A dynamic naive Bayes classifier (DNBC) is an extension of the popular probabilistic graphical model called hidden Markov model. Output variables are assumed to be statistically independent, which helps us in case of the curse of dimensionality occurring in high-dimensional space. Moreover, output variables that come from different probability distributions can be learned easier.

This thesis aims to create a parallel implementation of DNBC that can be easily executed on a computational cluster. For that reason, the algorithm will be implemented in the Scala language on top of Apache Spark.

1. Study DNBC and its possibilities of parallelism.

2. Implement DNBC that is applicable for both discrete and continuous output variables.

3. Parallelize the implementation on top of Apache Spark.

4. Evaluate the parallel implementation and compare it with the sequential implementation in terms of parallel scalability.

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Bachelor's thesis

Paralelní implementace dynamického naivního Bayesovského klasifikátoru

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April 22, 2018

Acknowledgements

Declaration

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Abstrakt

Dynamický naivní Bayesovský klasifikátor (DNBC) nachází využití v mnoha oblastech, například při rozpoznávání hlasu, písma, nebo při předpovídání počasí. DNBC je rozšířením skrytého Markovského modelu tím, že podporuje více pozorovaných proměnných. Předpokládá se, že tyto proměnné jsou vzájemně statisticky nezávislé. Tento předpoklad značně zjednodušuje výpočty a nedochází tak k jevu, který je znamý jako *prokletí dimenzionatily*. Klasifikátor byl naimplementován v programovacím jazyce Scala, nad platformou Apache Spark. Tato implementace využívá dostupných výpočetních zdrojů, kde práce je rozdělena na více procesorů. Díky paralelizaci se mi podařilo zkrátit čas potřebný pro učení na polovinu (oproti sekvenční verzi). Demonstroval jsem, že zrychlení lze dosáhnout nejenom vyšším počtem jader, ale i vyšším počtem strojů.

Klíčová slova   dynamický naivní Bayesovský klasifikátor, skrytý Markovův model, metoda maximální věrohodnosti, Scala, Apache Spark

Abstract

Dynamic naive Bayesian networks (DNBC) have many applications, such as in speech recognition, handwriting recognition or weather prediction. DNBC

extends a hidden Markov model by supporting multiple observed variables. It is assumed that these variables are mutually statistically independent. This assumption greatly simplifies computations and a phenomenon called *curse of dimensionality* does not occur. I have implemented the classifier in Scala language on top of Apache Spark. My implementation makes use of computational resources available, distributing work load across multiple CPUs. Thanks to parallelization, I have shorten the time needed for learning by half (in comparison to the sequential implementation). I have further demonstrated, that the speed up can be achieved not only by increasing the number of cores, but also by increasing the number of machines in a cluster.

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Introduction

Hidden Markov model (HMM) is a probabilistic model that is widely used in many fields, e.g. for speech recognition, handwriting recognition or weather prediction. The model considers a hidden random variable and an observed random variable. In case of speech recognition, the hidden variable would be an actual letter from the alphabet a person said. The observed variable could then be a tone pitch. To estimate the current letter of a word that the person said, the model takes into account the previously said letter and the current pitch level.

The model is first trained using labeled data—containing both hidden states and observed states.[1] Then an inference can be used to predict hidden states, knowing only observed states.

A limitation of HMM is that it only supports one observed random variable. In case of the speech recognition, there are more variables than just tone pitch that are relevant to letter estimation. One could increase the dimensionality of the observed variable. However, this would lead to a phenomenon called *curse of dimensionality* that would result in model training to be intractable.

Dynamic naive Bayesian classifier (DNBC) addresses this issue by supporting multiple observed variables. To avoid the curse of dimensionality, the observed variables are assumed to be statistically independent with each other. Due to the fact that the observed variables are statistically independent, the model can be easily trained in the parallel fashion.

However, there are no existing DNBC libraries written in Scala language. Although there exists a library for Bayesian networks, which is a super set of DNBC, it does not support parallelization on top of Apache Spark. Since Bayesian networks are above the scope of this thesis, I have decided to implement DNBC by myself.

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[1]This is true if using maximum likelihood estimation method for learning. In case of Baum-Welch algorithm, only observed states and list of possible hidden states are necessary.

In the first chapter, I briefly cover mathematical background used in this thesis—namely Gaussian distribution and Gaussian mixture distribution. Then I discuss parameter estimation of probabilistic models. This will be useful for training of HMM and DNBC later on.

In the Analysis chapter, I introduce foundations of DNBC. First, a Markov chain is introduced together with hidden Markov model. Afterwards, Bayesian networks and its derivatives, naive Bayesian classifier and dynamic Bayesian networks are discussed. This gives us enough foundation for defining dynamic naive Bayesian classifier.

DNBC is analyzed in terms of three basic operations that can be performed on it—learning, inference and scoring. I also provide an example problem and discuss limitations of DNBC.

The chapter 5 describes implementation details and design decisions I made when creating a DNBC library. Finally, I show experimental results on randomly generated data sets. The experiments are focused on learning and testing time. Scalability is measured as well. In the end, I show how well DNBC performs in terms of the inference accuracy on realistic data sets.

Goal of this thesis

There are two goals of this thesis. First, I provide the reader with definition of dynamic naive Bayesian classifier (DNBC) and algorithms used for learning, inference and scoring. To better understand DNBC, it is desired to mention the models this classifier is based on. It is also necessary to see whether use can be made of existing software solutions that implement DNBC in Scala programming language.

Second goal is to create a parallel implementation of DNBC that can be easily executed on a computational cluster. For that reason, the algorithm will be implemented in the Scala language on top of Apache Spark. Evaluation of the implementation is necessary to ensure correctness and to measure scalability potential.

Mathematical background

2.1 Probability density function

Probability density function (PDF) of a continuous random variable determines a likelihood that a given value occurs. Furthermore, 2.1 gives a probability of value being in interval $[a, b]$.

$$P(a \leq x \leq b) = \int_a^b \text{PDF}(x)dx \tag{2.1}$$

To satisfy the property that $P(-\inf < x < \inf) = 1$, the following has to hold:

$$\int_{-\inf}^{\inf} \text{PDF}(x)dx = 1. \tag{2.2}$$

2.2 Gaussian distribution

Gaussian (normal) distribution is defined by a probability density function

$$\text{PDF}_{\mathcal{N}(\mu, \sigma^2)}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}. \tag{2.3}$$

The distribution is defined by two parameters—mean μ and variance σ^2. Figure 2.1 provides a visualization of the probability density function.

Normal distribution is one of the most widespread distribution found in nature [4]. Imagine n independent, identically distributed (i.i.d.) random variables. For large $n > 30$, both sum and average of the variables converge to normal distribution. This phenomenon occurs because of the Central Limit Theorem. See book *Introduction to Probability* [5] for a proof.
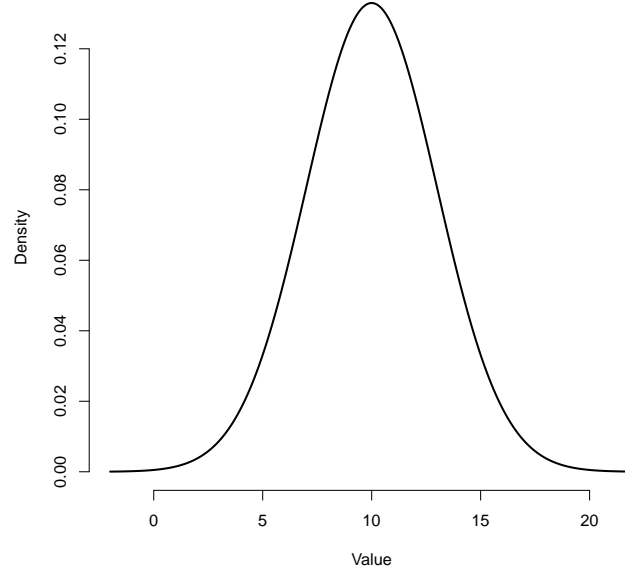
Figure 2.1: Visualization of Gaussian PDF with parameters $\mu = 10$ and $\sigma^2 = 3^2$.

2.3 Gaussian mixture distribution

Gaussian mixture distribution is a weighted sum of multiple components that follow normal distribution. The PDF is given by 2.4, where n is number of components.

$$\text{PDF}_{\mathcal{N}^*(\theta)}(x) = \sum_{i=1}^{n} w_i \text{PDF}_{\mathcal{N}(\mu_i, \sigma_i^2)}(x),\tag{2.4}$$

where w_i is a weight of particular component. The following conditions have to hold:

$$w_i \geq 0, 1 \leq i \leq n,\tag{2.5}$$

$$\sum_{i=1}^{n} w_i = 1.\tag{2.6}$$
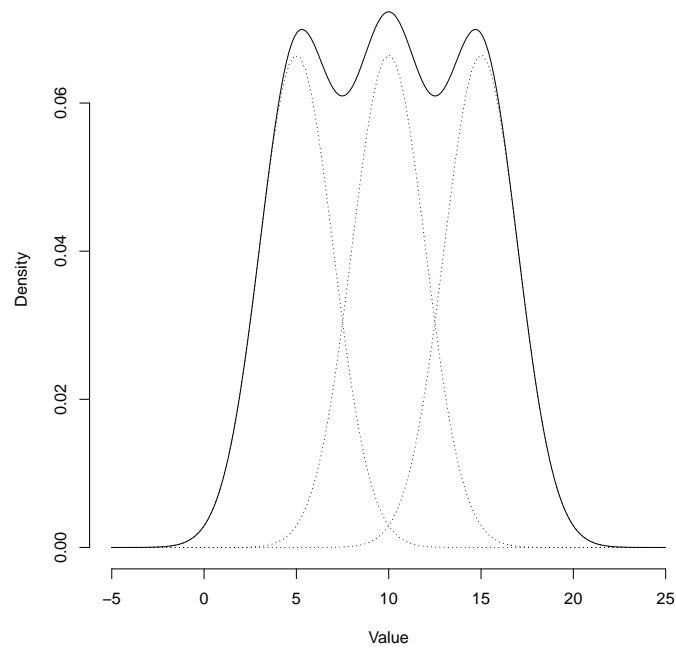
Figure 2.2: Visualization of a mixture with three components with parameters $\mu_1 = 5, \mu_2 = 10, \mu_3 = 15$ and $\sigma^2_{1,2,3} = 2^2$. Weights are $w_{1,2,3} = \frac{1}{3}$. Author: Smason79 [1].

Parameter estimation

In context of this chapter, the goal of parameter estimation is to estimate parameters of a probability distribution in a way that describes given data the best.

3.1 Maximum likelihood estimation

Maximum likelihood estimation (MLE) is a technique for finding parameters of a probabilistic distribution that best describe a random variable. The method aims to maximize the likelihood of all the learning data.

Formally $\text{argmax}_{\theta \in \Theta} \prod_{j=1}^{M} L(x_j, \theta)$, where:

- M is number of data points,

- $X = \{x_1, x_2, \ldots, x_M\}$ is a learning set of data points,

- L is a likelihood function (defined further),

- θ describes model parameters,

- Θ is a set of all model parameters.

3.2 Discrete distribution

Here I present a straightforward way of defining the likelihood function in case of discrete random variables. $L(x, \theta) = x_{cnt}/M$, where x_{cnt} is the number of times $x \in X$ occurs in learning data. Since the likelihood function does not depend on parameter θ, there is no expression to optimize.

There is a reason I did not choose any standard discrete probability distribution to define L. The random variable does not have to be $\mathbf{Z}$, nor $\mathbf{N}$. In fact it can be any abstract object, such as an animal. A type, where comparison
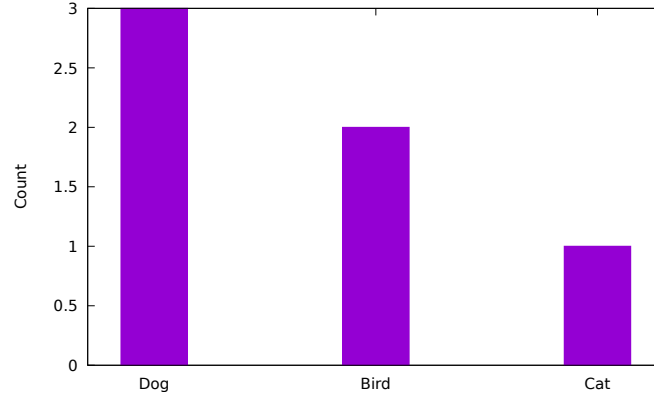
Figure 3.1: Frequency of data in a discrete data set.
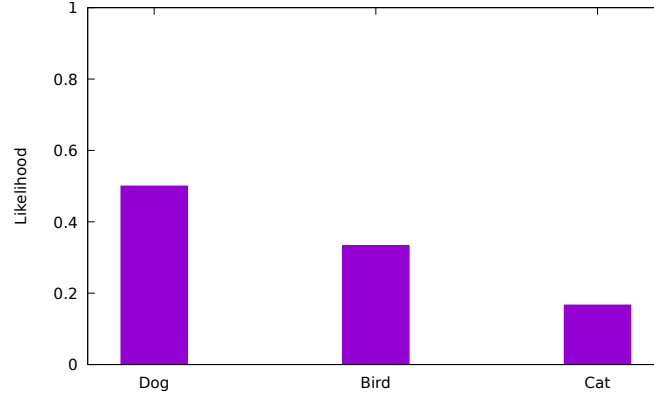
Figure 3.2: Likelihood function L of data in the discrete data set. Likelihood is zero at undefined states.

between two objects doesn't make sense. Therefore, it wouldn't make sense to assign non-zero probability to values that are not specified in learning phase.

As an example, consider the following data: {dog, bird, dog, cat, bird, dog}. Figure 3.2 shows a likelihood function L associated with the data.

3.3 Gaussian distribution

The normal distribution is defined by $\theta = \{\mu, \sigma^2\}$. In MLE, the goal is to find parameter $\theta \in \Theta$, such that the product in 3.1 is maximized.

$$\prod_{j=1}^{M} L(x_j, \theta) \tag{3.1}$$
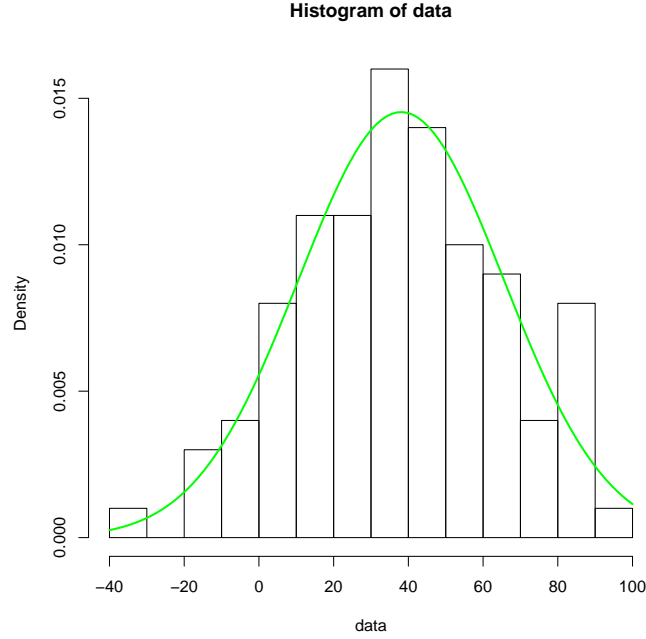
Figure 3.3: Histogram of randomly generated data from normal distribution $\mathcal{N}(40, 32^2)$. The green curve is a plot of normal distribution with the maximum likelihood estimate of θ parameters.

In the case of Gaussian distribution, the likelihood function L is defined by

$$L(x, \theta) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}},$$

where $x \in X$. Taking derivative of 3.1 with respect to μ equal to 0 yields

$$\sum_{j=1}^{M} x_j - M\mu = 0.$$

Maximum likelihood estimate of μ is therefore

$$\mu_{\text{est}} = \overline{X}_M.$$

Derivative of 3.1 with respect to σ^2 equal to zero results in MLE of σ^2 to be

$$\sigma_{\text{est}}^2 = \frac{1}{M} \sum_{j=1}^{M} (x_j - \overline{X}_M)^2.$$

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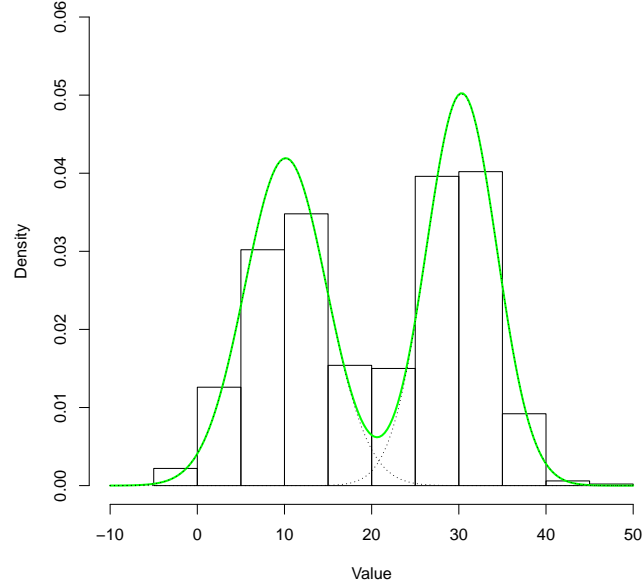
Figure 3.4: Histogram of randomly generated data from two normal distributions $\mathcal{N}(10, 5^2)$ and $\mathcal{N}(30, 4^2)$. The green curve is the best estimate, found using EM algorithm, of underlying normal mixture distribution. Dotted curves are estimates of individual Gaussian mixture components.

Figure 3.3 shows an example of MLE on a normally distributed random variable.

3.4 Gaussian mixture distribution

Given the number of components K components, there are component parameters $\theta_1, \theta_2, \ldots, \theta_K$ and weights $w_1, w_2, \ldots, w_K$ to estimate. In this section, I provide a description of expectation-maximization algorithm based on the lecture notes by Padhraic Smyth [6]. This algorithm provides an estimate of the aforementioned parameters.

Let's define a membership weight w_{jk}, of data point x_j in component k as

$$w_{jk} = \frac{\alpha_k \text{PDF}_{\mathcal{N}(\theta_k)}(x_j)}{\sum_{i=1}^{K} \alpha_i \text{PDF}_{\mathcal{N}(\theta_i)}(x_j)},$$

where α_k is a probability that a randomly selected x_j was generated by the component k. w_{jk} can be thought of as a level of certainty that x_j was generated by the component k. $\sum_{k=1}^{K} w_{jk} = 1$ holds.

The likelihood of all data points given Gaussian mixture parameters is defined as

$$l = \sum_{j=1}^{M} \sum_{k=1}^{K} \alpha_k \text{PDF}_{\mathcal{N}(\theta_k)}(x_j). \tag{3.2}$$

EM is an iterative algorithm, typically iterating until convergence is detected. Each iteration consists of two parts, an E-step and an M-step. In the E-step, weight w_{jk} is computed for each data point x_j and component k. Define $W_k = \sum_{j=1}^{M} w_{jk}$, the weight of all data points in component k. In the M-step, new model parameters are calculated as follows:

$$\alpha_k^{\text{new}} = \frac{W_k}{M},$$

$$\mu_k^{\text{new}} = \frac{\sum_{j=1}^{M} w_{jk} x_j}{W_k},$$

$$\sigma_k^{2\,\text{new}} = \frac{\sum_{j=1}^{M} w_{jk}(x_j - \mu_k^{\text{new}})^2}{W_k}.$$

Where μ_k^{new} resembles standard equation for estimating mean, and $\sigma_k^{2\,\text{new}}$ is similar to an equation for estimating variance. The differences are in weighting.

In the beginning of the algorithm, an initial guess of model parameters is necessary. This can be chosen randomly or through a heuristic.

Termination of the algorithm is determined by checking that the likelihood 3.2 of all data points hasn't improved enough in between iterations. In other words

$$l_{\text{cur}} - l_{\text{prev}} < \text{tol}.$$

One issue with the EM algorithm is that it does not guarantee to find a global optimum.

Analysis

4.1 Markov chain

4.1.1 Introduction

Markov chain describes possible sequences of events in which a probability of being at a state at given time depends only on value of previous state.

4.1.2 Description

A Markov chain is defined by

- set of states $S = \{S_1, S_2, \ldots, S_N\}$,

- transition matrix $A \in \mathbf{R}^{N \times N}$,

- initial probability vector $\pi \in \mathbf{R}^N$.

Where $a_{ij}, 1 \leq i, j \leq N$ is a probability of transitioning from state S_i into state S_j. π_i is a probability that the initial state is S_i.

Suppose a sequence of states $y_1, y_2, \ldots, y_T$, where $T \geq 2$. At time t, where $1 \leq t \leq T-1$, the transition probability a_{ij} is defined as $P(y_{t+1} = S_j | y_t = S_i)$.

4.1.3 Markov property

Markov chain satisfies a Markov property. This property says that $P(y_{t+1} = S_i | y_1 = s_1, y_2 = s_2, \ldots, y_t = s_t) = P(y_{t+1} = S_i | y_t = s_t)$. In other words, being at state S_i at time $t + 1$ only conditionally depends on being at state s_t at time t. Further history doesn't influence the probability.

Figure 4.1: Visualization of a Markov chain with three states.

4.1.4   Example

As an example, consider a Markov chain (MC) with three states: $S_1 =$ sunny, $S_2 =$ rainy and $S_3 =$ cloudy. This MC models how weather changes on every day. Suppose the following transition matrix:

$$A = \begin{bmatrix} 0.6 & 0.1 & 0.3 \\ 0.1 & 0.7 & 0.2 \\ 0.3 & 0.3 & 0.4 \end{bmatrix}. \tag{4.1}$$

If the weather is sunny, tomorrow will be most likely sunny as well. With probability 0.3, it will be cloudy. Rainy weather is very unlikely tomorrow. Consider the following initial probability vector:

$$\pi = \begin{bmatrix} 0.3 \\ 0.2 \\ 0.5 \end{bmatrix}. \tag{4.2}$$

The most likely weather on first day of measurement is cloudy.

4.1.5 Limitations

The previous example only takes into account weather at time t to predict weather at time $t + 1$. In reality, there are multiple factors that influence what the weather will be like. According to the example, if a weather is sunny now, it is unlikely it will start raining. If we, however, take into account humidity, we can improve the prediction. If we know that humidity is high, even though it was sunny, we can predict it started raining. Hidden Markov model addresses this issue.

4.2 Hidden Markov model

4.2.1 Introduction

Hidden Markov model (HMM) is an extension of Markov chain. The states are now called hidden states and every hidden state has an associated observed state.

4.2.2 Description

HMM is defined by: (based on paper by L. Rabiner [7])

- set of hidden states $S = \{S_1, S_2, \ldots, S_N\}$,

- set of observed symbols X,

- transition matrix $A \in \mathbf{R}^{N \times N}$,

- observation probability functions $B = \{b_1(o), b_2(o), \ldots, b_N(o)\}$,

- initial probability vector $\pi \in \mathbf{R}^N$.

The values of the X can be either discrete or continuous. The values of S are assumed to be discrete. The observation probability function $b_i(o)$ describes a probability $P(x_t = o | y_t = S_i)$. This probability function is also called an emission function.

Imagine a walk through a HMM graph (see figure 4.3 for an example graph). At time point t, there is a hidden state y_t and an observed symbol x_t. Value of the observed symbol conditionally depends on value of the hidden state. The dependency is described by emission function $b_i(o)$.

If $t \neq 1$ and $T > 1$, there is a hidden state y_t that conditionally depends on value of previous hidden state y_{t-1}. The dependency is described by transition a_{ij}. If $t = 1$, there is a hidden state y_1 that conditionally depends on initial transition π_i.
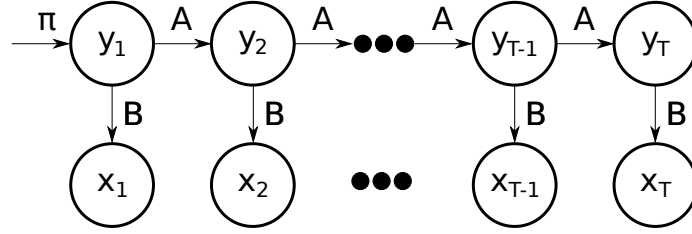
Figure 4.2: Visualization of a walk through a hidden Markov model. At each time point, there is a hidden state y_t and an observed symbol x_t.

4.2.3 Operations

There are three common operations that can be performed on HMM. Learning, inference and scoring.

4.2.3.1 Learning

Learning is used to estimate the model parameters $\{\pi, A, B\} = \lambda$. It is desired to estimate the parameters such that $\prod_{j=1}^{M} P(\mathbf{x}_j | \lambda)$ is maximized. Where $M \in \mathbf{N}$ is a number of sequences to be learned. $\mathbf{x}_j$ is a j-th sequence of observed symbols. In other words, it is desired to maximize the probability that given sequences of observed symbols were generated by the model.

4.2.3.2 Inference

Inference returns the most likely sequence of hidden states, given a sequence of observed symbols.

4.2.3.3 Scoring

Given a sequence of observed symbols $x_1, x_2, \ldots, x_T$, what is the probability that the sequence was generated by HMM with parameters λ? Scoring answers this question.

4.2.4 Learning

Initial transition function   The initial probability vector π can be viewed as a probability function π_i, assigning a probability to every hidden state $S_i \in S$. This is a function of discrete random variable that defines discrete probability distribution. As such, MLE technique (discussed in chapter 3) can be used to estimate the distribution parameters.

Transition function   Every row of A defines a probability function a_{ij} with parameter j. These functions are called transition functions. The function describes a probability of transitioning into state S_j form state S_i. The transition

functions define discrete probability distributions. Parameters of every such distribution can be estimated using MLE.

Emission function   The observation probability functions $b_i(o)$ are functions of either discrete or continuous random variable that takes on values in set of observed symbols X. For purposes of this thesis, it is assumed that continuous variables have Gaussian or Gaussian mixture distribution.

The functions $b_i(o)$ are also called emission functions (emissions). If values of the set of observed symbols X are discrete, then the emissions define discrete distributions and the parameters can be estimated through MLE. If the values of X are continuous, then the emissions define continuous probability distributions. As discussed earlier, parameters of Gaussian distribution can be estimated using MLE. Parameters of Gaussian mixture distribution can be estimated through EM algorithm.

Baum-Welch training   Baum-Welch training is an alternative learning algorithm that is not based on the MLE approach. It will not be covered in this thesis, but its existence should be noted in case you are a curious reader.

4.2.5   Inference

Given a sequence of observed symbols, what is the most likely associated sequence of hidden states? Viterbi algorithm answers this question. Let's define $\alpha_t(i)$ to be the maximum probability of sequence of hidden states and observed symbols up to time point t:

$$\alpha_t(i) = max_{y_1,y_2,\ldots,y_{t-1}} P(y_1, y_2, \ldots, y_{t-1}, y_t = S_i, x_1, x_2, \ldots, x_t | \lambda), \quad (4.3)$$

where λ are parameters of HMM model.

Initialization   At time point $t = 1$, the probability of being at hidden state S_i is simply the initial probability of being at that state and a probability of being at observed state x_1 given hidden state S_i. In other words:

$$\alpha_1(i) = \pi_i b_i(x_1). \quad (4.4)$$

Recursion   Taking into account the structure of HMM, the equation 4.3 can be rewritten recursively as

$$\alpha_t(j) = [\max_i \alpha_{t-1}(i) a_{ij}] b_j(x_t). \quad (4.5)$$

Hidden state at particular time point t is determined by

$$s_t = S_{\text{argmax}_i \, \alpha_t(i)}. \quad (4.6)$$

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Complexity   At each time point t and hidden state index j, the equation 4.5 loops through every hidden state index i. There are N hidden states. In addition, the recursion continues for every time point t. There are T time points. Thus, the overall complexity is $N^2 T$.

4.2.6   Scoring

In previous section, I have defined $\alpha_t(i)$ to be a probability of a sequence of hidden states up to time point t, where $y_t = S_i$, and a sequence of observed symbols up to time point t, given model parameters.

In order to compute the probability that sequence of observed symbols was generated by the HMM (score), take a look how $\alpha_T(i)$ is defined:

$$\alpha_T(i) = max_{y_1, y_2, \ldots, y_{T-1}} P(y_1, y_2, \ldots, y_{T-1}, y_T = S_i, x_1, x_2, \ldots, x_T | \lambda). \quad (4.7)$$

The score is then

$$\sum_{i=1}^{N} \alpha_T(i). \quad (4.8)$$

4.2.7   Example

Suppose an extension of an example mentioned in Markov chain chapter. i.e. there are three hidden states of weather: $S_1 =$ sunny, $S_2 =$ rainy and $S_3 =$ cloudy. Let's introduce a continuous observed random variable describing humidity level. It is easy to imagine that on sunny day, the humidity will be typically lower than on a rainy day. This observable variable can help in predicting future weather.

4.2.8   Limitations

There is only one observed variable, which may not be sufficient for successful prediction in real-life applications. One could increase the dimensionality of the observed variable. That would, however, lead to a problem called *curse of dimensionality*. As we would increase the dimensionality of observed variable, the learning time would increase greatly up to the point where it would no longer be tractable. Dynamic naive Bayesian classifier addresses this issue.

4.3   Bayesian network

Bayesian network is a probabilistic graphical model consisting of nodes and edges. The model is a directed acyclic graph (DAG). Every node describes a random variable which can be either discrete or continuous. Edges describe a conditional dependency among the nodes (variables).
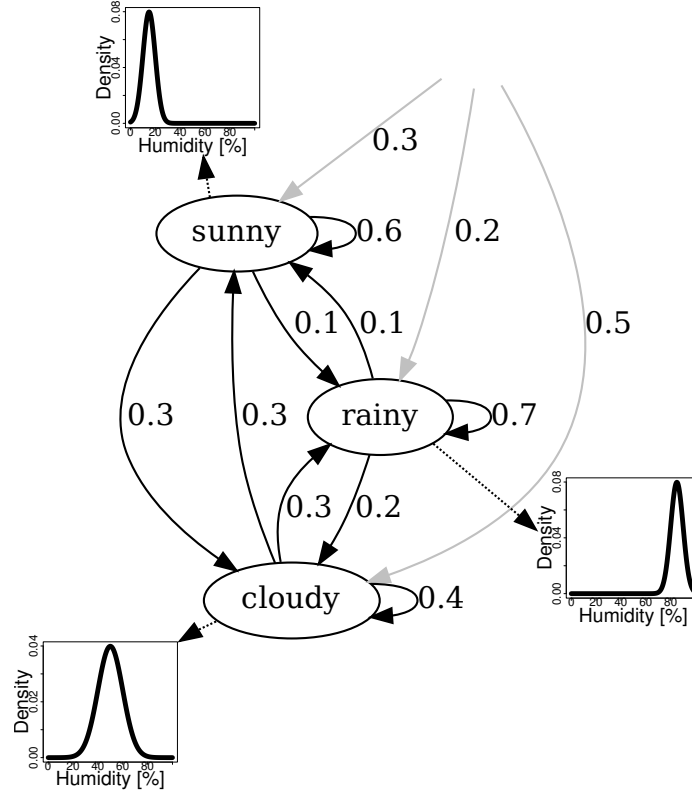
Figure 4.3: Visualization of a hidden Markov model with three states and a continuous observed variable.

As an example, consider a Bayesian network in figure 4.4. Every node represents a discrete random variable with two possible states—*true* and *false*. It can be imagined that dehydration can cause red skin, but it can also influence presence of cancer. In addition, red skin may signal a lack of water intake, or the skin may be red because of cancer cells. Every node defines a conditional probability table (CPT) given nodes it depends on.

4.4 Naive Bayesian classifier

Naive Bayesian classifier is a classifier (model that assigns class labels to given inputs) where features (random variables) are assumed to be conditionally independent of each other.

Imagine we would like to classify a class C_k given feature vector $\mathbf{x}$:

$$P(C_k|x_1, x_2, \ldots, x_n). \tag{4.9}$$
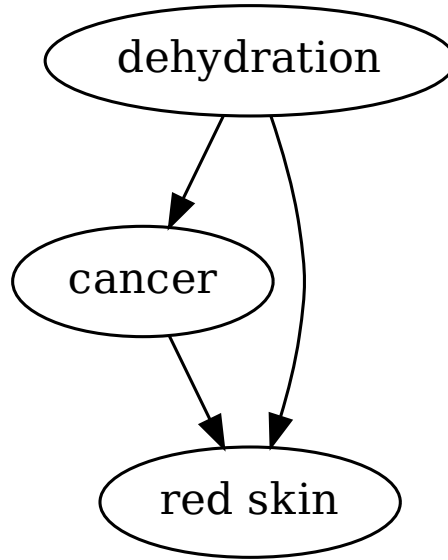
Figure 4.4: Visualization of a Bayesian network with three states.

dehydration	
true	false
0.1	0.9

Table 4.1: CPT for *dehydration*.

input	cancer	
dehydration	true	false
true	0.1	0.9
false	0.01	0.99

Table 4.2: CPT for *cancer*.

input		red skin	
cancer	dehydration	true	false
true	true	0.4	0.6
true	false	0.3	0.7
false	true	0.4	0.6
false	false	0.1	0.9

Table 4.3: CPT for *red skin*.
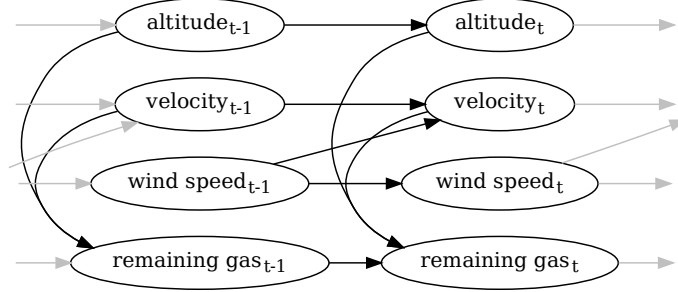
Figure 4.5: Visualization of a Dynamic Bayesian network with four variables at time t.

Using Bayes' theorem, the conditional probability can be rewritten as

$$P(C_k|\mathbf{x}) = \frac{P(C_k, \mathbf{x})}{P(\mathbf{x})} = \frac{P(C_k)P(\mathbf{x}|C_k)}{P(\mathbf{x})}. \tag{4.10}$$

Because the features are assumed to be conditionally independent of each other, the probability in numerator can be rewritten as

$$P(\mathbf{x}|C_k) = P(x_1|C_k)P(x_2|C_k)\cdots P(x_n|C_k). \tag{4.11}$$

Because of the independence assumption, learning of the classifier can be performed effectively, as mentioned in article by K. M. Leung [8].

4.5 Dynamic Bayesian network

Dynamic Bayesian network is a Bayesian network which accounts for time. At each time point t, the values of random variables can be computed based on values of associated random variables in time $t - 1$.

Consider figure 4.5 as an example. It can be imagined that velocity of an airplane at time t conditionally depends on velocity at time $t - 1$ as well as on wind speed at time $t - 1$. Remaining gas at time t conditionally depends on remaining gas at $t - 1$ and it is also influenced by altitude and velocity at current time t.

4.6 Dynamic naive Bayesian classifier

4.6.1 Introduction

Dynamic naive Bayesian classifier (DNBC) is an extension of hidden Markov model (HMM). The difference is that there may be a number of observed

Figure 4.6: Visualization of a Dynamic naive Bayesian classifier with two observed variables. At each time point, there is a hidden state y_t and two observed states: x_t^1 and x_t^2.

variables. In contrast, HMM is defined for only one observed variable. DNBC is dynamic, because it classifies sequences with variables at every time t. It is also naive, because the output variables are assumed to be conditionally independent of each other. Figure 4.6 demonstrates a walk through a model with 2 observed variables.
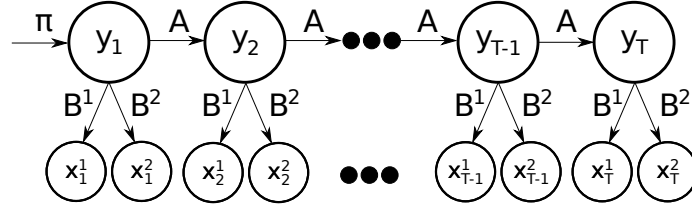
4.6.2 Description

DNBC is defined by

- number of observed variables M,

- set of hidden states $S = \{S_1, S_2, \ldots, S_N\}$,

- sets of observed symbols $X^j, j \in [1, M]$

- transition matrix $A \in \mathbf{R}^{N \times N}$,

- observation probability functions $B^j = \{b_1^j(o), b_2^j(o), \ldots, b_N^j(o)\}, j \in [1, M]$,

- initial probability vector $\pi \in \mathbf{R}^N$.

The values of particular set of observed symbols X^j can be either discrete or continuous. The values of S are assumed to be discrete. The observation probability function $b_i^j(o)$ describes a probability $P(x_t^j = o | y_t = S_i)$. $b_i^j(o)$ is called an emission function.

Imagine a walk through DNBC graph. At time point t, there is a hidden state y_t and M observed symbols x_t^j where $j \in [1, M]$. Value of every observed symbol conditionally depends on value of the hidden state. The dependency is described by emission function $b_i^j(o)$.

An important property of DNBC is that the observed variables are assumed to be independent of each other. Therefore, DNBC does not define any conditional dependency function between two observed variables.

If $t \neq 1$ and $T > 1$, there is a hidden state y_t that conditionally depends on value of previous hidden state y_{t-1}. The dependency is described by transition

a_{ij}. If $t = 1$, there is a hidden state y_1 that conditionally depends on initial transition π_i.

4.6.3 Operations

There are three common operations that can be performed on DNBC. Learning, inference and scoring.

4.6.3.1 Learning

Learning is used to estimate the model parameters $\{\pi, A, B^1, B^2, \ldots, B^M\} = \lambda$. It is desired to estimate the parameters such that $\prod_{j=1}^{M} P(\mathbf{x}_j|\lambda)$ is maximized. Where $M \in \mathbf{N}$ is a number of sequences to be learned. $\mathbf{x}_j$ is a j-th sequence of observed symbols. In other words, it is desired to maximize the product of probabilities that given sequence of observed symbols was generated by given model.

4.6.3.2 Inference

Inference returns the most likely sequence of hidden states, given sequences of observed symbols. Each sequence of observed symbols corresponds to particular observed variable. Each sequence thus has the same number of elements.

4.6.3.3 Scoring

Given sequences of observed symbols $x_1^j, x_2^j, \ldots, x_T^j, j \in [1, M]$ (one sequence per observed variable), what is the probability that the sequences were generated by DNBC with parameters λ? Scoring answers this question.

4.6.4 Learning

Maximum likelihood estimation This learning approach is similar to one described in case of HMM. The only difference is that there are multiple emission functions $b_i^j(o)$ where $j \in [1, M]$ and M is the number of observed variables. Therefore, there is now $M \times N$ continuous distributions to be learned. Each distribution is assumed to be Gaussian or Gaussian mixture.

4.6.5 Inference

Inference algorithm is again Viterbi. It is simply extended to support multiple observed variables. Let $\mathbf{x}_t^j$ be a sequence of observed symbols of variable j up to time point t.

$$\mathbf{x}_t^j = x_1^j, x_2^j, \ldots, x_t^j. \tag{4.12}$$

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Let's define $a_t(i)$ to be the maximum probability of sequence of hidden and sets of observed symbols up to time point t:

$$a_t(i) = max_{y_1,y_2,\ldots,y_{t-1}} P(y_1, y_2, \ldots, y_{t-1}, y_t = S_i, \mathbf{x}_t^1, \mathbf{x}_t^2, \ldots, \mathbf{x}_t^M | \lambda), \quad (4.13)$$

where λ are parameters of DNBC model.

Initialization At time point $t = 1$, the probability of being at hidden state S_i is equal to the initial probability of being at that state and probabilities of being at observed symbol x_1^j given hidden state S_i. In other words:

$$\alpha_1(i) = \pi_i \prod_{j=1}^{M} b_i^j(x_1^j). \quad (4.14)$$

Recursion Taking into account the structure of DNBC, the equation 4.13 can be rewritten recursively as

$$\alpha_t(j) = [\max_i \alpha_{t-1}(i) a_{ij}] \prod_{k=1}^{M} b_j^k(x_t^k). \quad (4.15)$$

Hidden state at particular time point t is determined by

$$s_t = S_{\mathrm{argmax}_i \, \alpha_t(i)}. \quad (4.16)$$

Complexity At each time point t and hidden state index j, the equation 4.15 loops through every hidden state index i and every observed variable index k. There are N hidden states and M observed variables. In addition, the recursion continues for every time point t. There are T time points. Thus, the overall time complexity is $N(N + M)T$.

4.6.6 Scoring

Scoring is performed the same way as in case of HMM. That is, the score can be calculated as

$$\sum_{i=1}^{N} \alpha_T(i). \quad (4.17)$$

4.6.7 Example

Consider a problem of weather prediction. Let's define a set of hidden states to be $S = \{S_1 = \text{sunny}, S_2 = \text{rainy}, S_3 = \text{cloudy}\}$. Let's consider the following observed variables: temperature, humidity and windiness. At every time t, the

hidden state conditionally depends on hidden state at time $t-1$. The three hidden variables at time t conditionally depend on hidden state t. These variables can help in predicting the hidden state.

4.6.8 Limitations

The observed variables are assumed to be conditionally independent of each other. While this assumption enables the use of algorithms with relatively low time complexity, it also limits the ability to describe more complicated relations among random variables. For example, the observed variables may be correlated in reality.

Implementation

There are no existing DNBC libraries written in Scala language. Although there exists a library for Bayesian networks [9], which is a super set of DNBC, it does not support computations on top of Apache Spark. Bayesian networks use different learning and inference algorithms than DNBC. Extending this library would thus be above scope of this thesis.

I have implemented a dynamic naive Bayesian classifier in Scala programming language that runs on top of Apache Spark. I named this software *dnbc-scala.*

5.1 Scala language

Scala is a programming language that combines functional and object-oriented programming. Scala code compiles into Java virtual machine (JVM) bytecode. This enables one to incorporate existing Java libraries into a Scala project.

5.2 Apache Spark

Apache Spark is an engine for cluster-computing. It provides application programming interface (API) that developers can use to execute computations on multiple nodes - processors or machines in a cluster. Spark is also fault-tolerant, meaning that if a computation fails at given node, another node will take over.

5.3 Project structure

The project is divided into 5 modules:

- *core*—main module containing DNBC interface, helper class for loading data set into required format and a class for measuring performance of DNBC on a data set,
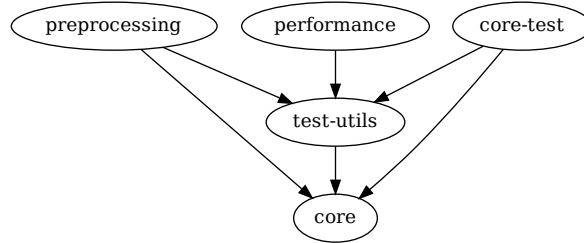
Figure 5.1: Dependencies among modules in *dnbc-scala* project.

- *core-test*—contains tests of *core* module,

- *performance*—provides command line interface for generating a parametric data set and measuring DNBC performance on it,

- *preprocessing*—transforms a predefined data set into data sets with different parameters,

- *test-utils*—provides commonly used functions in tests or in performance measurement.

Figure 5.1 provides overview of the project structure and module dependencies.

5.4 Usage

DynamicNaiveBayesianClassifier object *DynamicNaiveBayesianClassifier* object in *core* module serves as a factory for already learned class *DynamicNaiveBayesianClassifier*.

```
object DynamicNaiveBayesianClassifier {
  def mle(sc: SparkContext,
          sequences: Iterable[Seq[State]],
          continuousVariableHints: Option[List[Int]] =
            Option.empty)
          : DynamicNaiveBayesianClassifier = {
          // ...
          }
}
```

The function *mle* returns a learned (using MLE) model. *sequences* are sequences of *States* used for learning. Optional argument *continuousVariableHints* can be provided to set the number of components in Gaussian mixtures.

The implementation does not try to estimate the number. If the parameter is not provided, the continuous variables are expected to have normal distribution.

The model parameters (*Edges*) are learning in every sequence of states. After all the sequences have been processed, learning is finalized by calling *learnFinalize* on every edge. These functions are executed in parallel since they are not data-dependent with each other.

DynamicNaiveBayesianClassifier class   This class represents a DNBC model with known parameters.

```
class DynamicNaiveBayesianClassifier(
initialEdge: LearnedDiscreteEdge,
transitions: Map[String, LearnedDiscreteEdge],
discreteEmissions: List[Map[String, LearnedDiscreteEdge
    ]],
continuousEmissions: List[Map[String,
    LearnedContinuousEdge]]) {
def inferMostLikelyHiddenStates(observedStates: Seq[
    ObservedState]): List[String]
def score(observedStates: Seq[ObservedState]): Double
}
```

The *inferMostLikelyHiddenStates* function returns the most likely sequence of hidden states given a sequence of observed states. I am using Viterbi algorithm. The following is a function for Viterbi initialization.

```
  private def viterbiInitialize(observedStates: Seq[
      ObservedState]): Map[String,Double] = {
    var vcur = Map.empty[String,Double]
    for (hiddenState <- transitions.keys) {
      var emissionsSum = 0.0
      emissionsSum += discreteEmissions.zipWithIndex.map
          (z => Math.log(z._1(hiddenState)
        .probability(observedStates.head.
            DiscreteVariables(z._2)))).sum
      emissionsSum += continuousEmissions.zipWithIndex.
          map(z => Math.log(z._1(hiddenState)
        .probability(observedStates.head.
            ContinuousVariables(z._2)))).sum
      vcur += (hiddenState -> (emissionsSum + Math.log(
          initialEdge.probability(hiddenState))))
    }
    vcur
  }
```

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The *score* function returns a log-probability that given sequence of observed states was generated by the DNBC. It is internally using Viterbi algorithm to compute $\alpha_T(i)$.

The Viterbi algorithm is not implemented in parallel. The reason is that the algorithm proceeds by time points, and each time point depends on the previous one. At every time point, the parallelization is not worth it, since there is only a bunch of additions taking place.

State An observed state at given time point consists of observations of all the discrete and continuous variables. This is represented by *ObservedState* class.

```
class ObservedState(discreteVariables: List[String],
   continuousVariables: List[Double]) {
  def DiscreteVariables: List[String] =
     discreteVariables
  def ContinuousVariables: List[Double] =
     continuousVariables
}
```

A state at given time point consists of a hidden state and an *ObservedState*. Throughout the project, the hidden states are of *String* type.

```
class State(hiddenState: String, observedState:
   ObservedState) {
  def HiddenState: String = hiddenState
  def ObservedState: ObservedState = observedState
}
```

Edge An edge represents a particular random variable, parameters of which are to be learned.

```
trait Edge[T] {
  def learn(occurrence: T): Unit
  def learnFinalize(): LearnedEdge[T]
}
```

The *learn* function notifies an edge that *occurrence* occurred. User calls *learnFinalize* function to estimate the variable parameters based on previous occurrences.

There are two kinds of edges: *DiscreteEdge* and *ContinuousEdge*. As expected, *DiscreteEdge* represents a discrete random variable, whereas *ContinuousEdge* represents a continuous random variable.

To estimate the parameters of continuous random variables using MLE, I am using jMEF Java library. Previously I used Spark's MLlib library for estimating parameters of a Gaussian mixture model (GMM). The problem

with this is approach was that it can only estimate the parameters by making a computation across multiple nodes in a cluster. This is not a desired behavior since there are many estimations of small data that should run in parallel instead. Therefore, I ended up using jMEF library which estimates the parameters in sequential fashion.

LearnedEdge   A *LearnedEdge* represents a random variable which parameters have been already estimated. The *probability* function returns a probability that a state occurs.

```
trait LearnedEdge[T] {
  def probability(state: T): Double
}
```

RandomEdge   A *RandomEdge* generates random value given random variable parameters. This is useful for performance measurement, where data sets are randomly generated.

```
trait RandomEdge[T] {
  def next(): T
}
```

5.5   Underflow

Since the Viterbi algorithm is computing products of probabilities, the resulting value gets small in few iterations. To avoid underflow, one can compute a log-probability instead, using the following trick:

$$\log(abc) = \log(a) + \log(b) + \log(c). \tag{5.1}$$

Now instead of multiplying tiny numbers together, one can use addition.

5.6   Data set generation

The *test-utils* module contains a function *generatePerformanceDataSet*. This generates a random data set, given parameters, that can be used for measuring learning and testing time. The table 5.1 contains a list of supported parameters.

The initial edge probabilities are generated from a normal distribution and then normalized. The transition destinations are chosen randomly from a uniform distribution. The probabilities of transitions are then set the same way as in case of initial edge. Same approach is used for discrete emissions.

parameter
length of sequences
number of training sequences
number of testing sequences
number of hidden states
number of discrete observed variables
number of continuous observed variables
max number of components per mixture
transitions per hidden state

Table 5.1: Data set generation parameters

For continuous emissions, the components of GMM are chosen randomly in uniform fashion in range of these parameters:

$$\mu \in [-10, 10], \sigma^2 \in [1, 4]. \tag{5.2}$$

The weights in a *RandomContinuousEdge* are all equal.

Experiments

6.1 Unit tests

I am using a Toy Robot data set [2] as a base data set for unit tests. Imagine
a robot wandering through a maze. There are 12 hidden states. Every hidden
state is a 2D coordinate. Every hidden state has an associated color. The
color is a discrete observed variable consisting of 4 states: red, green, blue
and yellow. The initial state is chosen randomly. The data set contains of
200 training sequences and 200 test sequences. Every sequence consists of 200
time points. 10% of the data set observed states at time points are chosen at
random. This depicts robot's occasional failure to detect correct color.

Measurement For every data set in unit tests, an average success rate
(ASR) is measured. This average is the average percentage of hidden states
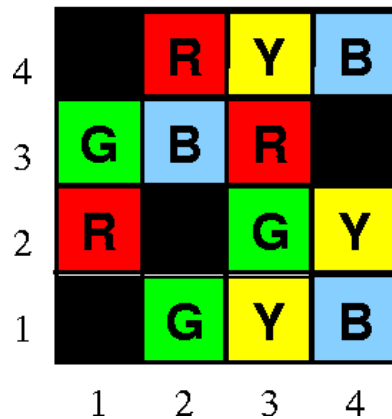inferred correctly in the testing phase.

Figure 6.1: Visualization of a Toy Robot data set [2].

CPU	2x 8-core Intel Xeon E5-2650 v2 2.6 GHz
RAM	96 GB
disk	2x500 GB HDD WD Velociraptor 10k SATA

Table 6.1: Machine specification [3]

Discrete variable   ASR on the Toy Robot data set is 65%.

Continuous variable   The Toy Robot data set is transformed to have a single continuous observed variable instead. Every color (discrete random variable) is replaced by temperature. The idea is that the 4 colors have different temperature distributions if sun is shedding light on the maze. ASR of this data set is 42%.

Discrete and continuous variable   A discrete observed variable is added to the continuous variable data set. This variable describes the quadrant of given 2D coordinate. It is assumed that these two variables are independent. ASR of this data set is 76%.

Gaussian mixture   A data set with single continuous observed variable is generated. Hidden states can take on two values: true and false. If the hidden state is true, observed state is generated from a Gaussian distribution. If the hidden state is false, observed state is generated from a Gaussian mixture distribution. Point of this test is to check that providing a variable hint describing the number of mixture components improves the ASR. ASR with correctly set variable hint is 3% higher compared to a case where no hint is set.

Scoring   A score is computed for a sequence of observed states that comes from a data set a DNBC was trained on. Another score is computed for a sequence of observed states that was generated randomly. Since the score is a log-probability, the values are negative. The following holds:

```
assert ( scoreReal * 1.5 > scoreRandom ).
```

6.2   Performance

In this section, I focus on learning and testing time given a generated parametric data set. The measurements were made on a machine specified in table 6.1. Every job was assigned 15 GB RAM and 10 GB disk space.

The base parameters used for data set generations and performance measurement are described in table 6.2.

number of processors	2
length of sequences	200
number of training sequences	1000
number of testing sequences	200
number of hidden states	10
number of discrete observed variables	5
number of continuous observed variables	5
max number of components per mixture	3
transitions per hidden state	5

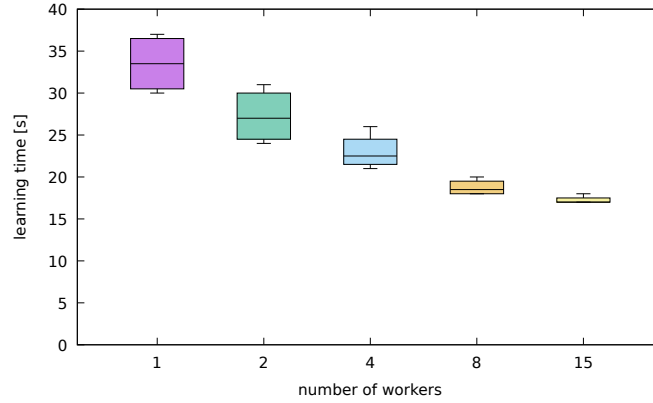Table 6.2: Base data set generation and evaluation parameters.

Figure 6.2: Learning time per number of workers.

Local scalability Goal of this measurement is to see how well the software scales as we increase number of processors. Figure 6.2 shows results of this measurement. Every configuration was measured 4 times to enable better understanding of the data. The data sets had 30 discrete and 30 continuous observed variables.

As it can be seen, the software does not scale particularly well. In fact, the majority of time is spent reading the data set data. This is not a parallel operation. Reading data is the bottleneck.

To focus on scalability of learning itself, figure 6.3 shows learning time of all continuous emissions, without the data loading. As it can be seen, this segment scales relatively well.

Cluster scalability In this experiment, I set up 8 independent worker nodes in a cluster. Every worker is assigned 15 GB RAM and 10 GB disk space. The goal is to measure scalability as the number of processors per node increases. The data sets had 100 discrete and 100 continuous observed variables. As it
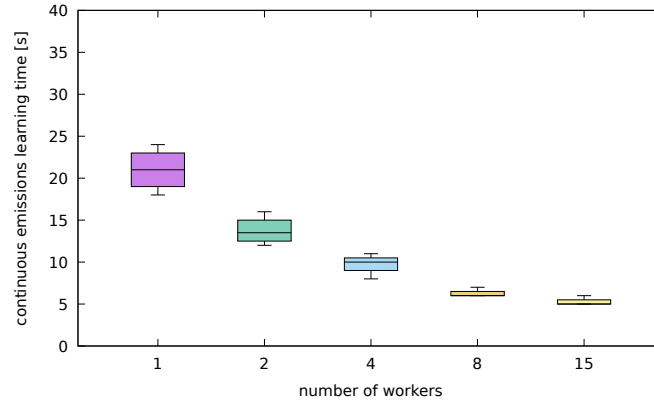
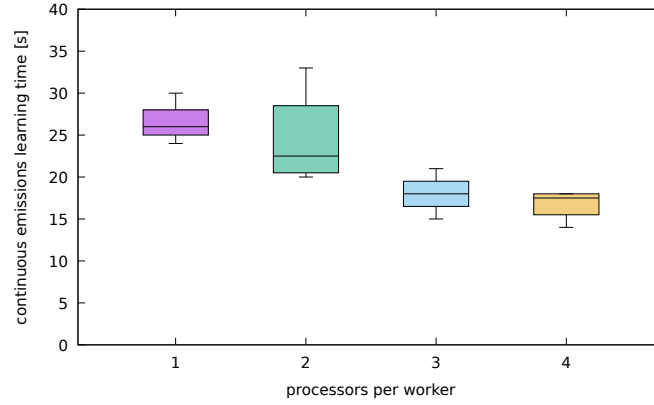Figure 6.3: Continuous emissions learning time per number of workers.

Figure 6.4: Continuous emissions learning time per number of processors per worker.

can be seen on figure 6.4, the continuous emissions learning time is about 45% lower when using 8×4 processors in comparison to using 8 processors.

Training sequences   Figure 6.5 shows approximately linear complexity as number of training sequences increases.

Hidden states   Interestingly, as we increase the number of hidden states, the learning time does not change. Testing time increases super-linearly. This can be see in figure 6.6.

Discrete variables   As the number of observed discrete variables increases, both learning and testing times increase approximately linearly. See figures 6.7 and 6.8.
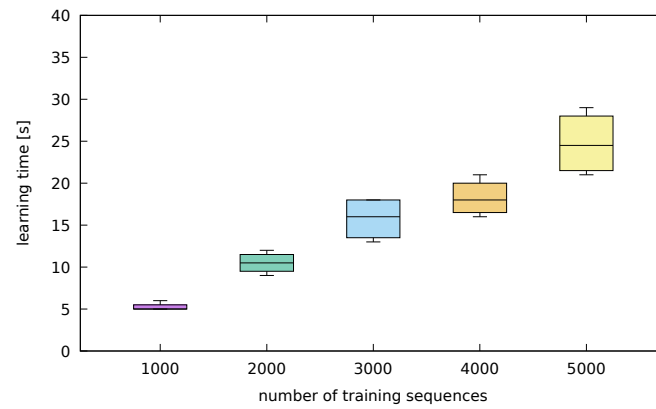
Figure 6.5: Learning time per number of training sequences.
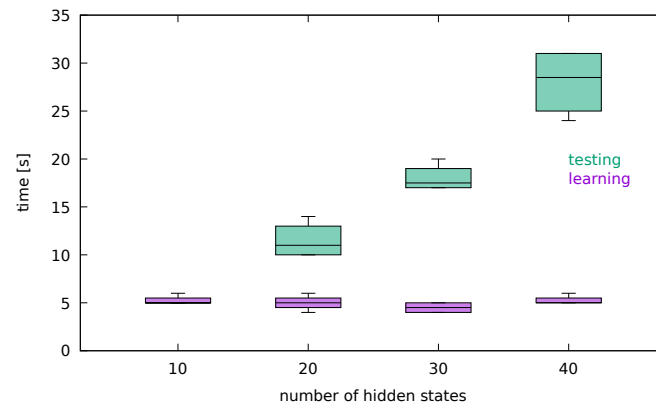

Figure 6.6: Learning and testing times per number of hidden states.

Continuous variables Similar phenomenon can be seen when the number of observed continuous variables increases. The plot looks very similar to the one where number of discrete variables is being increased.
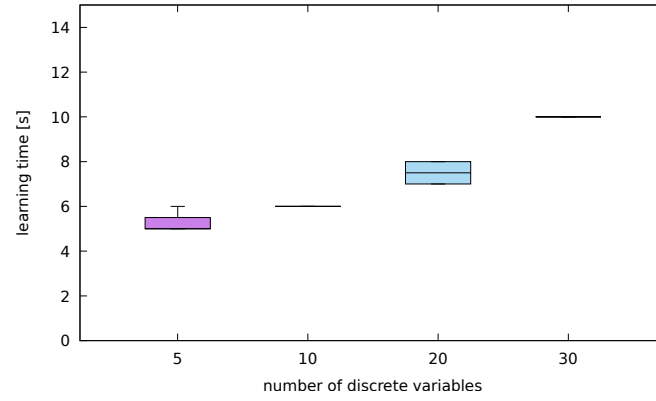
Figure 6.7: Learning time per number of observed discrete variables.
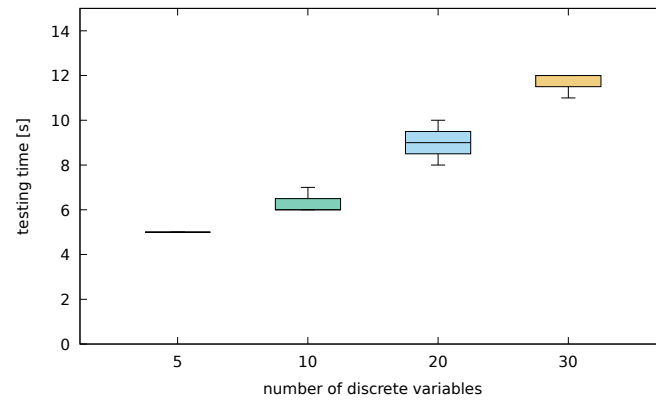

Figure 6.8: Testing time per number of observed discrete variables.

Conclusion

I have described the theory behind dynamic naive Bayesian classifier (DNBC) and other models it is based on. Since no known viable implementation currently exists in Scala, I have decided to implement DNBC by myself. I have demonstrated correctness of my implementation through unit tests. Furthermore, the software shows promising results in terms of speed up when used in a system with multiple processors. Future improvement could be to implement an alternative learning algorithm: Baum-Welch training, and compare it to existing maximum likelihood estimation (MLE) based learning.

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List of abbreviations

ASR average success rate

API application programming interface

CPT conditional probability table

DAG dynamic acyclic graph

DNBC dynamic naive Bayesian classifier

EM expectation-maximization

GMM Gaussian mixture model

HMM hidden Markov model

i.i.d. independent, identically distributed

JVM Java virtual machine

PDF probability density function

MC Markov chain

Obsah přiloženého CD

```
  readme.txt . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . stručný popis obsahu CD
 ─ exe . . . . . . . . . . . . . . . . . . . . . . . adresář se spustitelnou formou implementace
 ─ src
   ├─ impl . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . zdrojové kódy implementace
   └─ thesis . . . . . . . . . . . . . . . . . . . . . zdrojová forma práce ve formátu LaTeX
 ─ text . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . text práce
   ├─ thesis.pdf . . . . . . . . . . . . . . . . . . . . . . . . . . . text práce ve formátu PDF
   └─ thesis.ps . . . . . . . . . . . . . . . . . . . . . . . . . . . . . text práce ve formátu PS
```