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Deep Sequence Modeling for Drug Classification: A Stacked LSTM-RNN Approach to WHO ATC Prediction Stacked

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Abstract

The WHO Anatomical Therapeutic Chemical (ATC) classification system is a generally acknowledged drug classification scheme. The system is divided into five levels, each of which has multiple classes. Drugs were divided into classes based on their medicinal properties and effects. Predicting the drug's ATC code is critical in drug discovery and repurposing. For finding newer association data relating to ATC codes and drugs is still tough. Some compounds or drugs, in particular, may fall into 2 or more ATC classes. We presented a stacked LSTM-RNN model for ATC classification in order to resolve this concern. Thorough cross validation results have shown that staked LSTM achieved better results, compared to results achieved by the traditional ml algorithms which was represented in literature, specifically in AT (absolute true) rate, it is the most harsh and crucial metric for multi label systems.

Keywords: *ATC classification, Stacked LSTM, Multi label classifier, learned features, machine learning.*

INTRODUCTION

ATC (Anatomical Therapeutic Chemical) Classification System defines active compounds in medications based on organ of the body on which they work, their chemical, therapeutic, pharmacological qualities. ATC objective is to help monitor drug use as well as to do research work for enhancing medicine quality. ATC does not imply medication recommendation or efficacy [1].

The older version of ATC Classification System [7], was designed to help the pharmaceutical industry identify pharmaceutical medicines (rather than active ingredients). The EPHMRA (European pharmaceutical market research association) and Intellus created and manages ATC system. ATC was established in 1971 by EPHMRA and is operated by Intellus and EPHMRA. It has four different levels of codes [8]. The WHO's five-level approach is a revision and extension of the EPHMRA's. Improved ATC version was released for the first time in 1976 [2][3][4] by WHOCC (World health organization collaborating centre for drug statistics methodology).

ATC classification system follows a hierarchy [5], which means that each code must have only 1 parent code, with the exception of the 14 top-level codes, it has no parents. The codes are semantics identifier [5], which means they display information (The codes represent the entire lineage of parentage) in addition to functioning as identifiers. ATC has 6,331 codes until May-7-2020; the table 1 below shows its count for each level [6].

Levels in ATC	Different names	Code

First level	14	14
Second level	94	94
Third level	262	267
Fourth level	819	889
Fifth level	4363	5067

Table 1: ATC levels and its code counts for each level

ATC Classification

Drugs are divided into five main classes in ATC classification system [9].

The 1st level of code has one letter, denotes anatomical major category. There were 14 major categories [10], is shown in table 2. (e.g: C represents cardiovascular system). The therapeutic subgroup is indicated by the 2nd level of code, which contains 2 digits (e.g: C03 Diuretics). The pharmacological/therapeutic subgroup is indicated by the level 3 of the code, which contains 1 letter (*e.g*: C03C High ceiling diuretics).

The pharmacological/therapeutic/chemical subgroup is indicated by the 4th level of code, which consisting of 1 letter (e.g: C03CA Sulfonamides). Chemical substance was indicated by 5th level of code, which has 2 digits (e.g: C03CA*01* furosemide).

Code	Contents
V	Various
S	Sensory organs
R	Respiratory system
P	Antiparasitic products
N	Nervous system
M	Musculo skeletal system
L	Immunomodulating and Antineoplastic agents
J	Antiinfectives to systemic use
H	Systemic hormonal preparations
G	Genito urinary system
D	Dermatologicals
C	Cardiovascular system
B	Related to blood
A	Alimentary tract and metabolism

Table 2: Anatomical main categories

Different ATC classification systems available are: ATCvet (Anatomical therapeutic chemical classification system for veterinary medicinal products) for classification of veterinary drugs and HATC (Herbal ATC) is an ATC herbal substance classification.

WHOCC currently creates new drug listings to the ATC classification system solely in responding to requests by users such as regulatory agencies, researchers, and manufacturers, resulting in a severe gap in the system's drug coverage. Prediction of bioinformatics in ATC classification of drugs have recently been possible due to the introduction and aggregation of numerous data sources in drug studies like drug-induced gene expression, target proteins, chemical structures, and side effects[38][39]. The ATC classification prediction for drugs not just, helps to understand chemical, pharmacological, and therapeutic features of drugs, but it also gives useful information for finding drug side-effects and repurposing. Meanwhile, Prediction of ATC classification to chemical compounds is useful in the creation of new drugs, especially when combined with other virtual screening techniques[40][41].

LITERATURE SURVEY

Identifying ATC classifications for new drugs via analytical techniques is typically resource intensive and time taking. As a result, using machine learning approaches to predict ATC classes of a compound in silico is a popular topic in drug development and discovery.

For drug development, the "one drug, one target, one disease" approach was prevalent for a number of years. Many beneficial drugs, such as aspirin, and metformin [11,12], will affect several proteins, which is known as poly-pharmacology. Aspirin, the wonder drug, was first utilized as an anti-inflammatory and antipyretic agent before being used for the prevention of cerebrovascular and cardiovascular illnesses [13]. Aspirin was shown to reduce the risk of colorectal as well as different cancers in the future [14]. Metformin was discovered in 1950 to fight influenza and in 2008 to lower risk of cardiovascular strokes, in addition to its glucose lowering impact [26, 27]. As a result, network pharmacology got established at the perfect time with the mode of "multiple drugs, multiple targets, multiple diseases," which have used in drug discovery and repurposing [15]. Target based reposition is the indirect strategy for drug repurposing that identifies and verifies the target for particular validated therapeutic effects to existed drug [16,17]. Other strategy, which looks for direct effects among phenotypes and molecules, which is known as phenotyping. When compared to target based strategies, phenotype based strategies can skip the time-consuming target-validation procedure instead focuses on pharmacologic or direct therapeutic effects, saving time and money [18].

To predict ATC code, there have been numerous computational methods were developed. SuperPred, a website for target prediction and drug ATC code, was designed by authors in [19] in 2008. SuperPred's fundamental principle is that a drug with same structures has same biological effects. According to the authors, the similarity score of 0.85 or greater will have effective ATC predictions in 81 percent of cases [19]. Authors in [20] used the NLSP (Network Based Label Space Partition) technique to predict ATC code inside a multi label learning method in 2019. This model is on fingerprint and structural similarity of a chemical toward other's related to distinct categories of ATC.

Authors in [21] used random walk and shortest path techniques to estimate fourteen main categories in level 1 of ATC code classification system's. To identify level 1 to level 4 ATC codes, the authors in [22] analyzed SVM, Random Forest, Nave Bayes, Multilayer perception machine-learning methods on tiered-learning architecture. The authors in [23] developed dD-hybrid in 2015 as a method for predicting ATC code by adding drug's domain interaction network knowledge for prediction model. The authors found, medicines having similar domains will also have similar ATC codes.

The authors in [24] provided the dataset that they used. Authors discovered that approximately 75 percent of drug pairings will have shared similar ATC codes, when the target protein and chemical structure similarity scores greater than 0.8. The authors in [25] used SVM (support vector machine) to predict relationship between ATC code and drugs.

As per a recent detailed analysis in [28], we must examine the following techniques in order to develop a truly meaningful statistical predictor for the biological system:

1. Create or choose a suitable benchmark dataset for train and test the predictor;
2. Formulate a mathematical equation for samples that accurately reflects their intrinsic connection with target needed to get predicted.
3. In order to handle the prediction, construct or introduce a sophisticated engine/algorithm.
4. Cross validation tests should be used to properly validate the predictor's expected accuracy.

In the methods section, we'll go over each of these phases one after another.

Methods and results discussion

We proposed a ATC classification system in this paper, with stacked LSTM by combining multiple datasets and had different data like chemical to chemical associations, chemical structures, drug induced gene expression, side-effects, and target proteins. And also assessed its efficacy, accuracy with the goal of improving performance of ATC classification.

Descriptors and Data sets

The data set in [29] is fed into the proposed method. This data set consists of 3883 ATC-code drugs extracted from KEGG [31], a freely accessible drug database. A compound can only belong to six classes at a time. There are 4912 drugs having multiple labels in total. The drugs from the datasets are represented by the descriptors such as NRAKEL defines the drug using the 700D descriptor generated by Mashup algorithm [33], where it

produces output from 7 drug networks (2 on drugs similarity and 5 on chemical to chemical interaction). DDI assigns 3 mathematical equations to every drug, which has optimum structured similarity score, greater interaction scoring rate with drugs, and similarity score of molecular fingerprint, for each equation based on its relationship with level 1 of 14 major classes. As a result, resulting descriptor has the size 14*3[30]. FRAKEL presents every drug using ECFP fingerprint [32], is a 1024D binary vector. Drug is fed in to the RDKit, which is an open access ML toolbox to chemistry informatics, for obtaining the descriptor. The 64D categorical descriptor has been extracted from the 1024D binary vector, for every group represented in 16-bits integer.

Stacked LSTM based Operation Algorithm

Currently, LSTM neural-network is used to solve a variety of real-time problems such as speech processing, image labeling, machine translation, and sequence data analysis. The purpose of the paper is to predict the ATC classification of drugs using an LSTM neural-network for multi label classifiers. All the multi label classifier were trained on NRAKEL, DDI, and FRAKEL descriptors. Long short term memory units [34] were utilized to tackle RNN (Recurrent Neural Networks') vanishing gradient problem [35]. The LSTM uses 3 gates to determine what content is stored in the memory cell. Those same gates apply logistic functions to input's weighted sum. Back propagation is used to learn weights [36]. Forget and input gates will be in charge of handling cell state as well as providing the capacity to recall/remember for an extended period of time. This is denoted by equations below:

$$\begin{pmatrix} i_t \\ f_t \\ o_t \end{pmatrix} = \begin{pmatrix} \sigma(W_i[x_t, h_t - 1] + b_i) \\ \sigma(W_f[x_t, h_t - 1] + b_f) \\ \sigma(W_o[x_t, h_t - 1] + b_o) \end{pmatrix} \rightarrow (1)$$

$$c_t = f_t * c_{t-1} + i_t * \bar{C_t} \rightarrow (2)$$

$$h_t = o_t * f(c_t) \rightarrow (3)$$

Here,

o_t - output gate

f_t - forget gate

i_t - input gate

$\bar{C_t}$ - network candidate

σ - sigmoid function

x_t - current input at step t (time)

* - element wise multiplication

Four state vectors were: c – memory state, c_t - previous memory state, h_t- hidden state, h_{t-1} - previous hidden state

LSTM also includes a Tanh activation function for single layer network candidate $\bar{C_t}$. Activation functions [37] do non-linear transformation on previous layer's output before transferring to next layer.

Y = Activation $(\sum(\text{Weight} * \text{input}) + \text{bias})$ → (4)

Following is the procedure to update LSTM at t (time). By the given x_t , h_{t-1} and network's learnable weights U, b, then candidate layer $\bar{Ct}$ is

$$\bar{C_t} = Tanh(Uc\ x_t + Wc\ h_t - 1 + bc) \rightarrow (5)$$

The next memory cell is represented in equation 2. The output is the equation 3 of o_t as well as sigmoid of c_t. In terms of input, sorting input is not necessary, as all sequences were of same length. LSTM output will either be sequence last term or h_t (entire sequence). Parameters considered to train 2 stacked layers with similar sample sets were: mini-batch size is 27, number of classes are 14, number of hidden units are 100.

LSTM feature extraction is achieved by each pattern with activations from final layer, resulting in the feature vector by the dimension equals the total classes (14). Feature extraction is repeated multiple times by sorting original feature sets (utilized while training LSTM) randomly.

Classification By HML

The authors in [38] proposed the multi label classifier which combines the neighbor score and feature score. With global information available for entire training set, feature score determines whether the sample refers to a specific class or not. Neighbor score, on the other hand, determines class labels for samples which is dependent on assignment of class for its neighbors. By the regression model, feature score f1(x, g_j) feature score for the given pattern x to the g_j (anatomical group) has been estimated in order to determine that pattern relates to group g_j or not. Neighbor score f2(x, g_j) computes the importance of K neighbors' class membership to the pattern belongs to the particular group g_j. Neighbor score gets increased when there are higher x (neighbors) have more g*j* labels. Thereby, f2(x, g_j) is 1 when all of x's neighbors are related to g_j, and 0 otherwise.
Final x score is the weighted sum of 2 factors:

$$f(x,) = \alpha f1(x,gj)+(1-\alpha)f2(x,gj) \quad \rightarrow \quad (6)$$

Here,
k – represent number of neighbors
α – weight factor
For the proposed method we have used k value as 15, α with 0.5 as the default values.

Testing protocol

In order to obtain train as well as test sets, jackknife test protocol has been used. For the every iteration, 1 sample was put in test set and rest all samples in train set in jackknife test. The iteration process is repeated till every pattern had a shift in testing set [39].

Performance measures

Performance measures described in [39] were used to evaluate ATC classification is specified below. If 2 sets had same elements, then Δ return 1 else 0.

$$\text{Absolute False} = \frac{1}{N}\sum_{k=1}^{N}\left(\frac{||L_K \cup \acute{L_K}|| - ||L_K \cap \acute{L_K}||}{M}\right) \quad \rightarrow \quad (7)$$

$$\text{Absolute True} = \frac{1}{N}\sum_{k=1}^{N}\Delta\left(L_K, \acute{L_K}\right) \quad \rightarrow \quad (8)$$

$$\text{Accuracy} = \frac{1}{N}\sum_{k=1}^{N}\left(\frac{||L_K \cap \acute{L_K}||}{||L_K \cup \acute{L_K}||}\right) \quad \rightarrow \quad (9)$$

$$\text{Coverage} = \frac{1}{N}\sum_{k=1}^{N}\left(\frac{||L_K \cap \acute{L_K}||}{||L_K||}\right) \quad \rightarrow \quad (10)$$

$$\text{Aiming} = \frac{1}{N}\sum_{k=1}^{N}\left(\frac{||L_K \cap \acute{L_K}||}{||\acute{L_K}||}\right) \quad \rightarrow \quad (11)$$

Here,
$\acute{L_K}$ - predicted label
L_K - true label
N – total sample numbers
M – total classes

Achieved results by the proposed method

Classifiers like LIFT (Label-specific features, LSTM, HML (Hybrid multi label) were trained on NRAKEL, DDI, and FRAKEL descriptors and attained absolute true rates is shown in table 3. The proposed ensemble RNN-LSTM with HML has achieved 0.85 accuracy, 0.81 absolute true, 0.0129 absolute false, 0.93 aiming, 0.85 coverage.

Table 3: Attained absolute rates for the classifiers

Absolute True	**NRAKEL**	**FRAKEL**	**DDI**
LIFT	0.54	0.37	0.63

HML	0.71	0.61	0.59
LSTM	0.66	0.65	0.69

CONCLUSION

ATC (Anatomical Therapeutic Chemical) Classification System defines active compounds in medications based on organ of the body on which they work, their chemical, therapeutic, pharmacological qualities. ATC objective is to help monitor drug use as well as to do research work for enhancing medicine quality. Predicting the drug's ATC code is critical in drug discovery and repurposing. Some compounds or drugs, in particular, may fall into 2 or more ATC classes. To address this problem, proposed a ATC classification system in this paper, with stacked LSTM for multi label classifiers by combining multiple datasets and had different data like chemical to chemical associations, chemical structures, drug induced gene expression, side-effects, and target proteins. All the multi label classifier were trained on NRAKEL, DDI, and FRAKEL descriptors. Features extracted from LSTM were fed to HML for the multi label classification. In order to obtain train as well as test sets, jackknife test protocol has been used. The evaluations were put to the test against a benchmark data set consists of 3883 ATC-code drugs extracted from KEGG. The proposed ensemble RNN-LSTM with HML has achieved 0.85 accuracy, 0.81 absolute true, 0.0129 absolute false, 0.93 aiming, 0.85 coverage. In future, we wanted to improve the accuracy further.

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