# PH.D. RESEARCH PROPOSAL

# SEQUENCE LEARNING USING DEEP NEURAL NETWORKS WITH FLEXIBILITY & INTERPRETABILITY

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# 1   Aims & Objectives

1. Flexibility in modeling complex patterns with long-range dependencies

   (a) Capturing complex non-linear correlations without prior knowledge and assumptions

   (b) Encoding high dimensional input variables adaptively

   (c) Discovering long term dependencies of encoded inputs

2. Network architectures with better computational properties

3. Decoding/Encoding human intepretable representations from/into models

   (a) Approximating deep neural networks' input-output relationships using human intepretable models

   (b) Learning deep neural networks coupled with structured (potentially predefined) latent variable sequence

# 2   Synopsis

This project is focused on investigating sequence data learning using deep learning networks. We divide this project into three phases. We first aim to solve long-term dependencies issues by investigating RNNs based encoder-decoder models with attention mechanism. Then we will try to generalize those algorithms into broader network topologies such as CNNs and feed-forward networks to achieve better computational performance. The last goal of this project is to improve the interpretability of deep learning networks by using conventional human friendly machine learning techniques such as lasso regression, random forest and graphical models.

# 3   Background And Literature Review

One interesting task in machine learning is modeling complex sequences having long-term dependencies. Many applications such as machine translation, complex dynamical system analysis, activity recognition and behavioral phenotyping tools for neuro-science involved with capturing non-linear patterns in sequences. Sequence learning mainly have three difficulties: approximating non-linear relationship among sequences, feature selection and capturing long-term dependencies. Our primary aim of this proposal is mainly focused on demonstrating those three difficulties.

Despite substantial effort has been made for modeling sequences, many of those models are either unable to approximate non-linear relationships or have rigid assumptions due to the dependency on predefined form of prior function. For example, autoregressive moving average (ARMA) model [6] cannot capture non-linear relationships. Probabilistic Graphical Models [9, 10] (PGMs) are very well studied for the past decades. However, capabilities of approximating non-linear patterns of PGMs are also severely suffered from rigid assumptions over priors.

Deep Neural Networks [5] (DNNs) are powerful and flexible models that have outperforming performance on various difficult learning tasks. Despite the powerful capability of approximation, one significant limitation of DNNs is that they require fixed dimension of inputs and targets. Sutskever et al. [13] in 2014 demonstrated this difficulty as sequence to sequence problems. They introduced an encoder-decoder framework based on two Recurrent Neural Networks (RNNs) and achieved a very successful result in machine translation. The key ideas (as shown in Figure 1) behind encoder-decoder networks and its variants are that they first encode the whole sentence of words into a single, fixed length variable using encoder network. Then a decoder
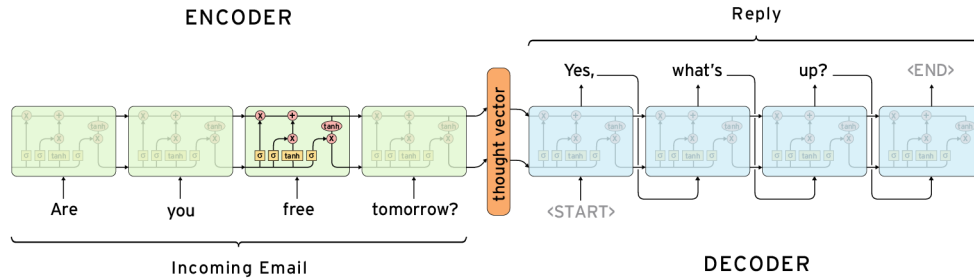
Figure 1: Encoder-Decoder Network

network is used to decode that variable and generate translation. One major drawback is that "indeed the performance of a basic encoder–decoder deteriorates rapidly as the length of an input sentence increases [1]". Since for many sequence learning applications there exists many long-term dependencies relationships, the question of solving this drawback remains open.

Other than long-term dependencies difficulty, DNNs contain a very large number of latent variables which make the training results very hard for a human to interpret [5]. Being able to explain the reasons behind such models plays a crucial role in tasks such as model comparison and deployment. It could also provide insights into the data set and model itself. Thus improving the interpretability of DNNs could also be a very interesting topic to investigate.

# 4 Proposed Methodology

We divide this project into three phases.

To commence we will investigate the mechanism of long-term dependencies in time-series and how to model them using deep neural networks. We will also investigate optimization algorithms which can jointly optimize neural networks together with feature selection.

With optimization algorithms in hand, at the second stage we will try to extend those algorithms into various network topologies such as CNNs and simple feed-forward neural networks. The goal of the second stage is to investigate novel network topologies which can preserve good approximation performance while having better computational properties, such as parallelization.

At the final stage, we will explore a large group of conventional machine learning methods (lasso regression, random forest, graphical model, etc.) aiming at explaining the learning results of neural networks. Outcomes at this stage not only improves the interpretability of neural networks but also give insights on how to encode expert prior knowledge into neural networks.

## 4.1 Modeling Long-term Dependencies And Feature Selection

As discussed in section 3, encoder-decoder networks based on RNNs outperform many other statistical machine learning models while suffering from short-term memories due to encoding global information into a single fixed length variable. One of the most popular ways is to introduce "attention mechanism" into encoder-decoder networks [1].

Bahdanau et al. [1] demonstrated long-term dependencies issue by introducing context vectors in the middle of encoder network and decoder network (as shown in Figure 2). Instead of encoding the global information into a single variable, attention mechanism enables encoder network to provide a sequence of encoded vectors on which decoder network can do soft-searches. As a result, decoder network is able to concentrate on the most relevant infor-
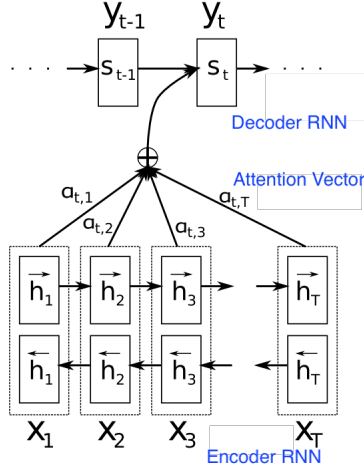
Figure 2: Attention Mechanism

mation represented by a subset of encoded vectors of arbitrary length. Thus encoder-decoder networks can have much better performance when dealing with long-term dependencies.

Qin et al. [11] extended Bahdanau et al. [1]'s work to adaptively select most relevant hidden states as well as most significant features simultaneously. They developed a dual stage RNNs (see Figure 3). Other than attention vector between encoder and decoder layer (so called "Temporal attention Layer" in Figure 3(b)), they adaptively weights input sequence $x_t^k$ which is the $k$th feature at $t$ step by attention $\alpha_t^k$ (see Figure 3(a)). The input attention mechanism is a feed-forward network. Thus the extended encoder-decoder network can weight features according to their importance while the whole network can still be trained jointly. However, their work is focused on regression. We will further investigate their methods by extending to classification cases.

(a) Input Attention Mechanism
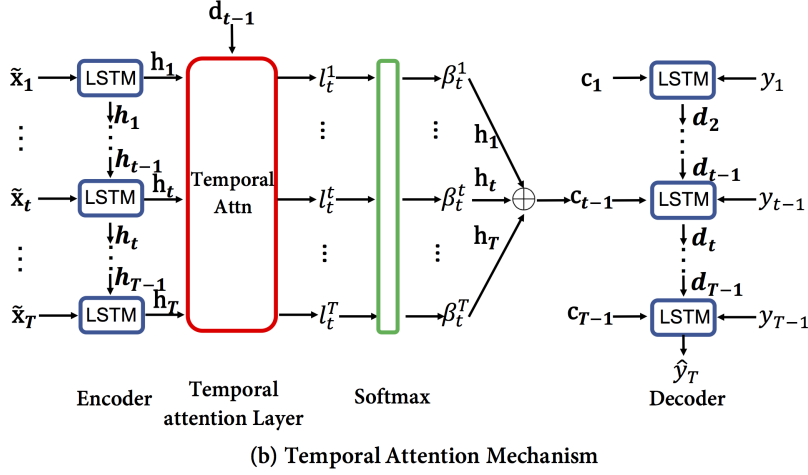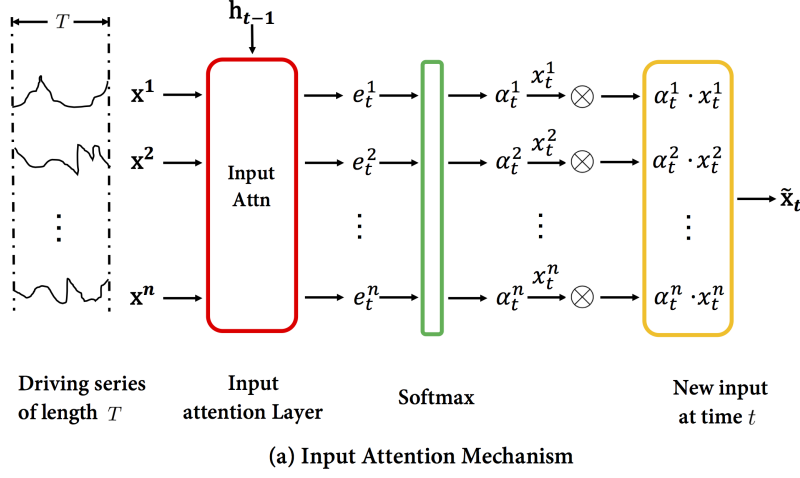


(b) Temporal Attention Mechanism

Figure 3: Dual-Stage Attention Based RNN

## 4.2 Topologies With Better Computational Properties

One major drawback of RNNs is computationally expensive. RNNs usually have a very deep recursive structure. It maintains hidden states of the entire past which prevents parallel implementation of the algorithm. On the contrary, Convolutional Neural Networks (CNNs) have a hierarchical structure and can fully exploit the GPU hardware by using parallel computing techniques. Gehring et al. [3] attempted to replace RNNs with CNNs in sequence modeling task by using a hierarchical structure CNNs. They captured correlations in length of $n$ sequence by applying $\mathcal{O}(\frac{n}{k})$ convolutional operations for kernels of width $k$ and constructed both of encoder and decoder networks using CNNs. Results of their model are slightly better than conventional encoder-decoder networks [1] on multiple data set but with a huge decreasing in training time.

Recently, numerous pure attention architecture have been proposed and achieved the state-of-the-art results in natural language processing problems. Vaswani et al. [14] dispensed CNNs and RNNs entirely and proposed a self-attention-based model. They extends the conventional attention mechanism to a so-called Multi-Head Attention (MHA) architecture by allowing each head to generate different distributions over encoder output. This novel network architecture has very concise topology representation and outperforms both RNNs and CNNs based sequence to sequence [14] models.

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In this project we plan to further investigate those network topologies. Besides, the question of creating attention mechanism in input layers (feature selection) in those architectures still remains open.

## 4.3  Interpretability

Substantial effort has been made for improving DNNs interpretability in recent years. There are mainly three different types of approaches:

- Explain local predictions directly

- Approximating DNNs using human interpretative models

- Joint learning probabilistic graphical models with DNNs

Ribeiro et al. [12] proposed a Local Interpretative Model-agnostic Explanations (LIME) method to interpret arbitrary machine learning models directly by explain individual outputs. They tried to approximate a human interpretative local estimator (Lasso in their case) by sampling around models' outputs and explain the reason behind those decisions by observing which features (input) are taking most responsibility in the local estimator. However, such approaches are limited to providing explanations for individual decision. A more challenging task would be providing a global insights of models.

Instead of explaining local predictions, Frosst and Hinton [2] use the DNNs to train a soft decision tree. One main difficulty of such model is that it requires exponentially large amount of training data with respect to the depth of the tree. However, with approximated DNNs in hand, sufficient amount of training data for soft decision tree can be provided by labeling unlabeled data using DNNs, sampling synthetic unlabeled data using generative approach [4] and distilling method [7]. Such soft decision tree could approximate DNNs to a reasonable extent while maintain human interpretability for further investigation.

More advanced approaches combines complementary strengths of Probabilistic Graphical Models (PGMs) and DNNs. Johnson et al. [8] proposed a combination of flexible deep learning feature models with structured Bayesian priors. They used deep auto-encoders to extract lower representation of non-linear observed data and used graphical models for latent variables sequence inference. A very efficient variational inference algorithm was developed to solve the joint learning problem. A very interesting view of their work is that other than providing better explanations, they also encoded human expert knowledge into DNNs through PGMs [8]. Investigation in this topic could provide very interesting insights for both DNNs and PGMs researches.

# 5   Work Plan

| Key Item | Date |
|---|---|
| Literature review and refine the scope of the project. | March - June 2017 |
| Re-implement models in section 4.1 and section 4.2 | July - December 2017 |
| Implement feature selection mechanism for models in section 4.2 | January - April 2018 |
| Explore various topologies to achieve better computational performance | May - September 2018 |
| Write up experiment results for conference paper | September - December 2018 |
| Re-implement models in section 4.3 | January - April 2019 |
| Investigating explanations of previous models | May - June 2019 |
| Write up experiment results for conference paper | July - October 2019 |
| Write up thesis | November - January 2020 |
| Draft submission of thesis to supervisor and rework based on feedback | Early February 2020 |
| Thesis presentation/defense and submission to assessors. Potentially rework based on feedback | March 2020 |
| Final submission of thesis | April 2020 |

Table 1: Estimated work plan

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