. However, we ran into issues with naive Bayes and TAN. Initially, we used quantiles, manual conversion, and discretization intervals to transform continuous information to discrete features. However, low accuracy and class imbalance were concerns with both naive Bayes and TAN. Quantiles did not have a class imbalance, but their accuracy was on the low side. As a result, when we attempted to convert from continuous to discrete manual, we ran across data imbalancing issues (unequal distribution of datapoints). When we employed discretization intervals, we ran into the same issue.

So, in order to solve both of these issues, we attempted to recreate the social connectedness index from the data. The accuracy of both naive Bayes and TAN was quite good, but we ran into the problem of data imbalancing again, and the confusion matrix had a big gap between the intervals. The next step was to try lowering the data's domain size and converting the continuous to categorical using the same procedures as before. However, the same issue of data imbalance arose. Furthermore, we tried a different method of reducing the domain size of the data, namely, deleting outliers and rows with missing data. Even then, the same problem occurred all over again.

4.3.2 Solution: structure learning

We used score-based Bayesian network structure learning to overcome the challenges we were having with naive Bayes and TAN. The manner the pre-processing was done, in particular, was different. To calculate the prior probability for both user and friend location, we employed a single variable (population feature). This is why the prior probabilities of both the user's location and the location of their friends are comparable. Furthermore, we regarded each country as a single entity. The network was also examined and assessed. Low precision and class imbalancing were no longer issues with the model.

Overall, the network functioned well in terms of accuracy, as seen by the calibration graphs acquired for scaledsci and distance km. The brier score was likewise close to zero, indicating that the model performed effectively. The BDe and BIC scores we obtained for k-fold cross-validation were likewise rather strong, demonstrating that the model worked. Many curves on the ROC curve computed were near to the top left corner, demonstrating that the model performed exceptionally well.

We also looked to see if the model could provide any relevant information. As a result, we analyzed the network using three different combinations of countries to observe how scaled sci and distancekm were distributed. The network was compared for the following country combinations: (Netherlands, Germany), (Netherlands, France), and (Netherlands, Spain) (Netherlands, Netherlands). We discovered that the distribution differed for each combination of countries and was not consistent.

4.3.3 Comparison with the naive Bayesian network

We also compared the search based network with the naive Bayes network. The same problem of data imbalance occurred for Naive Bayes and also the accuracy of the model was on the lower side. We also compared the model in terms of Log-Likelihood and the search based model performed well in terms of Log-Likelihood too.

4.3.4 Number of bins

The Bayesian network obtained by structure learning was also compared to the naive Bayesian network. The same problem of data imbalance plagued naive Bayes, and the model's accuracy was similarly on the low side. We also examined the models in terms of Log-Likelihood and found that the structure-learning model outperformed the others.

Furthermore, using fewer bins makes it impossible to gather information from the network, such as the distribution of scaledsci and distance for different sets of countries. As a result, when we tried to get data from the model, we used 20 bins and were able to examine the distribution for all possible combinations of countries. The figures 4.12, 4.13, and 4.11 can all be used to verify this. It is evident from these statistics that the distributions cannot be seen with 12 bins, 14 bins, or 17 bins, but only when bins higher than these are used.

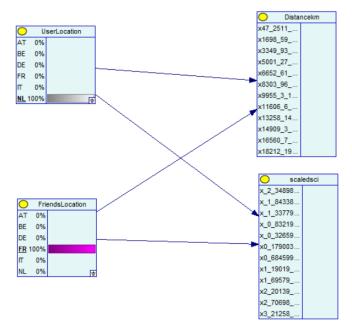


Figure 4.11: Network comparison for 12 bins

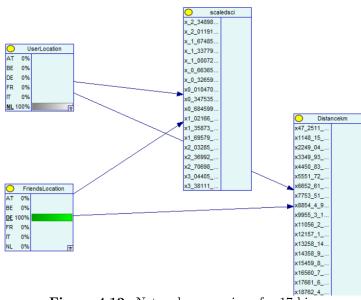


Figure 4.12: Network comparison for 17 bins

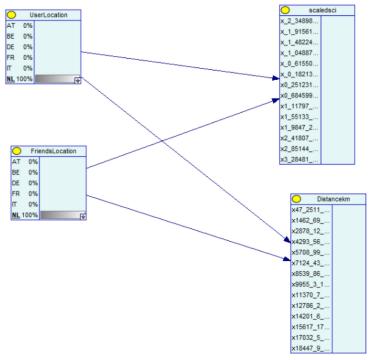


Figure 4.13: Network comparison for 14 bins

4.4 Future recommendations

On the basis of structure learning, we built a search-based network. We might also add more features to the network to see how it performs. However, the research findings suggest that moving forward using Bayesian networks for this problem is a good idea, as determining what kind of information is required took a lengthy time even with a traditional search-based network. When we first tried to build a TAN and a naive Bayes network at the outset of the research, we ran into a number of issues. We also tried a variety of strategies to solve the problem, but none of them were successful. Furthermore, we devised a method for constructing a network and extracted some relevant information from it. However, the findings of the study imply that building a Bayesian network for this problem will be extremely difficult, and that moving forward with Bayesian networks is not a good idea.

5. Conclusion

We strive to find the best Bayesian network topology for forecasting the Social Connectedness Index in this thesis (SCI). We attempted to learn a Bayesian network so that it would learn the parameters of the data. SCI reflects the strength between two countries, and we attempted to learn a Bayesian network so that it would learn the parameters of the data. So, to accomplish this, we first built a naive Bayes network, which we discovered performed poorly in terms of accuracy and also had the problem of data imbalance. Following that, we attempted to learn the Bayesian network using tabu search, which assisted us in determining the correct network structure. In order to accomplish this, we used the data's population feature to calculate the prior probability of user and friend location.

We also used K-cross validation and calibration plots to validate the network. The K-cross validation scores indicated that the model performed well, and the calibration plots for distancekm and scaledsci indicated that the model's calibration was good. We also used a confusion matrix and ROC curves to assess the network. The confusion matrix revealed that the model had an accuracy of 87 percent and that data imbalancing was not an issue. We discovered that the ROC curve is near to the top left corner, indicating that the model performed well. We also calculated the model's Brier score and discovered that it was close to 0, indicating that the model performed well.

We then compared the model to the naive Bayes network and discovered that the naive Bayes network performed poorly in terms of accuracy and Log-Likelihood. We acquired a 67 percent accuracy for naive Bayes, and the Log-Likelihood score was also higher. We also evaluated the network for different types of bins and discovered that as the number of bins grows, the accuracy falls and data imbalance becomes a problem. When we compared the network for other combinations of countries, we also tried to get some helpful information from it. This was only achievable when the number of bins was at least 20. Every combination of countries had a different distribution of scaledsci and distancekm. However, because the number of bins was increased, we had to sacrifice on accuracy.

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