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Active Learning for Text Classification

Aktivní učení pro klasifikaci textů

Masters's Degree Project

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I declare that this Masters's Degree Project is entirely my own work and I have listed all the used sources in the bibliography.

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Introduction

Chapter 1

Introduction

Easily speaking, decision can be defined as a set of actions. We are going to work with text data and solve text classification problem. Thus, our main purpose is to introduce precise mathematical abstractions for an automatic and optimal decision making.

Considering binary classification problem. We are seeking to find such set of actions that will assign each input value to its class.

We would like to commence our formal definition with the data. Let $\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^n$ and $\mathbf{y} \in \mathcal{Y} = \{(0, 1)^T, (1, 0)^T\}$, where \mathbf{x} are feature vectors of size n and \mathbf{y} are its labels assigned to the data from space \mathcal{X} . Each value from space \mathcal{Y} can be represented as a one hot representation that consist from ones and zeros $\mathbf{y} \in \{(0, 1)^T, (1, 0)^T\}$. Therefore, first class is represented as $\mathbf{y} = (1, 0)^T$ and second class is represented as $\mathbf{y} = (0, 1)^T$. As a good example of previous definition, \mathbf{x} can be a text document (represented in a mathematical form in order to meet a definition above) and \mathbf{y} can be its label that will show if the document is relevant or not. As seen from an example, label and text are forming a tuple. In this work we are also considering our data as tuples of variables $(\mathbf{x}, \mathbf{y}) \in \mathcal{X} \times \mathcal{Y}$.

1.1 Decision Theory

In this section we would like to define solution of a classification problem as finding such set of actions (decision) that minimizes classification error. This problem is still set up vaguely because neither decision nor minimization of classification error was properly defined.

Each classification problem can be summarized as finding the optimal boundary that will split the dataset with respect to labels. The boundary can be defined as an action that is done with respect to some conditions. Let $a \in \mathcal{A}$ is an action and \mathcal{A} is an action space. As mentioned previously, we would like to make a decision (action) that will split the dataset in two sets and we want this classification to be as good as possible. Quality of the classification can be measured with specific metrics which will be introduced in further sections. In our case we would like to minimize losses (error of classification). As a result, tandem of an action and loss minimization metric lets us to understand how good the action is. Subsequent step is an introduction of a loss function L . Loss function is dependent on action $a \in \mathcal{A}$. Formal definition of the loss function is shown next.

According to [1] loss function L can be defines as

$$L = L(\theta, a), \tag{1.1}$$

where $\theta \in \Theta$ is parameters' vector where Θ is parameters space and $a \in \mathcal{A}$ is an action where \mathcal{A} is an action space. In [1], it is also said that parameter θ can be understand as the true state of nature.

Definition above shows us loss with respect to one action and one true state of nature. Thus, we would like to define expected loss function.

Definition 1. [1] If $\pi^*(\theta)$ is believed probability distribution of θ at the time of decision making, the Bayesian expected loss of an action a is

$$\rho(\pi^*, a) = \mathbb{E}_{\pi^*}[L(\theta, a)], \quad (1.2)$$

$$= \int_{\Theta} L(\theta, a) \pi^* d\theta. \quad (1.3)$$

Basing on definition 1.2, the optimal action is the one that minimizes expected loss, which is defined as

$$a^* = \underset{a \in \mathcal{A}}{\operatorname{argmin}} \mathbb{E}_{\pi^*}[L(\theta, a)]. \quad (1.4)$$

However, how can we connect optimal action a^* with given data? Basing on the data definitions from previous part, we can assume that $\mathcal{X} \times \mathcal{Y}$ is an infinite set and (\mathbf{x}, \mathbf{y}) are samples from this set. Considering $\mathbf{x} \in \mathcal{X}$ and $\mathbf{y} \in \mathcal{Y}$ are random variables. If both \mathbf{x} and \mathbf{y} are random variables then tuple (\mathbf{x}, \mathbf{y}) is a sample from joint probability density function $p(\mathbf{x}, \mathbf{y})$. With the usage of conditional probability rule $p(\mathbf{x}, \mathbf{y})$ can be written as

$$p(\mathbf{x}, \mathbf{y}) = p(\mathbf{y}|\mathbf{x})p(\mathbf{x}). \quad (1.5)$$

At this part we are able to show which meaning this optimal action a^* has. In equation 1.5 $p(\mathbf{x})$ is given and $p(\mathbf{y}|\mathbf{x})$ is an unknown pdf that we want to estimate. The optimal action will lead us to an estimate of $p(\mathbf{y}|\mathbf{x})$.

1.2 Decision Theory for Supervised Learning

Supervised learning requires validation set of the data. Validation set is splitted on training and testing sets. Thus, we have to extend data definition.

Considering the data $\tilde{\mathbf{X}} \subset \mathcal{X}$ and its labels $\tilde{\mathbf{Y}} \subset \mathcal{Y}$. We define cartesian product $\tilde{\mathbf{X}} \times \tilde{\mathbf{Y}}$ as a validation set.

1.2.1 Decision Theory and Support Vector Machine Algorithm

In this subsection we will continue construction of the decision theory on the example of Support Vector Machine (SVM) method. For simplicity lets consider linearly separable dataset. From the theoretical perspective SVM constructs hyperplane in high dimensional space that separates two classes. In this case our decision (action) is a hyperplane that will separate two classes. Equation of the hyperplane can be written as $f(\mathbf{x}, \mathbf{w}, b) = \mathbf{w}^T \mathbf{x} + b$ where $\mathbf{w} \in \mathbb{R}^n$ is a set of hyperplane parameters and $b \in \mathbb{R}$ is a bias. As a result, action space is represented as $(\mathbb{R}^n, \mathbb{R}) = \mathcal{A}$ and as a consequence tuple $(\mathbf{w}, b) \in \mathcal{A}$. From this knowledge we can define $\theta = (\mathbf{x}, \mathbf{y})$ where tuple $(\mathbf{x}, \mathbf{y}) \in \mathcal{X} \times \mathcal{Y}$ is parameters and $\Theta = \mathcal{X} \times \mathcal{Y}$ is a parameters' space. However, for now we are limited on $\Theta = \tilde{\mathbf{X}} \times \tilde{\mathbf{Y}}$. Considering loss function 1.1 that can be written as

$$L = L(\mathbf{x}, \mathbf{y}, \mathbf{w}, b). \quad (1.6)$$

Following task is to understand how good is our action (hyperplane estimation) with respect to the dataset. We can choose different types of loss functions such as cross entropy, hinge loss, etc.. The most basic approach for SVM method is hinge loss function [2] which is defined as

$$L(\mathbf{x}, \mathbf{y}, \mathbf{w}, b) = \max(0, 1 - y\hat{y}(\mathbf{x}, \mathbf{w}, b)) \quad (1.7)$$

where $\hat{y}(\mathbf{x}, \mathbf{w}, b) = \mathbf{w}^T \mathbf{x} + b$ and $y = y_1$.

In terms of SVM method we want to find such hyperplane that will label input values as a first class if it is “above” the hyperplane and as a second class if it is “below” the hyperplane. At this point very important assumption will be introduced. In order to find an optimal hyperplane we assume that the data $\tilde{\mathbf{X}}$ and its labels $\tilde{\mathbf{Y}}$ fully describe spaces \mathcal{X} and \mathcal{Y} . Moreover, as mentioned earlier, we consider $\mathbf{x} \in \mathcal{X}$ and $\mathbf{y} \in \mathcal{Y}$ are random variables with joint probability density function $p(\mathbf{x}, \mathbf{y})$. We will also assume that $\forall i \in \{1, \dots, N\}$, $(\mathbf{x}_i, \mathbf{y}_i) \in \tilde{\mathbf{X}} \times \tilde{\mathbf{Y}}$ are independent identically distributed. As a result, with the usage of those data, probability density function $p(\mathbf{x}, \mathbf{y})$ can be estimated as

$$p(\mathbf{x}, \mathbf{y}) = \frac{1}{N} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i, \mathbf{y} - \mathbf{y}_i) \quad (1.8)$$

where $\delta(\mathbf{x} - \mathbf{x}_i, \mathbf{y} - \mathbf{y}_i)$ is Dirac delta function which is centered in $(\mathbf{x}_i, \mathbf{y}_i)$.

Using (1.2) we can evaluate expected loss function for SVM as follows

$$\begin{aligned} \mathbb{E}_{\pi^*} L &= \int_{\mathcal{X} \times \mathcal{Y}} L(\mathbf{x}, \mathbf{y}, \mathbf{w}, b) p(\mathbf{x}, \mathbf{y}) d(\mathbf{x}, \mathbf{y}), \\ &= \int_{\mathcal{X} \times \mathcal{Y}} \max(0, 1 - y_1 \hat{y}(\mathbf{x}, \mathbf{w}, b)) \frac{1}{N} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i, \mathbf{y} - \mathbf{y}_i) d(\mathbf{x}, \mathbf{y}), \\ &= \frac{1}{N} \sum_{i=1}^N \max(0, 1 - y_{1,i} \hat{y}(\mathbf{x}_i, \mathbf{w}, b)) \end{aligned}$$

where $\hat{y}(\mathbf{x}_i, \mathbf{w}, b) = \mathbf{w}^T \mathbf{x}_i + b$ and $y_{1,i}$ is first component of i -th vector \mathbf{y}_i . Expect loss function for SVM can be written as

$$\rho(\mathbf{x}_i, \mathbf{w}, b) = \frac{1}{N} \sum_{i=1}^N \max(0, 1 - y_i(\mathbf{w}^T \mathbf{x}_i + b)). \quad (1.9)$$

1.2.2 Decision Theory and Algorithm Based on Neural Network Function

Decision Theory construction for the algorithm, based on a neural network function, is mostly the same as in 1.2.1. However in this case our decision is to find estimate $\hat{\mathbf{y}} = \hat{\mathbf{y}}(\mathbf{x}, \mathbf{W}, \mathbf{b})$ of the probability density function $p(\mathbf{y}|\mathbf{x})$ where \mathbf{x} is the input data, \mathbf{W} is a set of all neural network function parameters and \mathbf{b} is a vector of biases. Action space \mathcal{A} will be parameters' and biases' space of $\hat{\mathbf{y}}$. Same as in 1.2.1 we can define (\mathbf{x}, \mathbf{y}) are parameters of the loss function and $\mathcal{X} \times \mathcal{Y}$ is a parameters' space. Another example of loss functions that we will use is cross entropy loss function, which is defined as

$$L(\mathbf{x}, \mathbf{y}, \mathbf{W}, \mathbf{b}) = -y_1 \ln(\hat{y}_1(\mathbf{x}, \mathbf{W}, \mathbf{b})) - y_2 \ln(\hat{y}_2(\mathbf{x}, \mathbf{W}, \mathbf{b})), \quad (1.10)$$

where $\mathbf{y} = (y_1, y_2)^T$ and $\hat{\mathbf{y}} = (\hat{y}_1, \hat{y}_2)^T$. Continuing using assumptions from ?? we consider $\mathbf{x} \in \mathcal{X}$ and $\mathbf{y} \in \mathcal{Y}$ are random variables with joint probability density function $p(\mathbf{x}, \mathbf{y})$. With the usage of the given dataset where $\forall i \in \{1, \dots, N\}$, $(\mathbf{x}_i, \mathbf{y}_i) \in \tilde{\mathbf{X}} \times \tilde{\mathbf{Y}}$ are independent identically distributed we can approximate $p(\mathbf{x}, \mathbf{y})$ as (1.8). Applying definition 1, expected loss for the algorithm based on a neural network function

is evaluated as

$$\begin{aligned}
\mathbb{E}_{\pi^*} L &= \int_{\mathcal{X} \times \mathcal{Y}} L(\mathbf{x}, y, \mathbf{W}, \mathbf{b}) p(\mathbf{x}, y) d(\mathbf{x}, y), \\
&= - \int_{\mathcal{X} \times \mathcal{Y}} \left(y_1 \ln(\hat{y}_1(\mathbf{x}, \mathbf{W}, \mathbf{b})) + y_2 \ln(\hat{y}_2(\mathbf{x}, \mathbf{W}, \mathbf{b})) \right) \frac{1}{N} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i, y - y_i) d(\mathbf{x}, y), \\
&= - \frac{1}{N} \sum_{i=1}^N \left(y_1 \ln(\hat{y}_1(\mathbf{x}, \mathbf{W}, \mathbf{b})) + y_2 \ln(\hat{y}_2(\mathbf{x}, \mathbf{W}, \mathbf{b})) \right), \tag{1.11}
\end{aligned}$$

where $\mathbf{y} = (y_1, y_2)^T$ and $\hat{\mathbf{y}} = (\hat{y}_1, \hat{y}_2)^T$.

1.2.3 Decision Theory and Naive Bayes Algorithm

Naive Bayes algorithm is a bit different to the algorithm based on Neural Networks and SVM. In the case of Naive Bayes we want to estimate $p(\mathbf{W}|\mathbf{x}, \mathbf{y})$ where $\mathbf{W} = (\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_n) \subset \mathcal{W}$ is an action ($a = \mathbf{W}$, $a \in \mathcal{A}$). The reason why we look for an estimate of the $p(\mathbf{W}|\mathbf{x}, \mathbf{y})$ but not $p(\mathbf{y}|\mathbf{x}, \mathbf{w})$ is due to the fact that in case of estimating $p(\mathbf{y}|\mathbf{x}, \mathbf{W})$ we would have to work with normalization constant would be dependent on the set of parameters \mathbf{W} . That fact would make our computations very complicated. Before continuing with a loss function construction we would like to go through Naive Bayes (NB) method.

1.2.3.1 Naive Bayes

Assuming binary classification problem. With the usage of Bayes rule we can rewrite $p(\mathbf{W}|\mathbf{x}, \mathbf{y})$ as follows

$$p(\mathbf{W}|\mathbf{x}, \mathbf{y}) = \frac{p(\mathbf{y})p(\mathbf{x}|\mathbf{y}, \mathbf{W})p(\mathbf{W})}{\int_{\mathcal{W}} p(\mathbf{x}, \mathbf{y}|\mathbf{W})p(\mathbf{W})d\mathbf{W}} \tag{1.12}$$

where \mathcal{W} is assumed as a space of \mathbf{W} .

Naive Bayes method introduces very strong assumption in equation 1.12. This assumption says that features of vector $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ are conditionally independent. As a result estimation of $p(\mathbf{W}|\mathbf{x}, \mathbf{y})$ can be estimated as

$$\tilde{p}(\mathbf{W}|\mathbf{x}, \mathbf{y}) = \frac{1}{Z} p(\mathbf{y}) p(\mathbf{W}) \prod_{i=1}^n (p(x_i|y_1, \mathbf{w}_i)^{y_1} p(x_i|y_2, \mathbf{w}_i)^{y_2}), \tag{1.13}$$

where $\mathbf{y} = (y_1, y_2)$, $\mathbf{W} = (\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_n)$, Z is a normalizing constant.

1.2.3.2 Decision Theory

We want to maximize probability $\tilde{p}(\mathbf{W}|\mathbf{x}, \mathbf{y})$. As a result, using 1.13, loss function L will be represented as

$$L(\mathbf{y}, \mathbf{x}, \mathbf{w}) = -\log(\tilde{p}(\mathbf{W}|\mathbf{x}, \mathbf{y})), \tag{1.14}$$

$$= \log(Z) - \log(p(\mathbf{y})) - \log(p(\mathbf{W})) - \sum_{i=1}^n \log(p(x_i|y_1, \mathbf{w}_i)^{y_1} p(x_i|y_2, \mathbf{w}_i)^{y_2}). \tag{1.15}$$

Same as in 1.2.1 and 1.2.2 we will assume that we can approximate $p(\mathbf{x}, \mathbf{y})$ as 1.8. From this moment everything is ready for deriving expected loss function. Expected loss function for Naive Bayes method

is derived as

$$\begin{aligned} \mathbb{E}_{\pi^*} L &= \int_{\mathcal{X} \times \mathcal{Y}} L(\mathbf{x}, \mathbf{y}, \mathbf{w}) p(\mathbf{x}, \mathbf{y}) d(\mathbf{x}, \mathbf{y}), \\ &= \int_{\mathcal{X} \times \mathcal{Y}} \left(\xi(\mathbf{W}, \mathbf{y}) - \sum_{i=1}^n \log(p(x_i|y_1, \mathbf{w}_i)^{y_1} p(x_i|y_2, \mathbf{w}_i)^{y_2}) \right) \frac{1}{N} \sum_{j=1}^N \delta(\mathbf{x} - \mathbf{x}_j, \mathbf{y} - \mathbf{y}_j) d(\mathbf{x}, \mathbf{y}), \\ &= \frac{1}{N} \sum_{j=1}^N \left(\xi_j(\mathbf{W}, \mathbf{y}_j) - \sum_{i=1}^n \log(p(x_{i,j}|y_{1,j}, \mathbf{w}_i)^{y_{1,j}} p(x_{i,j}|y_{2,j}, \mathbf{w}_i)^{y_{2,j}}) \right) \end{aligned} \quad (1.16)$$

where $\xi(\mathbf{W}, \mathbf{y}) = \log(Z) - \log(p(\mathbf{y})) - \log(p(\mathbf{W}))$ and $\xi_j(\mathbf{W}, \mathbf{y}_j) = \log(Z) - \log(p(\mathbf{y}_j)) - \log(p(\mathbf{W}))$.

1.2.4 Decision Theory and Random Forest Algorithm

In order to work with random forests we must precisely define decision trees and only then construct theory for random forests.

1.2.4.1 Decision Tree

In this section we expect our decision tree to give us an estimate $\hat{\mathbf{y}}(\mathbf{x}, \mathbf{w}) \in \{(0, 1)^T, (1, 0)^T\}$ where \mathbf{w} is a vector that describes tree (depth, branches, etc.), $\mathbf{x} \in \mathcal{X}$ and $\mathbf{y} \in \mathcal{Y}$. It is very important to mention that for different trees \mathbf{w} can have different dimensionality. Thus, for consistency we will assume that for all $\mathbf{w} \in \mathcal{W}$ exists upper bound, where \mathcal{W} is redefined as a space of tree parameters. As a result we will make all \mathbf{w} same length. If \mathbf{w} has spare elements, they will be filled with zeros. Parameter space will be same as in 1.2.1-1.2.3, whereas action $a \in \mathcal{A}$ will be represented as $\mathcal{A} = \mathcal{W}$. In order to understand when our tree is optimal we can use zero-one loss function. Zero-one loss function is defined as

$$L(\mathbf{x}, \mathbf{y}, \mathbf{w}) = \begin{cases} 1, & \mathbf{y} \neq \hat{\mathbf{y}}(\mathbf{x}, \mathbf{w}) \\ 0, & \mathbf{y} = \hat{\mathbf{y}}(\mathbf{x}, \mathbf{w}) \end{cases}. \quad (1.17)$$

With the usage of the given data where $\forall i \in \{1, \dots, N\}$, $(\mathbf{x}_i, \mathbf{y}_i) \in \tilde{\mathbf{X}} \times \tilde{\mathbf{Y}}$ are independent identically distributed we can approximate $p(\mathbf{x}, \mathbf{y})$ as (1.8). As a result, expected loss function for decision tree can be derived as

$$\begin{aligned} \mathbb{E}_{\pi^*} L &= \int_{\mathcal{X} \times \mathcal{Y}} L(\mathbf{x}, \mathbf{y}, \mathbf{w}) p(\mathbf{x}, \mathbf{y}) d(\mathbf{x}, \mathbf{y}), \\ &= \int_{\mathcal{X} \times \mathcal{Y}} L(\mathbf{x}, \mathbf{y}, \mathbf{w}) \frac{1}{N} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i, \mathbf{y} - \mathbf{y}_i) d(\mathbf{x}, \mathbf{y}), \\ &= \frac{1}{N} \sum_{i=1}^N L(\mathbf{x}_i, \mathbf{y}_i, \mathbf{w}) \end{aligned}$$

where $\sum_{i=1}^N L(\mathbf{x}_i, \mathbf{y}_i, \mathbf{w})$ is (1.17).

If we want to minimize expected loss we have to follow next steps. While construction decision tree we choose such feature $x_i \in (x_1, \dots, x_n)^T = \mathbf{x}$ that will bring as the highest information about the system. This feature will form first layer, then we add another feature with the highest informational gain and construct second layer. Basing of this method we construct nodes and add more and more layers (branches).

In the following part we are going to work with a set of decision trees. For this purposes we will define our decision tree as $\hat{\mathbf{y}} = (T_1(\mathbf{x}, \mathbf{w}_l), T_2(\mathbf{x}, \mathbf{w}_l))^T$ where index l represents set of parameters for l -th tree and indices 1, 2 represent first and second value of the one-hot vector.

1.2.4.2 Random Forest

Considering $\mathbf{x} \in \mathcal{X}$ and $\mathbf{y} \in \mathcal{Y}$ as random variables with joint probability density function $p(\mathbf{x}, \mathbf{y})$. We will also assume that $\forall i \in \{1, \dots, N\}$, $(\mathbf{x}_i, \mathbf{y}_i) \in \tilde{\mathbf{X}} \times \tilde{\mathbf{Y}}$ are independent identically distributed.

With the usage of $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}$ we will make $\{1, \dots, L\}$, $L \in \mathbb{N}$ sets where $\forall l \in L$, $\tilde{\mathbf{X}}_l \subset \tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}_l \subset \tilde{\mathbf{Y}}$. The data $\tilde{\mathbf{X}}_l$ and $\tilde{\mathbf{Y}}_l$ are created with random uniform sampling from $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}$. We also want each subset to contain strictly 60% of the data from $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}$. As a result parameter space for random forests will form tuples of sets $(\tilde{\mathbf{X}}_l, \tilde{\mathbf{Y}}_l)$. Basing on this theory we will construct L decision trees $\hat{y} = T(\mathbf{x}, \mathbf{w}_l)$, where $\mathbf{x} \in \tilde{\mathbf{X}}_l$. As a result for l -th decision tree

$$\mathbb{E}_{\pi^*} L = \frac{1}{N_l} \sum_{i=1}^{N_l} L(\mathbf{x}_{i,l}, \mathbf{y}_{i,l}, \mathbf{w}_l) \delta(\mathbf{x} - \mathbf{x}_{i,l}, \mathbf{y} - \mathbf{y}_{i,l}) \quad (1.18)$$

where $(\mathbf{x}_{i,l}, \mathbf{y}_{i,l}) \in (\tilde{\mathbf{X}}_l, \tilde{\mathbf{Y}}_l)$ and N_l is a number of the data in $\tilde{\mathbf{X}}_l$ and $\tilde{\mathbf{Y}}_l$. If we assume \mathbf{w}_l as a random variable then L decision trees form samples from probability density function $p(\mathbf{y}|\mathbf{x}, \mathbf{w})$. In other words

$$p(\mathbf{y}|\mathbf{x}, \mathbf{w}_l) = T_1(\mathbf{x}, \mathbf{w}_l)^{y_1} T_2(\mathbf{x}, \mathbf{w}_l)^{y_2} \quad (1.19)$$

where label \mathbf{y} is written as a one-hot representation $\mathbf{y} = (y_1, y_2)^T$. Thus, we can say that classification probability $p(\mathbf{y}|\mathbf{x})$ can be written as

$$p(\mathbf{y}|\mathbf{x}) = \int_{\mathbf{w} \in \mathcal{A}} p(\mathbf{y}|\mathbf{x}, \mathbf{w}) p(\mathbf{w}) d\mathbf{w}. \quad (1.20)$$

where \mathcal{A} is an action space. With the usage of samples \mathbf{w}_l we can approximate $p(\mathbf{y}|\mathbf{x})$ as

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{L} \sum_{l=1}^L T_1(\mathbf{x}, \mathbf{w}_l)^{y_1} T_2(\mathbf{x}, \mathbf{w}_l)^{y_2} \quad (1.21)$$

where each decision tree $(T_1(\mathbf{x}, \mathbf{w}_l), T_2(\mathbf{x}, \mathbf{w}_l))^T$ is constructed with the usage of (1.18).

Before continuing with further sections we define output of Random Forest as $\hat{\mathbf{y}} = \hat{\mathbf{y}}(\mathbf{x}, \mathbf{W})$, where $\mathbf{W} = (\mathbf{w}_1, \dots, \mathbf{w}_L)$ is set of parameters of specific Random Forest algorithm. We define vector $\hat{\mathbf{y}}$ as

$$\hat{\mathbf{y}} = \frac{1}{L} \sum_{l=1}^L (T_1(\mathbf{x}, \mathbf{w}_l), T_2(\mathbf{x}, \mathbf{w}_l)). \quad (1.22)$$

1.3 Decision Theory for Active Learning

Active learning problem is defined as a sequence of Supervised learning problems. In this part we will want to get not only set of parameters for specific model that minimizes its loss function but a probability distribution. We will explain how to get this probability distribution later. The reason why we want to get a parameters probability distribution because we have to integrate through a parameters space. More theory is explained further.

Specifically, we assume that labels $\mathbf{y} \in \tilde{\mathbf{Y}}$ are available only for $\mathbf{x} \in \tilde{\mathbf{X}}$. We have the possibility to select an unlabeled element from \mathbf{X} and ask for its label. Since it is expensive, we aim to have such questions that will maximize scores as fast as possible. Formally, we denote $J_0 = \{j_{01}, j_{02}, \dots, j_{0N}\} = \{1, \dots, N\}$ the initial set of N available labels. using only the labeled data, the supervised learning task is defined on sets $\mathbf{X}_0 = \tilde{\mathbf{X}} = \{\mathbf{x}_i\}_{i \in J_0}$ and $\mathbf{Y}_0 = \tilde{\mathbf{Y}} = \{\mathbf{y}_i\}_{i \in J_0}$. This set is sequentially extended with new labels gained from \mathbf{X} . We consider a sequence of U questions $u = \{1, \dots, U\}$, in each question, we select

an index j_u and ask to obtain the label \mathbf{y}_{j_u} for data record \mathbf{x}_{j_u} . The index set and the data sets are extended as follows

$$J_u = \{J_{u-1}, j_u\}, \quad \mathbf{X}_u = \{\mathbf{X}_{u-1}, \mathbf{x}_{j_u}\}, \quad \mathbf{Y}_u = \{\mathbf{Y}_{u-1}, \mathbf{y}_{j_u}\}.$$

The task of active learning is to optimize the selection of indices j_u to reach as good classification metrics with as low number of questions as possible. As a result we have to define expected loss for each question u that will be dependent on the action and parameter spaces. In this case we can define our action space \mathcal{A}_u as a space of the data indices with respect to the parameters space Θ_u for each question u . Parameters space is defined as a set of possible parameters from a specific model. It is very important to understand that we will need not only one set of parameters but parameters distribution. We need parameters distribution because we will integrate over the parameters space. As an example, if we talk about SVM method, then parameters space for active learning problem will be defined as a set of weights that form a hyperplane. If we talk about the algorithm that is based on a Neural Network function, then parameters space of the active learning problem will form weights from neurons. We wanted to highlight that parameters space will be different for each problem but the idea for each algorithm is same.

As a result our task can be written as

$$j_u^* = \operatorname{argmin}_{j \in J \setminus J_u} (\mathbb{E}_{\pi_u^*} L^*) \quad (1.23)$$

where $\mathbb{E}_{\pi_u^*} L^*$ is expected loss that is dependent on an action given question u and J is space of all indices. Expected loss for the active learning problem is defined as

$$\mathbb{E}_{\pi_u^*} L^* = \int_{\Theta_u} L^*(a, \theta) \pi_u^* d\theta \quad (1.24)$$

where $a \in \mathcal{A}_u$ and $\theta \in \Theta_u$ and L^* is a loss function for the active learning problem. Character “*” is used only for distinguishing active learning loss from the loss function which is used for different models. We will specify action space because it will be the same for all models that are used in the active learning section. Action space \mathcal{A} is a set of possible indices $j_u \in J_u$ where u is a specific question. Thus, (1.24) can be written as

$$\mathbb{E}_{\pi_u^*} L^* = \int_{\Theta_u} L^*(j_u, \theta) \pi_u^* d\theta. \quad (1.25)$$

Using this approach we will be able sequentially select indices from \mathbf{X} and ask for a label from \mathbf{Y} that will help us to get higher scores faster than in the case of random choice of indices.

1.3.1 Active Learning Loss Function

1.3.1.1 Entropy Based Loss

Considering that $\mathbf{y} \in \mathcal{Y}$ is defined with the usage of one-hot representation. Let $\hat{\mathbf{y}} = \hat{\mathbf{y}}(\mathbf{x}_{j_u}, \theta_u)$ is an estimate of \mathbf{y} . However, in this case output estimate $\hat{\mathbf{y}}$ is represented as a vector of probabilities that \mathbf{x}_{j_u} is assigned to different classes. As an example for well trained binary classifier, for specific \mathbf{x} that is assigned to $\mathbf{y} = (1, 0)^T$, classifiers estimate of \mathbf{x} can be $\hat{\mathbf{y}} = (0.95, 0.05)^T$. It is very interesting that before we can solve the optimization problem with choosing the index j_u we have to solve the optimization problem of finding $\hat{\mathbf{y}}$. This leads us to supervised learning models that we have discussed in previous sections.

We want to define our loss function as a negative entropy. Basing of the formal definition of the entropy we can write it as

$$-H(\hat{\mathbf{y}}|\mathbf{x}_{j_u}, \theta_u) = \sum_{r=1}^R \hat{y}_r(\mathbf{x}_{j_u}, \theta_u) \log(\hat{y}_r(\mathbf{x}_{j_u}, \theta_u)), \quad (1.26)$$

where \hat{y}_r is r -th element of the output estimate $\hat{\mathbf{y}}$ and θ is a vector of parameters for specific model. As done in Passive Learning sections we want to find expected loss based on entropy function. We want to find expected value over the parameter space. Thus, we have to define distribution

$$\pi_u^* = p_u(\theta_u|\mathbf{X}_u, \mathbf{Y}_u). \quad (1.27)$$

We do not have explicit form of the pdf. However, we assume that we have samples Q_u samples $\theta_{u,q} \in \{1_u, \dots, Q_u\}$ from $p_u(\theta_u|\mathbf{X}_u, \mathbf{Y}_u)$. As a result $p_u(\theta_u|\mathbf{X}_u, \mathbf{Y}_u)$ can be approximated as

$$\pi_u^* = \frac{1}{Q_u} \sum_{q=1}^{Q_u} \delta(\theta_u - \theta_{u,q}), \quad (1.28)$$

where $\delta(\theta_u - \theta_{u,q})$ is Dirac delta function centered in $\theta_{u,q}$. With the usage of previous knowledge we can derive expected entropy loss as

$$\begin{aligned} \mathbb{E}_{\pi_u^*} L^* &= \int_{\theta_u} -H(\hat{\mathbf{y}}|\mathbf{x}_{j_u}, \theta_u) p_u(\theta_u|\mathbf{X}_u, \mathbf{Y}_u) d\theta_u \\ &= \int_{\theta_u} -H(\hat{\mathbf{y}}|\mathbf{x}_{j_u}, \theta_u) \frac{1}{Q_u} \sum_{q=1}^{Q_u} \delta(\theta_u - \theta_{u,q}) d\theta_u \\ &= \frac{1}{Q_u} \sum_{q=1}^{Q_u} -H(\hat{\mathbf{y}}|\mathbf{x}_{j_u}, \theta_{u,q}) \\ &= \frac{1}{Q_u} \sum_{q=1}^{Q_u} \sum_{r=1}^R \hat{y}_r(\mathbf{x}_{j_u}, \theta_{u,q}) \log(\hat{y}_r(\mathbf{x}_{j_u}, \theta_{u,q})). \end{aligned} \quad (1.29)$$

1.3.1.2 Information Gain Based Function

TBD

1.3.2 Active Learning for Random Forests Algorithm

In Supervised Learning section 1.2.4 we have derived that $p(\mathbf{y}|\mathbf{x})$ for Random Forest (RF) algorithm is written as 1.21. Active Learning algorithm requires distribution over the parameters of the Random Forest algorithm. We will solve this problem the way that we will get samples from π_u^* and then approximate probability distribution as (1.27).

In order to estimate samples from π_u^* we define Ensemble Random Forest Algorithm. That means that we will use Q_u Random Forests in each step of Active Learning algorithm. In this case parameters of each $\hat{\mathbf{y}}_{q_u}$, where $\hat{\mathbf{y}}$ is Random Forest one-hot represented output and $q_u \in \{1_u, \dots, Q_u\}$, will be iid. Of-course RF algorithm is already ensemble of decision trees but in this case we create ensemble algorithm from ensemble algorithms. Previously we defined for each decision tree T_l where $l \in \{1, \dots, L\}$, that \mathbf{w}_l is a vector of parameters of l -th decision tree. Thus, let $\mathbf{W} = (\mathbf{w}_1, \dots, \mathbf{w}_L)$ is set of parameters of specific

Random Forest algorithm. Thus, for $\hat{\mathbf{y}}_{q_u}$ we have $\mathbf{W}_{q_u} = (\mathbf{w}_{q_u,1}, \dots, \mathbf{w}_{q_u,L})$. As a result we can approximate π_u^* as

$$\pi_u^* = \frac{1}{Q_u} \sum_{q_u=1}^{Q_u} \delta(\mathbf{W} - \mathbf{W}_{q_u}). \quad (1.30)$$

Another important point is to define $\hat{\mathbf{y}}_{q_u} = \hat{\mathbf{y}}(\mathbf{x}_{j_u}, \mathbf{W}_{q_u})$. We formally define each element \hat{y}_{r,q_u} of vector $\hat{\mathbf{y}}_{q_u}$ as

$$\hat{y}_{r,q_u} = \frac{1}{L} \sum_{l=1}^L T_r(\mathbf{x}_{j_u}, \mathbf{w}_{q_u,l}),$$

where r is r -th class T_r is r -th element of a decision tree vector.

With the usage of the theory from section 1.3.1 we can write expected loss for Active Learning Random Forest Algorithm as

$$\mathbb{E}_{\pi_u^*} L_u^* = \frac{1}{Q_u} \sum_{q=1}^{Q_u} \sum_{r=1}^R \hat{y}_r(\mathbf{x}_{j_u}, \mathbf{W}_{q_u}) \log(\hat{y}_r(\mathbf{x}_{j_u}, \mathbf{W}_{q_u})). \quad (1.31)$$

Conclusion

Text of the conclusion...

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