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Denoising Autoencoder based Long non-coding RNA-Disease Association Prediction

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Abstract

Long non-coding RNAs (lncRNAs) are recent listing in RNA Bioinformatics, which is getting more popular due to their important functional roles. According to the available research, lncRNAs play an essential role in multiple complex diseases. Determining the function of lncRNAs in diseases will help to comprehend many missing links in the disease mechanism. Predicting lncRNA-disease association (LDA) is a crucial stage in this process which is getting at most research interest nowadays. The developments in machine learning and deep learning technologies influenced recent research on LDA models. Most of the methods analyse the interactions of lncRNA with other molecules such as microRNA (miRNA), messenger RNA(mRNA), and proteins. Deep learning models, specifically from autoencoder classes, used extensively in unsupervised learning of features from these associations. This research paper proposes a denoising autoencoder (DAE) based LDA prediction approach. The proposed model uses DAE to learn lncRNA-disease representations from multiple biological networks such as lncRNA-miRNA, miRNA-disease, and disease-lncRNA interactions. The experiments show that the model outperforms other state-of-the-art LDA models concerning the area under the ROC curve (AUC-ROC, 0.94) and the area under precision-recall (AUPR, 0.9592).

Keywords: Long non-coding RNA; Autoencoder; Denoising autoencoder; Representation learning; Deep learning; Function similarity network;

1. Introduction

Central Dogma of Molecular Biology views RNAs as arbitrators between DNA and proteins. The human genome project and studies on genome organism sequencing have identified an unusual amount of biological transcripts. Although most of them do not translate into proteins, they play an essential role in synthesizing and regulating trans-

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lation. Such transcripts are called non-coding RNAs (ncRNA), and long non-coding RNAs (lncRNAs) are recent entries. Identifying and analysing the biological significance of ncRNAs is a new challenge in Bioinformatics.

Long non-coding RNAs are ncRNA transcripts with length more than 200 nucleotides [6]. It is reported that lncRNAs regulate a wide range of biological processes, and any dysregulation leads to complex diseases such as cancers, heart failure [21], malignancies [10] and Alzheimer's disease [14]. Therefore, determining the role of lncRNAs in diseases will aid in better understanding disease mechanisms and bring new insights into their treatments. Though the knowledge about lncRNA functionalities is incomplete, it is understood that lncRNA interactions with other molecules like DNA, protein, and other ncRNAs (like microRNA) have a significant role in the disease mechanisms. Researchers are still tackling the issue of developing a better lncRNA-disease association model.

This paper proposes a denoising autoencoder (DAE) based model for LDA prediction task. Autoencoders are popular deep learning models for unsupervised representation learning. Denoising models, a variant of autoenders improve the learning capability of the autoencoder by introducing noise in the input. DAE-based models have successfully been employed to predict drug-target interactions and phenotype prediction yet have not been used to predict LDA. Following the architecture of DBNLDA [16], the proposed model uses a multi-modal network approach by constructing individual interaction networks for lncRNA-miRNA, disease-miRNA, and lncRNA-disease. Stages of denoising autoencoders learn lncRNA-disease representations from these networks. A classifier takes these representations to predict the association. Evaluations show the proposed model outperforms several recent LDA models in terms of Area under the ROC curve (AUC-ROC) and Area under the Precision-Recall curve (AUPR).

The main objectives of this paper are as follows:

1. Propose a denoising autoencoder based model lncRNA-disease association prediction.
2. Compare the effectiveness of various autoencoder models in LDA prediction.

The rest of the paper is organized as follows. A technical background of autoencoders and DAE are discussed in the following subsections 1.1 and 1.2. Section 2 presents a comprehensive review of deep learning based LDA prediction models. Section 3 discusses the proposed architecture. Experiments and results are discussed in Section 4, and Section 5 concludes the paper.

1.1. Autoencoder

An autoencoder(AE) is a feed forward, non-recurrent neural network that uses an input layer and an output layer coupled with a stack of hidden layers. Input layer and output layer have same number of neurons. Autoencoders learn to reconstruct the given input at the output nodes using two functions encoder and decoder. Encoder function takes a vector $\mathcal{G} \in \mathbb{R}^n$ as input and maps to a p-dimensional hidden representation $\mathbf{h} \in \mathbb{R}^p$ such a way that $\mathbf{h} = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b})$, where $\mathbf{W}$ and $\mathbf{b}$ are the learning parameters, σ is a non-linear activation. The function of decoder is to reconstructs the input from the $\mathbf{h}$. Let $\mathbf{X}'$ is the output of decoder reconstructed.

In the decoder part the $\mathbf{h}$ gets reconstructed back to $\mathbf{G}^{'}$ where $\mathbf{G}' = \sigma'(\mathbf{W}'\mathbf{h} + \mathbf{b}')$. $\mathbf{W}'$,$\mathbf{b}'$ and σ' are the parameters of the decoder. The Equation 1 shows the computation of reconstruction loss in the autoencoder.

$$\mathcal{L}(\mathbf{G}, \mathbf{G}') = \left\|\mathbf{G} - \mathbf{G}^{'}\right\|^2 = \left\|\mathbf{G} - \sigma'(\mathbf{W}'(\sigma(\mathbf{W}\mathbf{x} + \mathbf{b})) + \mathbf{b}')\right\|^2 \tag{1}$$

Once the autoencoder model is trained, the representation learned by encoder can be used as latent features for further machine learning tasks [15, 9, 19].

1.2. Denoising autoencoder

Denoising autoencoders (DAE) is a variant of standard autoencoder. which try to improve the reconstruction function by introducing a noise factor in the input data [7]. Using this algorithm,the given input $\mathcal{G}$ was corrupted by applying stochastic mapping techniques to $\mathcal{G}'$. The corrupted input $\mathcal{G}'$ is then transformed to a latent space using the conventional standard autoencoder algorithm as discussed in Section 1.1. Further, the model reconstructs the noise

free input from the hidden representation at the output. Additive isotropic Gaussian noise is one example through which the input data gets corrupted while training. In addition to compressing data(like a standard autoencoder), a denoising autoencoder learns to eliminate noise signals from data. This makes DAE to learn better data representation than ordinary autoencoder.

Nomenclature

ϕ	Encoder part of autoencoder.
ψ	Decorder part of autoencoder.
$\mathcal{X}$	Input vector to autoencoder.
$\mathcal{F}$	Decomposed latent varibles.
$\mathbf{W}$	Weight vector of autoencoder.
$\mathbf{b}$	Bias vector of autoencoder.
σ	Activation function.
L_{lm}	Embedding feature matrix from LM network.
D_{dm}	Embedding feature matrix from DM network.
LD_{ldm}	Combined feature matrix from LM and DM.
LD_{ld}	Embedding matrix from LD network.
LD_{dae1}	Output features from denoising autoencoder subnetwork1.
LD_{dae2}	Output features from denoising autoencoder subnetwork2.
LD_{dae}	Output features from combined DAE network.
LD_v^{at}	Recalculated embedding matrix after passing through attention layer

2. Related Works

An array of computational methods, mainly from the machine learning genre, for the lncRNA-disease Association (LDA) prediction have been proposed in the literature, with varying degrees of effectiveness. Initial models for LDA were trying to characterize lncRNA-disease association by building a lncRNA functional similarity network. For example, methods such as IRWRLDA [3], RWRlncD [20], and BRWLDA [27] were proposed the use of various random walk algorithms for LDA prediction. More recent studies used a diversified interaction of lncRNAs and diseases with messenger RNA(miRNA), lncRNA, and micro RNA (mRNA). These interactions were usually represented as networks, and features were extracted using various graph-theoretical properties. Finally, the analysis used machine learning algorithms like SVM [11], Random Walk [25], and Laplacian regularised least square approach. However, the appropriate modeling of lncRNA-disease characteristics was intricate in the above mentioned methods.

The introduction of deep learning models enabled unsupervised representation learning, eliminating the necessity for feature extraction. Deep learning based LDA models generally uses a model for learning the representation of lncRNAs and diseases from heterogeneous interaction networks. For example, CNNLDA [23], and GCNLDA [24] used CNNs and GCNs to learn latent features of diseases, lncRNAs, and miRNAs. Similarly, GAMCLDA [22] employed graph autoencoder and matrix completion technique to develop a lncRNA-disease association. The use of Deep Belief Networks (DBN) to predict the lncRNA-disease association was discussed in [16]. Researchers are experimenting with new deep learning models to improve the prediction and optimize the model parameters.

3. Materials and Methods

Similar to the architecture used in [16], the proposed architecture uses functional similarity, co-expression and known lncRNA-disease interactions to make predictions. The methodology contains 3 main stages namely- (i) construction of interaction networks, (ii) DAE based feature learning, and (iii) LDA prediction. The architecture of the proposed model is shown in Fig 1.

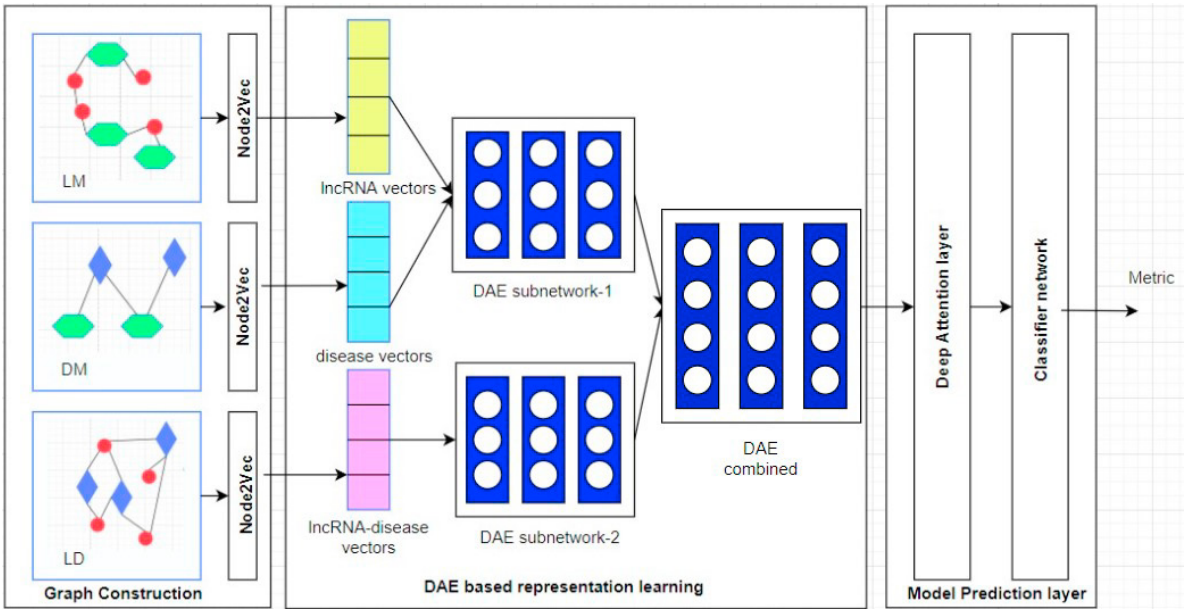

Fig. 1. Proposed architecture of DAE based lncRNA-disease association prediction

3.1. Dataset

Dataset used in recent works [23, 24, 16] are used for getting lncRNA, miRNA, and disease interaction. The lncRNA-disease interactions were collected from LncRNADisease [1], lnc2cancer[17] databases. Similarly the miRNA interactions with lncRNA and disease were collected from Starbase[12], and miRNet[4] databases. All the collected interactions and associations consist of 412 diseases , 495 miRNAs and 240 lncRNAs. The datasets contains 2697 experimentally validated interaction between lncRNA and diseases, which constitutes the positive samples. All the other lncRNAs-disease pairs, not in the positive samples are considered as negative samples. To make the dataset balance, we randomly picked 2697 negative interaction pairs.

3.2. Construction of interaction networks and node embedding

The initial process in the proposed method is the development of three networks : lncRNA-miRNA (LM), disease-miRNA (DM) and lncRNA-disease (LD). Let *dn*, *mn* and *ln* respectively be the number of diseases, miRNAs and lncRNAs. LM network is constructed based on lncRNA-lncRNA similarity and lncRNA-miRNA interactions. Similarly, disease-disease similarity and disease-miRNA interactions are used for the constructions of DM network. While construction of the above networks, functional similarities between lncRNAs and miRNAs are estimated using Chen's method [2]. According to this method, a positive similarity score between two nodes is represented by an edge in the network. In the construction of LD network, an undirected edge represents the known, experimentally validated lncRNA-disease association.

To further process these networks using deep learning models, the above networks need to be embedded into a vector space. Node2Vec [8] algorithm is used to create node embeddings from each networks. Node2Vec creates embedding vectors from the networks through neighbourhood information. Initially, *LM* network is passed through Node2Vec algorithm and the embedding matrix for lncRNA, represented as $L_{lm} \in \mathbb{R}^{ln \times j}$, is calculated, where j is the embedding dimension. For diseases, similar embedding feature matrix is obtained from *DM* network,represented as $D_{dm} \in \mathbb{R}^{dn \times j}$. For each disease-lncRNA pairs (say *l-d*) in the dataset, lncRNA vector from L_{lm} and disease vectors from D_{dm} are concatenated to get combined matrix $LD_{ldm}[ld] \in \mathbb{R}^{2j}$. The resultant embedding matrix can be represented as $LD_{ldm} \in \mathbb{R}^{n \times 2j}$, where n is the total number of lncRNA-disease pairs in the dataset. Similarly, the embeddings obtained from LD network can be represented as $LD_{ld} \in \mathbb{R}^{n \times 2j}$ embedding matrix.

3.3. DAE based representation learning

Denoising autoencoder (DAE) based feature learning is implemented after the Node2Vec embedding layer. DAE is used in this work to project the lncRNA and disease nodes to another latent dimension i ,where $i \geq j$. The work follows a multi-modal learning approach, where two DAE subnetworks are used to learn lncRNA-disease features. The *DAE subnetwork-1* takes LD_{ldm} as input, added with a mixture of Gaussian noise with 0.2 noise factor, and generates $LD_{ldm'}$ as output. Likewise, *DAE subnetwork-2* receives LD_{ld}, with same Gaussian noise, and generates $LD_{ld'}$ as output. The combined embedding features are then passed into a third DAE (named as *DAE combined*) and generates $LD_{dae'} \in \mathbb{R}^{n \times x}$, as the final representation of lncRNAs and diseases.

3.4. Attention layer for features

There is a risk of losing feature relevance in the representation learnt by the DAE layers since the architecture uses sparse networks. The attention mechanism is used to tackle this problem by recalculating feature from the available data so that their importance might be unique. Here, $LD_{dae'} \in \mathbb{R}^{n \times x}$, feature matrix learnt by *DAE-combined* is applied with an attention technique similar to that used in previous work [16]. Let $LD_{dae'_v} = \left[ld_v^1, ld_v^2, \ldots, ld_v^{x'}\right]$ represents the v^{th} entry in the data after DAE based learning, where $ld_v^k \in \mathbb{R}, \forall k = 1, 2, \ldots x'$. For $LD_{dae'_v}$, the attention score for each element is computed based on equation 2.

$$\alpha_v^{at} = Soft\max\left(H^{at} \cdot \tanh\left(W^{at} LD_v + b^{at}\right)\right) \tag{2}$$

where $H^{at} \in \mathbb{R}^{x' \times x'}$, $W^{at} \in \mathbb{R}^{x' \times x'}$ and $b^{at} \in \mathbb{R}^{x'}$ represents the attention weight parameters for the calculation of the updated score. Then the updated feature values are recalculated using equation 3.

$$LD_v^{at} = \alpha_v^{at} \otimes LD_{dae_v} \tag{3}$$

For association prediction, the matrix LD^{at} is given as an input.

3.5. Prediction Module

The final component in the proposed architecture is an ANN classifier that predicts the lncRNA-disease association. The module has 1-2-1 structure, with x nodes receiving input from LD^{at} and a single neuron predicting the association score at the output layer.The association score is estimated using a sigmoid function in the output layer. The network employed a binary cross-entropy loss and an ADAM optimizer with a learning rate of 0.001. All layers except the output used ReLu as activation function.

3.6. Hyperparameter tuning

The performance of the proposed model is determined by a number of hyperparameters such as node embedding dimension, number of nodes in DAE, and number of nodes in the hidden layer of classifier module. Hyperparameter tuning was performed systematically using grid search method to optimize the performance of the model. Based on the experiments, embedding dimension in Node2Vec was fixed as 64 and rest of the values were kept as reported in [8]. The number of input nodes in DAE subnetworks were taken as 128 and that of the DAE combined was 256. Higher scores were obtained while changing the no of epochs (30,40,50,100 and 200) in the neural network-based classifier. Figure 4 depicts the summary of AUPR scores obtained while doing hyperparameter tuning of the proposed model .

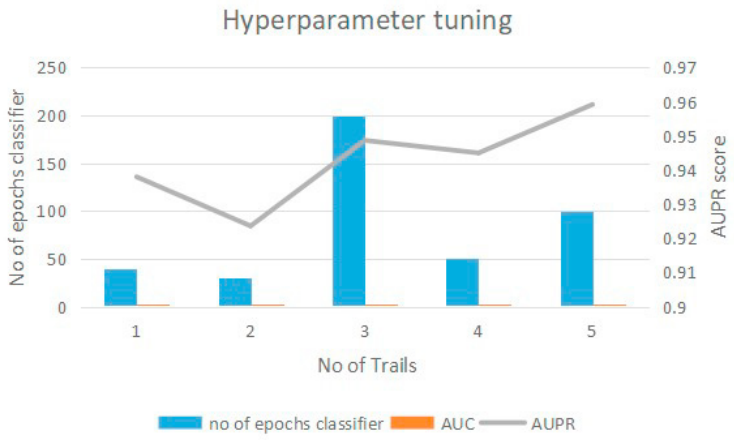

Fig. 2. Hyperparameter tuning of proposed model

4. Experiments and Results

4.1. Experimental Setup

The performance of the proposed model was evaluated using AUC-ROC and AUPR scores over 5-fold-cross validation, as explained in [16]. A detailed comparison with state-of-the-art deep learning models were conducted on the same dataset. To analyse the effectiveness of autoencoder based feature learning models for LDA prediction, experiments were performed with stacked autoencoders and denoising autoencoders. The implementation of both stacked and denoising autoencoder models were done using tensorflow library. We tried experiments on two network approaches: single-stage (SS) and multi-modal (MM) architectures. The SS architecture had a single combined network of lncRNA-disease-miRNA and a single feature learning algorithm. Multi-modal approach is explained in the previous section.

4.2. Results

4.2.1. Results of the proposed model

The DAE subnetworks were trained for 100 epochs and the loss-epoch graph (shown in Figure 3) showed compatible behaviour throughout the cross validation. The proposed model reported an average AUC of 0.9479. The model gave an average accuracy of 0.9479 and AUPR score of 0.9592. Figures 3 and 4 depict a summary of the performance of the model in 5-fold cross-validation.

4.2.2. Comparison with state-of-the-art methods

The proposed model was compared with other methods such as LDAP [11], GCNLDA [24], MFLDA [5], Ping's Method [18] , SIMCLDA [13], CNNLDA [23], RFLDA [26] and GAMCLDA [22] on the basis of AUPR and AUC-ROC scores. The above methods follow a network based feature learning approach for lncRNA-disease association prediction. A through analysis of the performance of these methods with the proposed model shows the proposed DAE based model gave near best performance with reference to AUC (second rank) and best performance based on AUPR scores. The results of the comparison are shown in Table 1. The AUC value of the proposed model is very close to the highest reported result from random forest based lncRNA-disease association (RFLDA, 1.1% less) and higher than rest of the methods. In terms of AUPR value, the suggested model outperforms all other techniques with a score of 0.9592 (18 % more than RFLDA) as shown in Table 1. Thus, these results proves the efficiency of the proposed DAE based learning for predicting lncRNA-disease association.

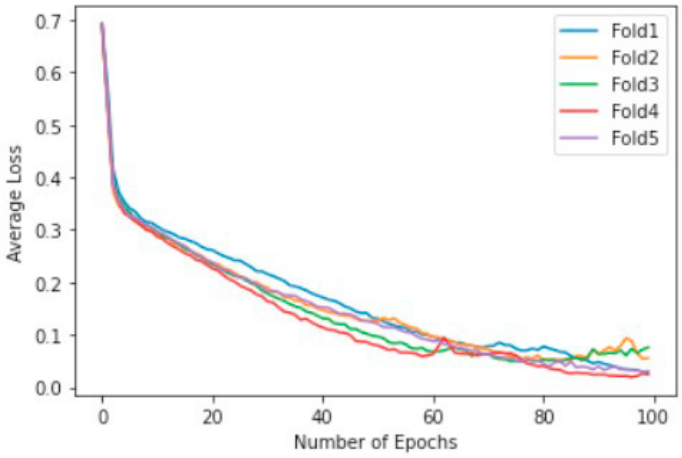

Fig. 3. Learning curve of proposed model over five-fold cross validation

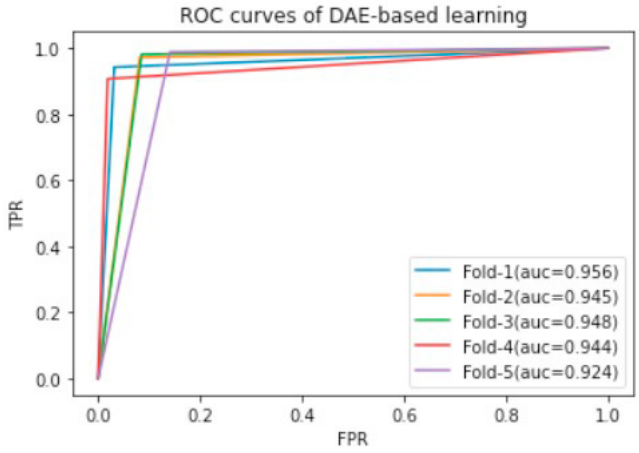

Fig. 4. ROC curve of DAE based learning

Table 1. Comparison with state-of-the-art methods

Methods	AUPR	AUC
MFLDA [5]	0.066	0.626
SIMCLDA [13]	0.095	0.746
LDAP [11]	0.166	0.863
Ping's Method[18]	0.219	0.871
GAMCLDA[22]	0.037	0.907
CNNLDA[23]	0.251	0.952
GCNLDA[24]	0.223	0.959
RFLDA[26]	0.779	0.976
Proposed model	**0.959**	**0.948**

4.2.3. Comparison with different AE models

To analyse how DAE-based representation learning increases the performance of the model predictions, experiments were repeated on different AE models such as stacked autoencoders and DAE. Results in Table 2 explicitly show that the incorporation of DAE-based learning considerably increased the model performance. It was also ob-

served that the number of parameters used in denoising autoencoder(DAE) was comparatively less than that of stacked autoencoder(AE).

A comparison between single-stage and multi-modal approach also conducted. It is evident from Table 2 that the proposed multi-modal approach has better performance in both stacked AE and DAE. Studies also shows that splitted networks (LM,DM and LD) based feature learning have higher model performance and accuracy.

Table 2. Results of experiments on various AE models

Experiments	Features	AUC	AUPR
Exp1	Single-stage(AE)	0.53	0.751
Exp2	Single-stage(DAE)	0.6581	0.749
Exp3	Multi-modal,subnetwork-1(AE),subnetwork-2(AE),combined(AE)	0.701	0.793
Exp4	Multi-modal,subnetwork-1(DAE),subnetwork-2(DAE),DAE	0.9479	0.959

5. Conclusion

This paper proposed a denoising autoencoder based model for predicting lncRNA-disease associations. The model learned lncRNA-disease representations from heterogeneous networks formed from interactions and functional similarities between lncRNAs, miRNAs, and diseases. A multi-modal approach with combinations of denoising auto encoders were used to extract lncRNA-disease representations from above networks. The experimental analysis and evaluations confirm that the proposed model achieves a comparable performance with the contemporary methods for LDA prediction. To highlight this further, a comparative study of various autoencoders for LDA were experimented. The proposed work can be enhanced with more biological interactions such as protein-lncRNA and protein-diseases. Experiments can be extended with recent developments in graph based neural networks.

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