Tutorial _PGMPY__statement

October 4, 2024

1 Bayesian Networks

This TP provides an excellent opportunity to gain further exposure to relevant topics and applications of Bayesian Networks (diagnosis, prediction, etc.).

Objectives: Students will be able to: - Create Bayesian Networks. - Learn Bayesian Networks from real-world problems and datasets. - Determine inferences from Bayesian Networks.

Technology Requirements: - Linux (windows user may install virtual machines) - Python 3.8 or higher (due to pgmpy compatibility) - Download and install pip and then install pgmpy: \$ pip install pgmpy - If the previous did not work, this can be done manually after downloading the code source:

```
$ git clone https://github.com/pgmpy/pgmpy
$ cd pgmpy/
$ sudo pip install -r requirements.txt
$ sudo python setup.py install
```

*Note: if you encountered problems installing pip or pgmpy, refer to the pgmpy Installation Page: https://pgmpy.org/started/install.html

[]: !pip install pgmpy

```
[]: import pgmpy
import pgmpy.models
import pgmpy.inference
import pgmpy.estimators
import pgmpy.inference

import networkx as nx
import matplotlib.pyplot
import xgboost

import pandas as pd
import time

from sklearn.metrics import ConfusionMatrixDisplay, accuracy_score
```

1.1 Part 0: Building a model from scratch: Monty Hall Problem

You might know about the famous Monty Hall, or three doors problem (https://en.wikipedia.org/wiki/Monty_Hall_problem). This is a TV game where a contestant Contestant interacts with a host Host to find a price Price hidden behind one of three closed doors. The contestant makes a first choice of one door they would like to open. The host will then help the contestant by opening one of the doors, leaving the contestant to choose again amongst 2 doors. If the chosen door hides the price, the constestant wins.

The host rules for choosing a door to open are: - never open the door behind which the price is hidden - never open the door chosen by the contestant

A mathematician states: "Selecting in the second step the door that wasn't chosen in the first step, has a 66% probability of granting the price to the contestant". We want to use Bayesian Network modeling to affirm or infirm this statement.

We will model this problem with a three states Bayesian Network. - Contestant is a random variable with 3 possible values (the first chosen door by the contestant) - Price is a random variable with 3 possible values (the price door) - Host is a random variable with 3 possible values (the opened door by the host)

The price is placed before the contestant make its first choice, and the contestant has no indication on its location.

Question: From your understanding of the statement, write the independence and conditional independence relations you expect about Contestant, Price, Host, in the form "X indep Y" or "X indep Y | Z". (A relation "X indep Y" means that X and Y value are set independently, without any link or interaction. A relation "X indep Y | Z" means that X and Y have been chosen with respect to a same information which is the value of Z, but other than that, there is no further link between the value of X and Y.)

TODO 0.1 Instantiate an object you will name monty_hall, from the class pgmpy.models.BayesianNetwork (https://pgmpy.org/models/bayesiannetwork.html). Add edges with its .add_edge method, corresponding to each edge in the Monty Hall graph.

Run the cell after to visualize the network.

```
[]: # TODO

[]: # RUN THIS CELL

def plot_bayesian_network(bn):

    # Convert to a directed graph for visualization
    G = nx.DiGraph(bn.edges())

# Draw the graph
    nx.draw(G, with_labels=True, pos=nx.circular_layout(G))

plot_bayesian_network(monty_hall)
```

TODO 0.2: BayesianNetwork objects have a method that allows to find automatically the inde-

pendence relations: .get_independencies (https://pgmpy.org/base/base.html). Verify that the relations encoded in the network match your answer to the first question.

If the relations differ, try to explain your reasoning (no point will be deducted for an explained incorrect answer).

```
[ ]:  # TODO
```

Since we have specified the structure of the bayesian network in monty_hall, we must now provide the conditional probability distribution.

We assume that both Contestant and Price are chosen randomly (with probability uniformly $\frac{1}{3}$).

TODO 0.3 Use pgmpy.factors.discrete.CPD.TabularCPD (https://pgmpy.org/factors/discrete.html) to specify the conditional probability distribution of *Contestant* and of *Price*. Name the TabularCPD of "Contestant" as cpd_c and "Price" as cpd_p.

Hint: a coin toss can be modeled by TabularCPD("coin_toss", 2, [[0.5], [0.5]])

The name of each variable (in first argument) must be identical to the corresponding node in the BayesianNetwork graph montly_hall.

```
[ ]:  # TODO
```

Run the following cell.

Question: From the table, what is the value of $\mathbb{P}(Host = 0 | Contestant = 1, Price = 2)$? How do you interpret this value with respect to the problem setting?

Question: How many numerical parameters in total were created to build this Bayesian Network? How many would be needed to create the entire joint probability table of $\mathbb{P}(Contestant, Price, Host)$?

Run the following cell to add the probability tables to the monty_hall object.

```
[]: # RUN THIS CELL
```

```
# We now add the conditional probability distributions (cpd) to the bayesian_
network.

monty_hall.add_cpds(cpd_c, cpd_p, cpd_h)

# Verify that the model is correctly specified

assert monty_hall.check_model()
```

If the previous cell throws an error, you may have mispecified either the monty_hall graph (todo 0.1) or the CPD of *Contestant* and *Price* (todo 0.3).

You can check how check_model verifies the BayesianNetwork in its documentation (https://pgmpy.org/models/bayesiannetwork.html)

1.1.1 Application

Suppose that you, as a contestant, have chosen Contestant = 0 as your first guess.

The host might open door Host = 1, or Host = 2 as a result (but never door 0 as it was chosen by the contestant).

TODO 0.4 Using pgmpy.inference.ExactInference.VariableElimination (https://pgmpy.org/exact_infer/ve.html), compute the exact conditional probability distribution of $\mathbb{P}(Price|Contestant=0, Host=1)$ and $\mathbb{P}(Price|Contestant=0, Host=2)$.

Once a VariableElimination object has been set, you can use the class method VariableElimination.query with adequate variables and evidence parameters. The remaining arguments can be set to their default values.

```
[]: inference = pgmpy.inference.ExactInference.VariableElimination(monty_hall)
# TODO
```

Question: According to the two result tables, should you maintain your choice of door Contestant = 0, or select the remaining door?

Question: Even though the contestant final choice has one of two doors, why are the probability of success not (0.5, 0.5)?

1.2 Part 1: Bayesian Modeling of a credit risk dataset

This part is dedicated to learning a Bayesian model (graph and distribution) to model Credit risk in Germany. In this part, we will not specify the structure by hand, instead it will be learned from the data.

We will see how to: - open and inspect a dataset as a DataFrame - handle missing values with and without domain knowledge - apply binning to variables with lots of possible values with and without domain knowledge - separate data into training and validation sets

First, run the following cell to open the data in the form of a pandas. DataFrame.

Question: What do rows represent? What do columns represent?

Question: What is the name (in the data) of the variable that we want to model?

Question: Are there categorical variables? Continuous? Discrete?

1.2.1 Data Preparation

Before we can use the dataset to model credit risk, we must prepare the data to ensure that it can be used properly. This generally involves three steps. - Ensuring that there are no missing values - Ensuring that all columns have a type that allows Bayesian Network structure learning and estimation. Specifically, all variables should be discrete, with a sufficiently low number of possible values (https://pgmpy.org/index.html). - Separing the data into training and validation sets. The training set is used for structure learning and parameter estimation. The validation set is used to compare different learned models on a prediction task.

We will first handle missing (NaN) values. - A domain expert tells us that missing values in "Saving accounts" are valid. A NaN values show that the credit seeker does not have a saving account. We will replace this value by "no account".

TODO 1.1: Is there any other column with missing values? You can use the DataFrame.isnull() method to check if a value is null, and the DataFrame.sum(axis=0) method to get the number of nonzero values in each column.

```
(https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.isnull.html) (https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.sum.html)
```

If there is any missing value remaining, remove the corresponding rows from the DataFrame, using the .dropna() method.

(https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.dropna.html)

Now that we have dealt with missing values, we must ensure that variables are discrete with low number of possible values. We will arbitrarily say that **above 10 values** is too many.

When a variable has too many values, we must apply binning to it. Binning means grouping together values under new names, into a small number of categories. There are different strategy to binning.

- A domain expert might create meaningful binning from prior knowledge. For instance, age is usually grouped in 18-25, 26-45, 46-65, 65+ categories. - When no prior knowledge is available, a common strategy on ordered data (where a "lesser than" notion makes sense) is to create bins of equal population with ordered values. For instance, age could be grouped in three groups from 18 to 30, 31 to 37, 37+ if each group correspond to roughly the same number of observations (rows).

The following cell iterates over the columns of the dataset, and for each of them, prints the number of unique values contained in the column. It uses pd.DataFrame.columns (https://pandas.pydata.org/docs/reference/frame.html) and pd.Series.unique (https://pandas.pydata.org/docs/reference/series.html).

Question Which columns seem to have too many unique values to handle like categorical variables?

TODO 1.2: Apply the function pandas.qcut (https://pandas.pydata.org/docs/reference/api/pandas.qcut.html), with quantiles q=[0, .33, .66, 1] to make three equally populated bins, for Age, Credit amount, and Duration.

You should replace the previous column with the new value: syntax dataframe[column] = pd.qcut(...).

```
[]: # TODO

[]: # RUN THIS CELL

# verify that Age, Credit amount and Duration have been correctly prepared
for variable in ["Age", "Credit amount", "Duration"]:
    assert len(german_credit[variable].unique())==3
    print("Variable '{}' has the following list of possible values: {}".

Gormat(variable, german_credit[variable].unique()))
```

TODO 1.3: To separate our Train/Validation sets, use the method DataFrame.sample (https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.sample.html) to sample without replacement a fraction 0.9 of the dataset german_credit, called train_set. Use the method DataFrame.drop (https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.drop.html) with indexes train_set.index to create a validation set val_set. IMPORTANT for reproducibility, make sure to seed your sample selection with parameter random_state.

```
[]: # TODO

[]: # RUN THIS CELL

assert len(train_set)==900
assert len(val_set)==100
```

We will put aside the validation set for the remainder of part 1 and part 2.

1.2.2 Model learning

To learn a Bayesian Network structure fitting the data, pgmpy provides several algorithms. We will use Hill Climb Search (https://pgmpy.org/structure_estimator/hill.html). This algorithm: - is greedy: a scoring function is optimized by making gradual modification to a Directed Acyclic Graph, until no modification can improve the score (hence, hill-climbing). - is heuristic: the scoring function represents some sort of belief of what a best network structure would be. For instance, a best graph would both fit the data well while having a small description length (an encoding of this graph should be as small as possible) (BIC score, AIC score). Another best graph concept would rely on fitting the data well while maximizing a probability over a distribution of graphs (K2 score, DBE score...). See http://www.lx.it.pt/~asmc/pub/talks/09-TA/ta pres.pdf for more details.

TODO 1.4: Instanciate pgmpy.estimators.HillClimbSearch on the training set. Apply the method HillClimbSearch.estimate on the instance, with k2score, and otherwise default parameters. Finally, reuse plot_bayesian_network defined in part 0 to plot the learned network.

[]: # TODO

TODO 1.5: The estimate method argument tabu_length controls how many of the last graph modifications are impossible to modify. Run another graph estimation while setting tabu_length=1. Is there any change to the graph?

[]: # TODO

TODO 1.6: As mentionned before, different scoring functions encode different beliefs of what an optimal graph would look like. Apply the estimate method with bicscore scoring method. The BIC (Bayesian Information Criterion) penalizes graphs with a lot of edges, under the belief that the simplest structure is the most likely (Occam's razor https://en.wikipedia.org/wiki/Occam%27s_razor).

[]: ## TODO

Question To your opinion, which graph is simpler to interpret?

Question To your opinion, which graph is faster to evaluate?

We will now use the graph produced by the **bicscore** method. We now need to learn a set of factor functions to model the joint probability distribution. Precisely, for each node V with parents (in-going edges) Pa(V), we learn $\mathbb{P}(V|Pa(V))$.

The library pgmpy provides several parameter estimation algorithms, each with different particularities. The one we will use is the following: - Maximum Likelihood Estimation (https://pgmpy.org/param_estimator/mle.html): estimates joint probabilities by using the frequency/count of each configuration of values. It needs all variables to be observed in the data.

There are other methods, that do not apply to our case: - Expectation Maximization (https://pgmpy.org/param_estimator/em.html): Used in the presence of *latent* variables, i.e. variables in the graph for which there is no data. Expectation Maximization does not maximize the likelihood of the joint distribution, but the expectation of this likelihood. - Bayesian Estimation

(https://pgmpy.org/param_estimator/bayesian_est.html): Used when domain knowledge, or belief, is known beside what is recorded in the data. This knowledge is specified to the algorithm in the form of *priors*. Due to the additional information, parameter estimates typically require less observations than Maximum Likelihood Estimation.

TODO 1.7: Apply MLE (https://pgmpy.org/param_estimator/mle.html) with its .get_parameters() method to estimate the parameters of the Bayesian Network. Add the parameters to a model object (class pgmpy.models.BayesianNetwork) built from the graph structure obtained with bicscore. You will name this model model. Use the training data only.

```
[ ]:  # TODO
```

```
[]: # RUN THIS CELL
assert model.check_model()
```

1.3 Part 2: Bayesian Inference

In this part, we will use the previous model to analyse the mechanisms behind Credit Risk attribution by banks.

We will first examine relations between Gender and Risk.

TODO 2.1: Use Variable Elimination to print the joint distribution $\mathbb{P}(\text{Gender}, \text{Risk})$. Use Variable Elimination to print the conditional distribution $\mathbb{P}(\text{Risk}|\text{Gender})$ for both Gender values.

Question: Are gender differences associated to lowered risk? What is hidden in the conditional distribution, that is apparent in the joint distribution? What prior would be needed to deduce the joint distribution $\mathbb{P}(\texttt{Gender},\texttt{Risk})$ from the conditional distributions $\mathbb{P}(\texttt{Risk}|\texttt{Gender})$?

TODO 2.2: Examine how some of the other variables are associated to varying Risk (using conditional distributions). Write down your conclusions.

```
[ ]: # TODO
```

BONUS Question Job categories go from "0 - unskilled" to "3 - highly skilled". Does the risk evolution in function of the Job attribute correspond to your expectations? If not, what could be the reason for the difference?

The Bayesian Network associated to german credit has 9 variables. The previous joint and conditional distribution only involve 2 of them. Therefore, the algorithm has eliminated 7 variables.

The computation time of the inference might change depending on the order in which variables are eliminated. The elimination order is controlled by the parameter elimination_order of the .query method.

TODO 2.3 For an identical query of joint probability $\mathbb{P}(Risk,.)$ between the Risk and an arbitrary variable, measure the time spent when given different elimination orders (greedy, MinFill, MinNeighbors, MinWeight). You may use time.time() to obtain the current time.

```
[ ]:  # TODO
```

The Bayesian Network can help us with *Feature Selection*. The goal of feature selection is to select a subset of variables that contain all the necessary information about Risk, i.e., the *Markov Blanket*.

For instance, variable Job might have information on Risk (i.e., not independent), but this information might already be contained in another variable, making Job redundant.

TODO 2.4 To know which variables can be made independent from Risk by conditioning on other variables, it is possible to use the graph structure. Find a Markov Blanket of Risk. The method BayesianNetwork.get_markov_blanket (https://pgmpy.org/base/base.html) is ready made for this task.

[]: ## TODO

Question Interpret the markov blanket information: what is a markov blanket and what does it mean regarding how banks attribute credit risk rating?

BONUS: causal inference This bonus part covers an application of Bayesian Network not covered during the CM. You may go to part 3 directly then come back to it later.

We will now consider the variable Job, for which we observe that Risk is different depending on the category. We can say clearly that Job and Risk aren't **independent**. What we cannot say while looking uniquely at the conditional probability distribution, is whether Job influences (is a cause of) Risk. Indeed, variables can be associated but not causated.

It is generally difficult to determine causal relationships from observed data. Assuming that causal effects are linear (meaning that if Job has an influence on Risk, then this influence can be correctly modeled by a linear regression model), the causal inference framework (https://pgmpy.org/exact_infer/causal.html) allows to estimate whether two associated variables have a causal influence on each other (Average Treatment Effect https://en.wikipedia.org/wiki/Average_treatment_effect). The question it solves is the following: "if a credit seeker's job category were to increase due to a job change, how much would Risk increase?"

Precisely, the ATE is the difference between the expected Risk when the job stays the same, compared to the expected Risk when the job category increases.

TODO 2.6: Apply pgmpy.inference.CausalInference with its method .estimate_ate on training data, to infer if Job has an influence on Risk.

[]: #TODO

Question: Is Job category causaly linked to Risk?

We now consider the variable Duration. We can confirm that it is associated to Risk, with higher credit amount related to greater proportion of 'bad' risk. Again, we would like to know if this is a cause-effect relation.

We will now use another way of quantifying causal relationships: do-calculus with counterfactuals. The question it solves is: "if all credit seekers were to be attributed the same duration by the bank, how would risk be distributed?" If Duration and Risk are not causaly linked, then the resulting distribution of Risk will be identical for all durations.

TODO 2.7: Use CausalInference.query to estimate the Risk after a do operation on Duration for each category of duration (specify do={"Duration":value} for appropriate values).

[]: #TODO

Question: Is Duration causaly linked to Risk?

1.4 Part 3: Bayesian models as predictive models

Now that we have learned a model of the training data, we can apply it to validation data to evaluate how it works as a predictive model. We can use Maximum A Posteriori inference, to find out what Risk is most likely considering the values of the other variables. Formally, for a given validation sample s where Risk is removed, we want to estimate $\arg \max \mathbb{P}(Risk|Gender, ..., Housing = s)$.

TODO 3.1: Use VariableElimination.map_query (https://pgmpy.org/exact_infer/ve.html) to predict and store credit risk for each sample in the validation set. You can iterate over samples by using val_set.to_dict(), each row being converted to a dictionary. Make sure to not include Risk in the evidences.

You will need to store the true risk in a list y_true for each sample, and store the corresponding predicted value into a list y_pred.

[]: #TODO

Run the next cell to visualize the classification performance.

[]: # RUN THIS CELL print("Classification accuracy:", accuracy_score(y_true, y_pred)) ConfusionMatrixDisplay.from_predictions(y_true, y_pred)

Question The previous snipet plots a Confusion Matrix. Briefly explain what it means.

Question What is the link between the confusion matrix and the accuracy metric?

Question What would be False Positive and False Negative in this confusion matrix? Which one would you rather minimize if you were to work for a bank?

We would like to compare the previous map_query predictive model to a standard machine learning model.

We will use XGBoost, one of the main libraries of simple learning models based on "boosting" and specifically "gradient boosting" (https://xgboost.readthedocs.io/en/stable/).

XGBoost is a library that can only manipulate numerical values. Columns "Gender", "Housing", "Saving accounts", "Purpose", and "Risk" contain strings, so we need to transform them. For each of these columns, the next cell creates a new column with suffix "_numerical" (i.e. "Gender_numerical"), where each of the string values is replaced by an integer. This can be done with .apply (https://pandas.pydata.org/docs/reference/api/pandas.Series.apply.html) and a function, or .map (https://pandas.pydata.org/docs/reference/api/pandas.Series.map.html) and a dictionary.

```
[]: # Run this cell.
     #method 1
     label_mapping = {'good': 0, 'bad': 1}
     val_set['Risk_numerical'] = val_set['Risk'].map(label_mapping)
     train_set['Risk_numerical'] = train_set['Risk'].map(label_mapping)
     #method 2
     label_mapping = dict([(value,index) for index,value in_
      ⇔enumerate(german_credit["Gender"].unique())])
     val_set['Gender_numerical'] = val_set['Gender'].map(label_mapping)
     train_set['Gender_numerical'] = train_set['Gender'].map(label_mapping)
     #method 3
     label_mapping = lambda x: german_credit["Housing"].unique().tolist().index(x)
     val_set['Housing_numerical'] = val_set['Housing'].apply(label_mapping)
     train set['Housing numerical'] = train set['Housing'].apply(label mapping)
     label_mapping = lambda x: german_credit["Saving accounts"].unique().tolist().
      \rightarrowindex(x)
     val_set['Saving accounts_numerical'] = val_set['Saving accounts'].
      →apply(label_mapping)
     train_set['Saving accounts_numerical'] = train_set['Saving accounts'].
      →apply(label_mapping)
     label_mapping = lambda x: german_credit["Purpose"].unique().tolist().index(x)
     val_set['Purpose_numerical'] = val_set['Purpose'].apply(label_mapping)
     train_set['Purpose_numerical'] = train_set['Purpose'].apply(label_mapping)
```

Run the next cell. Its purpose is to make XGBoost and Pandas aware of the categorical nature of some columns.

```
train_set['Risk_numerical'] = train_set['Risk_numerical'].astype("category")
val_set['Risk_numerical'] = val_set['Risk_numerical'].astype("category")
train_set['Duration'] = train_set['Duration'].astype("category")
val_set['Duration'] = val_set['Duration'].astype("category")
train_set['Age'] = train_set['Age'].astype("category")
val_set['Age'] = val_set['Age'].astype("category")
train_set['Credit amount'] = train_set['Credit amount'].astype("category")
val_set['Credit amount'] = val_set['Credit amount'].astype("category")
```

TODO 3.2 In the next cell, create an XGBClassifier model (https://xgboost.readthedocs.io/en/stable/python/python_api.html#xgboost.XGBClassifier) with adequate parameter values. Train (.fit, https://xgboost.readthedocs.io/en/stable/python/python_api.html on train_set with the columns full_variables to predict "Risk_numerical". Predict (.predict, https://xgboost.readthedocs.io/en/stable/python/python_api.html#xgboost.XGBClassifier.predict) on the validation set val_set, and store the result as y_pred.

Hint: for categorical values to be handled, a parameter "enable_categorical" must be set to true at model declaration.

```
[]: full_variables = ["Purpose_numerical", "Saving accounts_numerical", "

"Housing_numerical", "Gender_numerical", "Credit History", "Age", "Job", "

"Credit amount", "Duration"]

## WRITE YOUR CODE BELOW
```

Run the next cell to evaluate the performance of the model.

```
[]: y_true = val_set["Risk_numerical"].values
    print("Classification accuracy:" , accuracy_score(y_true, y_pred))
    ConfusionMatrixDisplay.from_predictions(y_true, y_pred)
```

TODO 3.3 Train and evaluate another XGBClassifier, this time with input data restricted to the markov blanket found in TODO 2.4.

```
[]: ## WRITE YOUR CODE BELOW

[]: # Run the following

y_true = val_set["Risk_numerical"].values
print("Classification accuracy:", accuracy_score(y_true, y_pred))
```

Question: Conclude: did removing columns decrease the information on Risk contained by the dataset? Was this an expected behaviour?

Question: Did removing column increase accuracy? Suggest an explanation why.

ConfusionMatrixDisplay.from_predictions(y_true, y_pred)

Question: Conclude on the predictive performance of bayesian modeling versus XGBoost for this dataset.