ANALYSING THE EFFECTS OF DATA AUGMENTATION AND HYPER-PARAMETERS FOR TEXT CLASSIFICATION WITH CONVOLUTIONAL NEURAL NETWORKS

JONATHAN K. QUIJAS

Department of Computer Science

APPROVED:
Olac Fuentes, Chair, Ph.D.
Monika Akbar, Ph.D.
David Novick, Ph.D.

Charles Ambler, Ph.D.

Dean of the Graduate School

©Copyright

by

Jonathan K. Quijas

2017

to my

FAMILY

 $thanks\ for\ everything$

ANALYSING THE EFFECTS OF DATA AUGMENTATION AND HYPER-PARAMETERS FOR TEXT CLASSIFICATION WITH CONVOLUTIONAL NEURAL NETWORKS

by

JONATHAN K. QUIJAS

THESIS

Presented to the Faculty of the Graduate School of

The University of Texas at El Paso

in Partial Fulfillment

of the Requirements

for the Degree of

MASTER OF SCIENCE

Department of Computer Science $\begin{tabular}{ll} THE UNIVERSITY OF TEXAS AT EL PASO \\ May 2017 \end{tabular}$

Acknowledgements

Abstract

Convolutional neural networks have seen much success in computer vision and natural language processing tasks. When training convolutional neural networks for text classification tasks, a common technique is to transform an input sequence of words into a dense matrix of word embeddings, or words represented as dense vectors, using table lookup operations. This allows for the inputs to be represented in a way that the well-known convolution/pooling operations can be applied to them in a manner similar to images. These word embeddings may be further incorporated into the neural network itself as a trainable layer to allow fine-tuning, usually leading to improved model predictions. The drastic increase of free parameters however, leads to overfitting if proper regularization is not applied or the size of the training set is not large enough.

We give an overview of popular convolutional and recurrent network architectures, describe their basic functions, and discuss their observed advantages and shortcomings on our task and data. We follow this discussion with an overview of our final choice of architecture, based on a combination of these architectures.

We train our neural networks using abstracts from multiple science and engineering fields, each set of abstracts comprised of multiple topics. The number of publications available for our task is moderate, in the mid thousands for each topic. We analyse the effect of using word embeddings with our models in terms of fit and prediction. We then propose embedding "trainability" schemes to alleviate overfitting, improve performance and achieve faster convergeance. We conclude our study proposing several data augmentation techniques designed for text sequences in an attempt to further mitigate overfitting and improve generalization. Finally, we provide discussion on our empirical results as well as future work.

Table of Contents

		P	age
A	cknow	rledgements	V
Al	ostrac	±	vi
Та	ble o	f Contents	vii
Li	st of	Figures	ix
\mathbf{C}	apte	er	
1	Intro	oduction	1
	1.1	Training a Neural Network	1
	1.2	Minimizing Non-Convex Functions: Gradiant-Based Learning	2
	1.3	Bias-Variance Tradeoff	2
	1.4	Weight Regularization	4
		1.4.1 Dropout	5
2	Text	Classification with Deep Neural Networks	6
	2.1	Brief Overview of Deep Learning	6
	2.2	Word Embeddings	7
	2.3	Convolutional Neural Networks	8
		2.3.1 Input Representation: Word Embeddings for Convolutional Networks	9
3	Mod	lel, Dataset, and Final Pipeline Description	11
	3.1	Layer Descriptions	11
		3.1.1 Embedding Layer	11
		3.1.2 Feature Maps: Convolution + Pooling	12
		3.1.3 Gated Recurrent Unit Layer	13
		3.1.4 Dense Layer	14
	3.2	Model Description	14
4	Tow	ards Improving Model Performance: Embeddings and Data Augmentation	17

	4.1	Freezing the Embedding Layer	17
	4.2	Principal Component Analysis and Dimensionality Reduction of the Embed-	
		dings	18
	4.3	Dataset Augmentation: Shuffling and Noise Injection	19
		4.3.1 Shuffling	20
		4.3.2 Noise Injection	21
	4.4	Dataset Augmentation: Padding	21
		4.4.1 Wrap Padding	23
	4.5	Reducing Data Granularity: From Abstract to Sentences	23
5	Exp	erimental Results	24
	5.1	Dataset Descriptions	24
	5.2	Freezing the Embeddings: Results	24
	5.3	Data Augmentation Results	26
	5.4	Astrophysics	26
	5.5	Physics	26
	5.6	Mathematics	27
	5.7	Computer Science	27
	5.8	Quantitative Biology	28
6	Con	cluding Remarks	29
	6.1	Significance of the Result	29
	6.2	Future Work	29
Re	eferen	ces	30
Cı	ırricu	lum Vitae	33

List of Figures

1.1	Visualization of overfitting. Training error decreases as epochs progress,	
	eventually reaching zero. Validation error starts increasing, indicating over-	
	fitting. The best model is shown at the dotted line, where validation error	
	reached its minimum	4
2.1	Visualization of embeddings using the t-distributed stochastic neighbor em-	
	bedding (t-SNE) dimensionality reduction algorithm. Words with similar or	
	related meanings tend to lie close to each other in embedding space	8
2.2	Visualization of a feature map with a single kernel. In this example, the	
	kernel convolves tri-grams, or windows of three words. After convolution	
	with all possible trigram context windows, max pooling is applied to reduce	
	dimensionality. Here, the pool size is 3. This process is repeated as many	
	times as there are kernels in the layer and their outputs are concatenated	
	horizantally to yield a matrix of size $num\ filters \times (input\ length\ -\ pool\ size$	
	+ 1)	10
3.1	Visualization of an embedding layer. Word indexes are mapped to word	
	embeddings. This layer outputs a matrix comprised of stacked embeddings,	
	one for each index	12
3.2	Visualization of a recurrent layer. Each hidden layer \boldsymbol{h}^t is a function of	
	the previous hidden layer h^{t-1} , the present input signal x^t . The weights are	
	shared across time steps in order for the model to generalize better	13
3.3	Model Architecture: embedding layer, followed by a feature map, and a	
	recurrent layer. At the end, we have a fully connected layer with a softmax	
	activation, which will output class probabilities	16

Chapter 1

Introduction

This work is an early step towards fascilitating interdisciplinary research within the University of Texas at El Paso. In the future, we wish to design a system to automatically assign or recommend faculty to interdisciplinary research communities based on their publication data. For this task, we want to learn models that capture important and high-level features from the raw inputs in order to make decisions as accurate and meaningful to the faculty members as possible. Neural networks are effective at learning said complex features. This study is to better understand deep convolutional and recurrent networks for the task of classifying scientific publication abstracts.

1.1 Training a Neural Network

A neural network is a function $f(x; \theta)$ that maps an input x to some response variable y. When we *train* a neural network, we *learn* the model parameters, or weights, θ that minimize some cost function $J(\theta)$. For a regression task, where the model's output is a continuous variable, a common cost function is the **Mean Square Error**:

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} (y_i - f(\boldsymbol{x}_i; \boldsymbol{\theta}))^2$$

For categorical or discrete output variables found in classification tasks, we normally use the Categorical Cross-Entropy:

$$J(\boldsymbol{\theta}) = -\mathbb{E}_{\boldsymbol{x}, y \sim \hat{p}_{data}} \log p(y|\boldsymbol{x}; \boldsymbol{\theta})$$

Given a training set of observations x_i and their true labels y_i , we compute weights that minimize the cost, or error, via maximum likelihood (ML) estimation:

$$oldsymbol{ heta}_{ML} = rgmax_{oldsymbol{ heta}} \sum_{i}^{m} \log P(y_i | oldsymbol{x}_i; oldsymbol{ heta})$$

which one can see is equivalent to computing the weights that *minimize* the cross-entropy cost function.

1.2 Minimizing Non-Convex Functions: Gradiant-Based Learning

Due to the non-linearities associated with a neural network, the loss function to be minimized becomes non-convex. Non-convex optimization is in general more difficult than convex optimization, so we usually rely on gradient-based methods for the task. Gradient based optimization provides a sound theoretical framework and a practical and well tested methodology for learning deep neural networks. This gradient-based learning process involves moving, or updating, the weight values in the direction opposite of the cost function's gradient, repeating this process for a series of **epochs**, or training iterations. These updates should be small, scaled by a learning rate, and can make learning a lengthy process. Gradient based learning is also scalable to datasets of enourmous size. The gradients and updates may be computed using small random batches of the training set at a time rather than the entire dataset (e.g. Stochastic Gradient Descent) [2].

1.3 Bias-Variance Tradeoff

Given a set of i.i.d. observations $\{x_1, ..., x_n\}$, we wish to compute the set of weights $\hat{\theta}$ that is as close as possible to θ , the set of weights that truly parametrize the data generating

process $p_{data}(\boldsymbol{x};\boldsymbol{\theta})$. This concrete parameter value (in contrast to a density over possible values) is called a **point estimator**, or statistic, of the true set of parameters. Unless the data generating process is known exactly the parameter estimators will have error. Two different measures of error in an estimator are its bias and variance. The **bias** measures the expected deviation between $\boldsymbol{\theta}$ and the estimator $\hat{\boldsymbol{\theta}}$, this expectation over the data:

$$Bias(\hat{oldsymbol{ heta}}) = \mathbb{E}(\hat{oldsymbol{ heta}}) - oldsymbol{ heta}$$

$$= \mathbb{E}[\hat{oldsymbol{ heta}} - oldsymbol{ heta}]$$

The **variance** is a measure of the deviation from the expected estimator, caused by the randomness in the sample, or how much the estimator will vary as a function of the data sample:

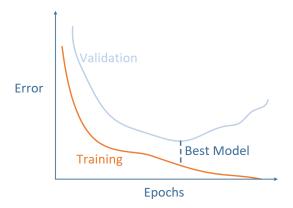
$$Var(\hat{\boldsymbol{\theta}}) = \mathbb{E}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^2$$

When learning a neural network's weights, we use a training set so that we can later generalize previously unseen data with high accuracy (or some other determined metric). That means that during training, we obtain $\boldsymbol{\theta}_{ML}$ by minimizing $J_{train}(\boldsymbol{\theta})$, but we care about having low $J_{test}(\boldsymbol{\theta})$ i.e. low cost on test data points.

Overfitting occurs when a network is able to predict its training set extremely well (i.e. very close to zero error), but fails to predict unseen data points. This is because the network's weights have been extremely fine-tuned to fit its training data, but do not fit or represent data points outside of its training samples. An overfitted model is said to have large variance and small bias. Conversely, underfitting occurs when the model fails to predict the training set because it generalizes too much. This model is said to have large bias and small variance. When training a neural network, we aim to find a balance between training cost and test cost, between overfitting and underfitting.

Because of the commonly large number of weights in deep convolutional networks, it is easy to overfit a moderate size training set [7]. It has been shown that when using a large

Figure 1.1: Visualization of overfitting. Training error decreases as epochs progress, eventually reaching zero. Validation error starts increasing, indicating overfitting. The best model is shown at the dotted line, where validation error reached its minimum.



enough dataset, neural networks are trained without overfitting, and thus generalize well to new unseen data. Because of the abundance of data today, it is usually easy to acquire large datasets, although this is not always the case. In this work, we consider the case then the sizes of available datasets are moderately sized (e.g. tens of thousands examples).

1.4 Weight Regularization

One way to regularize a model is to impose a constraint on its weights. By adding a penalty term to the cost function, we can decrease the magnitude of our weights to to prevent them from *blowing up* and overfitting the training set. L_2 regularization adds the L2 norm of the weights to the cost function:

$$J(\boldsymbol{\theta}) = -\mathbb{E}_{\boldsymbol{x}, y \sim \hat{p}_{data}} \log p(y|\boldsymbol{x}; \boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_{2}$$

where λ is the regularization control parameter. Higher values of λ penalize more and a value of 0 leads to no regularization.

1.4.1 Dropout

A recently proposed and highly effective way to regularize a neural network is via **dropout**[7][19]. Dropout "deactivates" a neuron or unit with probability p_{drop} . We deactivate a unit by setting its output to 0. This forces the network to not rely on combinations of activations, since any unit will only be *active* with probability $1 - p_{drop}$.

Chapter 2

Text Classification with Deep Neural Networks

2.1 Brief Overview of Deep Learning

Deep convolutional neural networks have seen much success on a wide array of application, from scene interpretation to self-driving vehicles and art generation. Natural language processing tasks are no exception to the range of problems deep learning can solve, from sentiment analysis to language modeling. One very useful function of deep neural networks is their ability to learn high-level features at each consecutive layer [12].

One type of neural networks that is particularly good at learning features from the data is the convolutional neural network (CNN)[13][15][5]. A CNN learns a set of weights, or kernels, that are normally much smaller than the input size. The difference in size forces the weights to have **sparse interaction**, or interaction on a subregion of the input, versus the dense interaction between every input with every output in traditional neural networks (i.e. vector-matrix multiplication). This sparse interaction allows for features to be detected locally within the input (e.g. edge detection). **Parameter sharing** allows for distinct outputs to be computed using the same set of weights. This drastically reduces the number of unique weights and allows for significant increases in network depth (i.e. deep networks) without the need to increase the amount of training data. These two design principles make CNN's poweful and efficient feature extractors.

Another type of deep neural network that has seen much success is the recurrent neural network (RNN). RNN's are designed to model data that display temporal structure, such

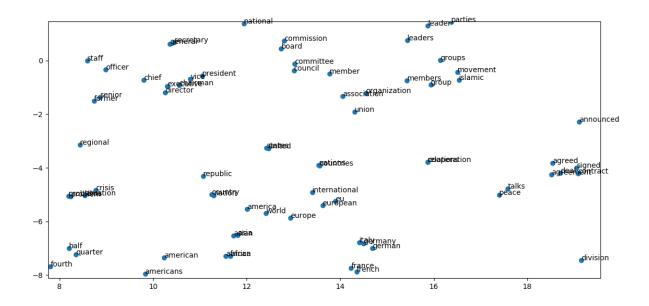
as text and speech. By unfolding time-steps as a computational graph, the network can learn to model data along the time dimension, using at each time step the raw input plus the output of the last time step's layer [Siegelman and Sontag 1995]. Because of the usually very deep structure of the recurrent network, computation of the gradient via back propagation can lead to the vanishing gradient problem, where the gradient starts to shrink and become very close to zero as we back-propagate the errors. [8] proposed the Long Short-Term Memory (LSTM) recurrent network, a type of recurrent that essentially solves this problem with recurrent networks. A recent and simpler variation of the LSTM network is the Gated Recurrent Unit (GRU), which performs comparably well [4].

2.2 Word Embeddings

Another significant achievement of deep learning for natural language processing is the neural probabilistic language model. [1] proposed a neural network to model the probability of a word given its context $P(w_t|w_{t-k},\ldots,w_{t-1})$

In their work, they addressed the curse of dimensionality, manifested by the fact that a test word sequence (w_{t-k}, \ldots, w_t) is likely to be different from all training sequences, by learning distributed representations of words. Words are represented as dense continuous vectors called **word embeddings**. Using word embeddings to model the likelihood of word sequences allowed generalization because the language model would give high probability to unseen word sequences if they were made up of words semantically similar to already seen words. Because of the of the underlying algorithm used to learn these word embeddings, similar words tend to lie closer to each other on embedding space. Thus, word embeddings are said to capture semantic relations and encode more information than just a word identifier (e.g. a bag-of-words or one-hot vector representation).

Figure 2.1: Visualization of embeddings using the t-distributed stochastic neighbor embedding (t-SNE) dimensionality reduction algorithm. Words with similar or related meanings tend to lie close to each other in embedding space.



2.3 Convolutional Neural Networks

As described previously, convolutional neural networks are known for their abilities to learn high-level features from raw data. As input signals advance forward through the network, they produce latent signals as linear combinations with learned parameters, have non-linearities applied to them, and have a pooling or selection mechanism based on simple functions such as the average or maximum operations [22].

When dealing with image data, images are convolved with multiple filters, each convolution applied to overlapping subimages called as receptive fields. This localized convolution process leads to discovery of low level features of images in the training set such as edges. As data flows forward through the model, higher level features are discovered (e.g. wheels or headlights in a vehicle image dataset).

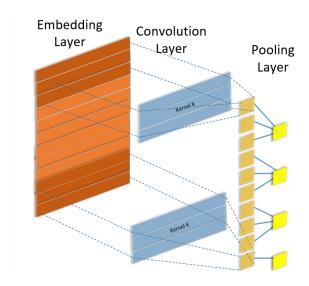
These convolutional neural networks are comprised of feature maps. A feature map is

a **convolution** layer paired with a **pooling** layer afterwards. The convolution stage creates *activations*, whereas the pooling stage reduces dimensionality and creates translation invariance.

2.3.1 Input Representation: Word Embeddings for Convolutional Networks

We can take advantage of word embeddings to apply convolutions to text in a fashion similar to convolutions with image data and exploit the semantic information in the embeddings [10]. We apply the convolutions to overlapping sub-regions of the input text i.e. bi-grams, tri-grams, etc. After convolution, we apply a non-linear function such as max(0,x) and reduce data dimensionality by pooling such as $x_{pool} = max(x_1, ..., x_n)$. Given a set of documents $s_1, ..., s_m$, we build a vocabulary $\mathbb V$ and a bag-of-words model from $\mathbb V$ to create a mapping $BoW : \mathbb V \mapsto \{1, ..., |\mathbb V|\}$. We represent a training document s as a sequence of integers $BoW(s) = s = s_1, ..., s_k$, each integer being simply a word index in $\mathbb V$. When the convolutional network receives this input sequence, each word index will be mapped to a corresponding embedding vector.

Figure 2.2: Visualization of a feature map with a single kernel. In this example, the kernel convolves tri-grams, or windows of three words. After convolution with all possible trigram context windows, max pooling is applied to reduce dimensionality. Here, the pool size is 3. This process is repeated as many times as there are kernels in the layer and their outputs are concatenated horizantally to yield a matrix of size $num\ filters \times (input\ length\ -\ pool\ size\ +\ 1)$.



Chapter 3

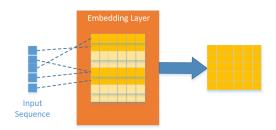
Model, Dataset, and Final Pipeline Description

3.1 Layer Descriptions

3.1.1 Embedding Layer

An **embedding layer** maps an word index, or integer, into its corresponding embedding. This layer is usually the first layer in a neural network that processes input such as text. Given input text s, this layer receives as input a sequence of word indexes $BoW(s) = x = x_1, ..., x_k$ and maps each word into an embedding. Thus, for an input text s, we transform it into a sequence of integers x, and from there into $\mathbf{E} \in \mathbb{R}^{n \times d}$, where d is the embedding size. These embeddings are further fine-tuned during training. Because of the large number of parameters in this layer (number of words allowed times embedding size), it is usually a good idea to use L_2 regularization or dropout in order to avoid or mitigate overfitting.

Figure 3.1: Visualization of an embedding layer. Word indexes are mapped to word embeddings. This layer outputs a matrix comprised of stacked embeddings, one for each index.



3.1.2 Feature Maps: Convolution + Pooling

We refer to a convolutional layer followed by a pooling layer as a feature map. Since our data are text sequences and thus have temporal structure, we use a one-dimensional convolutional layer to convolve with embedding n-grams through the input sequence [20]. As in Figure 2.2, we stride only along the time dimension. This is in contrast to the usual two-dimensional convolution schemes with image data, where the kernels stride along the width and height dimensions of the input data. After the convolution step, we apply a non-linearity to each computed feature. We chose the rectified linear activation (**ReLU**) function

$$ReLU(x) = max(0, x)$$

Although simple, this non-linearity is quite effective and thus widely used. We then use a max pooling operation to output a single value for each kernel similar to [14]. Besides the huge dimensionality reduction, we do this so that we pass to the next layer the single strongest activation from each kernel i.e. a strong feature selection mechanism.

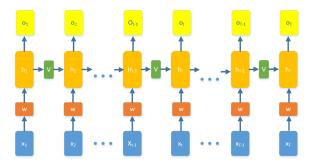
3.1.3 Gated Recurrent Unit Layer

A recurrent layer is designed to process data with temporal structure i.e. sequences [17]. This recurrent layer is in itself a network, where the hidden layer values at time t depend on the previous hidden layer's values, the input corresponding to time t, and a shared parameter set:

$$\boldsymbol{h}^t = f(\boldsymbol{h}^{t-1}, \boldsymbol{x}^t, \boldsymbol{\theta})$$

This is implemented by *unrolling* the layer along the time dimension as a sequence of layers, each corresponding to the next in time. Because of this design, back propagation of error through the unrolled layer can result in the vanishing gradient problem.

Figure 3.2: Visualization of a recurrent layer. Each hidden layer h^t is a function of the previous hidden layer h^{t-1} , the present input signal x^t . The weights are shared across time steps in order for the model to generalize better.



A Gated Recurrent Unit layer is a type of recurrent layer designed to combat this condition [4]. It is a simplified version of the earlier LSTM layer [8], also designed to mitigate the vanishing gradient problem, and in practice it performs comparably well. This layer models the latent features computed by the feature map as a time sequence. This means that it does not assume indepences between activation and learn to model the temporal structure of the previous layer's output. This property makes the layer an adequate choice, since we deal with text data which inhibits temporal structure.

3.1.4 Dense Layer

The last layer in our model is the classical **dense**, or fully connected layer. The number of units in this layer is equal to the number of classes in our dataset. Given the output of the network's second to last layer h, we can compute the unnormalized log probabilities

$$z = W^T h + b$$

for some bias vector \boldsymbol{b} .

Each z_i is a log probability of the input corresponding to class i. The **softmax** activation function is then applied to the all units, to finally output class probabilities:

$$\hat{y}_i = softmax(\boldsymbol{z})_i = \frac{exp(z_i)}{\sum_j exp(z_j)}$$

 $\hat{y}_i = P\{y = i | \boldsymbol{x}\}$

3.2 Model Description

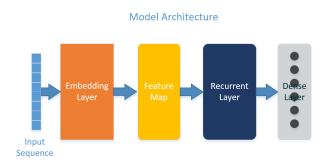
[21] provide an overview of typical neural models used for natural language processing. A standard architecture for convolutional neural networks for text sequence classification is the one proposed by [10]. This model has an embedding layer followed by a feature map and a dense layer with a softmax activation to output class probabilities. This model has parameter sharing and sparse interaction properties inherent of convolutional neural networks, and thus is a good choice for efficiently extracting features from the data via convolutions and non-linearities. The pooling operation provides data dimensionality and acts as a translation invariance mechanism. This reduction makes forward propagation an even more efficient process. Convolutional neural networks, however, are not designed to consider the data as having temporal structure, as is the case with text sequence data.

Another popular neural model for text classification is the recurrent neural network. This architecture is explicitly designed to treat data to display temporal structure. Because of this, the recurrent neural network is an excelent choice for text sequence data. At a basic level, this architecture is comprised of an embedding layer (to transform input sequences into word embeddings) followed by a recurrent layer e.g. LSTM or GRU, then a dense layer with the softmax activation to output probabilities.

In our experiments, a purely convolutional neural network displayed great efficiency relative to the recurrent network. Because of the convolution and pooling operations, the CNN normally processed the data around 10 times as fast as the RNN. The RNN, although slower, always achieved around 4% higher accuracy on all experiments, due perhaps to its ability to model sequential data.

After testing both architectures, the model we use in the rest of this work is a mixture of these two standards. After the embedding layer, we add a feature map to extract features from the raw inputs, then we add a GRU layer. This design choice incorporates the sequence modeling power of the RNN with the fast and efficient feature extraction of the CNN. This combination always led to the higher accuracy achieved with the RNN, with training times orders of magnitude shorter as with the CNN. We further extended our pooling operation to be global. Out of all the features computed by a kernel, we select only the single strongest one (i.e. highest value). The pooling layer's output size is therefore equal to the number of kernels in our convolutional layer. In order to create a one-to-one correspondance between the network's inputs (the word indices in the input sequence) and the units in the recurrent layer, we chose to have a number of kernels equal to the network's input size (i.e. length of input sequence). This design choice proved to be very efficient and reached the highest accuracy percentages during our experiments.

Figure 3.3: Model Architecture: embedding layer, followed by a feature map, and a recurrent layer. At the end, we have a fully connected layer with a softmax activation, which will output class probabilities.



The final network's architecture is as follows:

- Input layer: word index vector
- Embedding layer: maps word index vector to embedding matrix
- Feature Map:
 - Convolution layer: kernel size=5, ReLU activation
 - Global MaxPooling layer: Outputs a scalar per kernel
- Gated Recurrent Unit layer with tanh activations
- Dense layer with *softmax* activations

Chapter 4

Towards Improving Model Performance: Embeddings and Data Augmentation

As mentioned in section 3.1.1, we can fine-tune the word embeddings via back-propagation and gradient descent (or some other gradient-based optimizer), just as any other weights in the neural network. In this case, the number of free parameters in our model increases drastically. It is easier to overfit a model with more free parameters when the amount of training data is limited, as is the case in our task. Another important aspect to consider when fine-tuning the embeddings is whether we lose the semantic information originally present in them. It is therefore a good idea to evaluate the effect of training the embeddings. In the following sections, we propose various ways treat the embedding layer in our neural network in order to mitigate overfitting. We also consider reducing the dimensionality of the embeddings via Principal Component Analysis (PCA). Finally, we propose data augmentation techniques inspired by computer vision tasks but designed for text data with temporal structure, as is the case with our data.

4.1 Freezing the Embedding Layer

When we make our model's embeddings trainable, its number of free parameters highly increases. With inputs of size n, and embeddings of size d, we introduce $n \times d$ new parameters into the model. We therefore propose multiple embedding trainability schemes to quantify

how much the embeddings help increase (or decrease) test accuracy and overfitting.

• Frozen Embeddings

- With this scheme, we freeze the embedding layer altogether. We do not update the embedding vectors, so the model relies completely on its other parameters to fit the data.

• Freeze-Unfreeze

- With the freeze-unfreeze scheme, we train the model with its embedding layer frozen until some stopping criterion is met. After this, we unfreeze, or make the embedding layer trainable, and retrain the model.

• Flash-Freeze

- In the *flash-freeze* scheme, we allow the embedding layer to be trainable for a small number of epochs (e.g. three), then freeze it and retrain the model.

• Unfrozen Embeddings

- We allow the embeddings layer to be trainable from the beggining to the end.
We will refer to a model trained with unfrozen embeddings and without any of our proposed data augmentation schemes as the baseline model.

4.2 Principal Component Analysis and Dimensionality Reduction of the Embeddings

Principal Component Analysis (PCA) is a very popular linear transformation commonly used to reduce dimensionality of a dataset [18]. It projects the data to a representation where the variables are linearly uncorrelated. Concretely, PCA projects the data onto new axes called principal components. These axes, or dimensions, are orthogonal and selected

in a way that minimizes reconstruction mean square error. Given a data matrix X with n dimensions, its principal components are the eigenvectors of the covariance matrix X^TX . The first principal component is the direction of most variation. The second principal component is the direction with the next largest variation, and so on. We can then choose to retain only the k < n principal components that contain the most variation in the data.

We propose to apply PCA to the word embeddings in order to linearly decorrelate their dimensions and reduce their dimensionality. By reducing the dimensionality while preserving the majority of the variance in them (e.g. 95%), we will reduce the number of parameters introduced to the model while retaining most of the information from the original embeddings.

4.3 Dataset Augmentation: Shuffling and Noise Injection

Another common practice aimed to reducing overfitting is to **augment** the dataset. Data augmentation refers to any transformation of the input data in a way that the label value does not change. Data augmentation is ubiquitous in computer vision tasks. Example transformations include translations, rotations, and color intensity jitters via Pricipal Component Analysis [11]. All these transformations should be subtle enough that the overall structure is preserved, but allow for the model to process more distinct training data points.

The data augmentation techniques mentioned above are common practive in computer vision tasks such as image classification. In order to introduce more variance into our dataset, we propose data augmentation techniques inspired by computer vision by designed for text sequence data. We propose to **shuffle** by randomly changing the order of words within a **context windows**, or non-overlapping neighborhood of words in the input text sequence. We further propose to inject small amounts of **noise** to the input sequence by randomly replacing words with words taken from the training vocabulary.

As long as the overall structure of the data (and label) is preserved, data augmentation normally lead to improved task performance [3] [11][9][6]. With that same rationale, we expect our proposed augmentation techniques to yield increase accuracy percentages. In other words, we expect that our changes will be subtle enough for the label to be preserved, but effective enough that we introduce more variance into our dataset and help cope with the limited number of training examples.

4.3.1 Shuffling

We propose to augment our dataset by making small *context* changes that don't change the global structure of the input sequences. Concretely, we move a *context window* along non-overlapping neighborhoods the input sequence, randomly shuffling the words indexes inside it. For example using a context window of size 2 i.e. *bi-gram*, an input sequence

$$\mathbf{x} = x_1, x_2, x_3, x_4, x_5, x_6$$

could be shuffled to:

$$\boldsymbol{x}' = x_2, x_1, x_3, x_4, \underbrace{x_6, x_5}_{\text{bi-gram}}$$

In the first pass, the first two indexes get shuffled. The second pass led to no changes in ordering. The third and final pass shuffles the last two indexes.

As it is common practice in computer vision tasks to apply small translations and rotations to images, we perform this operation to slightly perturb the temporal structure of our text sequence data. The rationale for this dataset augmentation technique is that small changes in the ordering of the words will result in a larger training sample; a training input sequence has a low chance of being repeated as its length increases. Smaller context windows preserve the most structure. This method will preserve most of the original context structure in the sequence, as long as the shuffling is not to harsh e.g. a complete random permutation of the sequence.

4.3.2 Noise Injection

One common augmentation technique for image datasets is to add small amount of noise. By replacing a relatively small number of pixel values with noise, the model gets to process and train on a different but similar instance. The noise should be subtle enough as to not distort the image too much, otherwise we could potentially train the model using mostly noise. We propose to augment our dataset by injecting noise to each training sample. Again, we aim to simulate a larger training sample while avoiding harsh changes to the original inputs. Concretely, each word in a text sequence gets replaced with a specified probability with a word randomly chosen from our training vocabulary.

```
Algorithm 1 Add noise to input sequence
```

```
1: procedure NoiseInjection(\boldsymbol{x} = [x_1, ..., x_n], \mathbb{V}, p_{noise})
2: for k = 1 to n do
3: if p_k \sim U(0, 1) \leq p_{noise} then
4: x_k \leftarrow x_k' \in \mathbb{V}
5: end if
6: end for
return \boldsymbol{x}
7: end procedure
```

4.4 Dataset Augmentation: Padding

In order to enforce uniform input size for our neural networks, we apply **zero-padding**. For any arbitrary training instance $BoW(s) = \mathbf{x} = x_1, ..., x_k$, we enforce that k = n, for the specified input size n. Thus, if k < n, we transform it into $\mathbf{x}_{pad} = x_1, ..., x_k, 0_{k+1}, ..., 0_n$. Conversely, if k > n, we simply truncate \mathbf{x} to be of size n. The input length introduces another model hyper-parameter that should be fine-tuned, but a reasonable approach is to pad enough to fully accommodate the length of most input sequences i.e. its preferrable to

pad than truncate and lose information.

Our network's input is a sequence of integers, each integer being a word index: a number representing a word in our vocabulary V. Word indexes range from 1 to |V|, and the index 0 being left for out-of-vocabulary words. When we pad our input sequence with 0s, we dont add any additional information; we simply create a constant input length. We propose that if instead we add values that characterize or help describe the input sequence more thoroughly, we may increase the amount information available during neural network training.

Consider a very simple input sequence, and assume its true label can be determined from a single word:

"This paper is about computer graphics"

where the label is "Graphics" i.e. a publication about computer graphics. In this simple case, the label is determined by the word "graphics". To the human reader, this single informative word is enough for the classifier to predict the label correctly although it is only 1/6 of the entire text.

Now consider a the padded version, where we enfore an input length of 10:

"This paper is about computer graphics PAD PAD PAD"

In the padded version, the word graphics is now only 1/10 of the entire text. If we could pad the sequence using this informative word instead of some meaningless token e.g. 0's, we could increase the likelihood of the model extracting features from it. In other words, make important words be present more frequently. We propose to pad input sequences with values found already within the input text sequence instead of 0's only.

4.4.1 Wrap Padding

Our proposed padding scheme is to *wrap around* the text, repeating words once we reach the padding portion. Referring back to the first example, the input sequence:

"This paper is about computer graphics PAD PAD PAD"

would then be

"This paper is about computer graphics This paper is about"

One thing to observe is that using this simple scheme, we remove all 0's i.e. non-informative padding indexes from the text sequence, but we also don't have selection mechanism and can miss useful words such as missing the word "graphics" in this example. Nonetheless, it is a simple approach to pad our data and increase the likelihood of encountering informative words during feature extraction.

4.5 Reducing Data Granularity: From Abstract to Sentences

Our last proposed dataset augmentation scheme is break each training abtract into a set of sentences, and train the network using this finer text granularity. For example, training a model using single sentences, another using sentence pairs, and another using sentence triplets. During testing, we break a test abstract into sentence sets and classify each set individually. We then assign the class with the largest mean.

Chapter 5

Experimental Results

In this chapter we will show our results.

5.1 Dataset Descriptions

We gathered a scientific publication abstract dataset from Arxiv.org. Concretely, we obtained publications from the physics, mathematics, computer science, and quantitative biology disciplines. For each discipline, we considered each **topic** as a class. For example, when considering computer science publications, we considered the "computational complexity" topic as one class, "artificial intelligence" as another class, and so on. Each class has 5000 examples. Because of this class balance, it is appropriate to report the prediction accuracy on the test set. We use a 70/30 split for training and testing. We apply simple preprocessing to the texts by removing non-alphanumeric characters, and converting to lower case characters. The dataset distribution is shown in the table below.

We used the GloVe embedding set for our pretrained embeddings [16]. This set consists of 400,000 words, each represented as a vector of size 100.

5.2 Freezing the Embeddings: Results

We tested the four different proposed embedding training approaches. The first method is to leave the embeddings frozen throughout training i.e. non-trainable parameters. The second approach is to freeze the embeddings until convergeance, then retrain with the embeddings

Department	Number of Labels	Training Size	Testing Size
AstroPhysics	5	17500	7500
Physics	13	45015	19293
Computer Science	20	63396	27170
Mathematics	26	87705	37588
Quant. Bio	5	11006	4717

Table 5.1: Dataset distribution. We obtained 5000 abstracts for each class. We use 70% of the data for training and 30% for testing.

unfrozen. The third proposed approach is to train with the embeddings unfrozen for a small number of epochs (e.g. three), then freeze the embeddings and retrain the model. The last approach is to simply train with the embeddings as trainable parameters from the beggining to the end.

Dataset	Training Set Size	Frozen	Not-Frozen	Freeze-Unfreeze	Flash-Freeze
AstroPhysics	17500	0.757(8)	0.765(6)	0.758(7)	.775(6)
Physics	45000	0.740(11)	0.774(13)	0.767(27)	0.789(6)
Computer Science	63400	0.647(17)	0.682(10)	0.682(16)	.701(6)
Mathematics	87700	.590(22)	.685 (21)	.678(72)	.684(6)
Quant. Bio	11000	.805 (5)	0.823(9)	0.820(7)	.841 (6)

Table 5.2: Accuracy results on all datasets with proposed embedding training schemes. The numbers in parenthesis represent the number of epochs until the model converged.

We observe that the Flash-Freeze method achieves relatively faster convergence, with accuracy competent or better than the accuracy of all other methods. We observed that when using the *flash-freeze* embedding training method, we reached a good stopping point after a small number of epochs (e.g. 6). This is useful because it removes the need to use

a validation split for early stopping. From here on, all our models are trained using the *flash-freeze* technique for 6 epochs: 3 epochs training the embeddings and 3 epochs with the embeddings frozen.

All other methods required a validation split for early stopping. We used a 90/10 split for training and validation respectively.

5.3 Data Augmentation Results

In this section we show the experimental results obtained using the proposed data augmentation techniques. Our model hyper-parameters are as follows: number of training words=20000, kernel size=3, learning rate=0.001, regularization rate=0.00001, dropout rate = 0.2, maximum sequence length = 250. We refer the model trained using the *non-frozen* scheme and without any of the proposed augmentation techniques as the **baseline**.

5.4 Astrophysics

	Astrophysics Test Accuracy							
	No Change Embedding PCA Wrap Padding PCA & Padding Sentence Sp							
No Aug	0.773	0.774	0.778	0.777	0.769			
Noise	0.771	0.779	0.768	0.777	0.765			
Shuffle	0.772	0.768	0.770	0.764	0.766			
Ensemble 0.771 0.777 0.770 0.777 0.770								
Baseline: 0.765								

5.5 Physics

	Physics Test Accuracy								
	No Change Embedding PCA Wrap Padding PCA & Padding Sentence Spli								
No Aug	0.789	0.789	0.790	0.790	0.786				
Noise	0.774	0.757	0.783	0.782	0.743				
Shuffle	0.772	0.761	0.787	0.787	0.766				
Ensemble	Ensemble 0.783 0.775 0.789 0.789 0.765								
	Baseline: 0.774								

5.6 Mathematics

Mathematics Test Accuracy								
	No Change Embedding PCA Wrap Padding PCA & Padding Sentence Split							
No Aug	1	2	3	1	2			
Noise	1	2	3	1	2			
Shuffle	1	2	3	1	2			
Ensemble 1 2 3 1 2								
Baseline:								

5.7 Computer Science

	Computer Science Test Accuracy							
	No Change Embedding PCA Wrap Padding PCA & Padding Sentence Sp							
No Aug	1	2	3	0.702	2			
Noise	1	2	3	1	2			
Shuffle	1	2	3	1	2			
Ensemble 1 2 3 1 2								
Baseline: 0.682								

5.8 Quantitative Biology

Quantitative Biology Test Accuracy									
	No Change Embedding PCA Wrap Padding PCA & Padding Sentence Splin								
No Aug	0.836	0.837	0.839	0.838	0.833				
Noise	0.827	0.835	0.837	0.834	0.812				
Shuffle	0.831	0.827	0.831	0.829	0.820				
Ensemble 0.839 0.840 0.840 0.840 0.830									
Baseline: 0.828									

Chapter 6

Concluding Remarks

- 6.1 Significance of the Result
- 6.2 Future Work

References

- [1] Yoshua Bengio, Réjean Ducharme, Pascal Vincent, and Christian Jauvin. A neural probabilistic language model. *Journal of machine learning research*, 3(Feb):1137–1155, 2003.
- [2] Léon Bottou. Large-scale machine learning with stochastic gradient descent. In *Proceedings of COMPSTAT'2010*, pages 177–186. Springer, 2010.
- [3] Nitesh V Chawla, Kevin W Bowyer, Lawrence O Hall, and W Philip Kegelmeyer. Smote: synthetic minority over-sampling technique. *Journal of artificial intelligence research*, 16:321–357, 2002.
- [4] Junyoung Chung, Caglar Gulcehre, KyungHyun Cho, and Yoshua Bengio. Empirical evaluation of gated recurrent neural networks on sequence modeling. arXiv preprint arXiv:1412.3555, 2014.
- [5] Alexey Dosovitskiy, Jost Tobias Springenberg, Martin Riedmiller, and Thomas Brox. Discriminative unsupervised feature learning with convolutional neural networks. In Advances in Neural Information Processing Systems, pages 766–774, 2014.
- [6] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pages 770–778, 2016.
- [7] Geoffrey E Hinton, Nitish Srivastava, Alex Krizhevsky, Ilya Sutskever, and Ruslan R Salakhutdinov. Improving neural networks by preventing co-adaptation of feature detectors. arXiv preprint arXiv:1207.0580, 2012.
- [8] Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. *Neural computation*, 9(8):1735–1780, 1997.

- [9] Max Jaderberg, Karen Simonyan, Andrew Zisserman, et al. Spatial transformer networks. In *Advances in Neural Information Processing Systems*, pages 2017–2025, 2015.
- [10] Yoon Kim. Convolutional neural networks for sentence classification. arXiv preprint arXiv:1408.5882, 2014.
- [11] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolutional neural networks. In *Advances in neural information processing systems*, pages 1097–1105, 2012.
- [12] Quoc V Le. Building high-level features using large scale unsupervised learning. In Acoustics, Speech and Signal Processing (ICASSP), 2013 IEEE International Conference on, pages 8595–8598. IEEE, 2013.
- [13] Yann LeCun, Bernhard Boser, John S Denker, Donnie Henderson, Richard E Howard, Wayne Hubbard, and Lawrence D Jackel. Backpropagation applied to handwritten zip code recognition. *Neural computation*, 1(4):541–551, 1989.
- [14] Min Lin, Qiang Chen, and Shuicheng Yan. Network in network. *CoRR*, abs/1312.4400, 2013.
- [15] Maxime Oquab, Leon Bottou, Ivan Laptev, and Josef Sivic. Learning and transferring mid-level image representations using convolutional neural networks. In *Proceedings* of the IEEE conference on computer vision and pattern recognition, pages 1717–1724, 2014.
- [16] Jeffrey Pennington, Richard Socher, and Christopher D. Manning. Glove: Global vectors for word representation. In *Empirical Methods in Natural Language Processing* (EMNLP), pages 1532–1543, 2014.
- [17] David E Rumelhart, Paul Smolensky, James L McClelland, and G Hinton. Sequential thought processes in pdp models. *Parallel distributed processing: explorations in the microstructures of cognition*, 2:3–57, 1986.

- [18] Jonathon Shlens. A tutorial on principal component analysis. CoRR, abs/1404.1100, 2014.
- [19] Nitish Srivastava, Geoffrey E Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: a simple way to prevent neural networks from overfitting.

 Journal of Machine Learning Research, 15(1):1929–1958, 2014.
- [20] Alexander Waibel, Toshiyuki Hanazawa, Geoffrey Hinton, Kiyohiro Shikano, and K Lang. Phoneme recognition: neural networks vs. hidden markov models vs. hidden markov models. In Acoustics, Speech, and Signal Processing, 1988. ICASSP-88., 1988 International Conference on, pages 107–110. IEEE, 1988.
- [21] Wenpeng Yin, Katharina Kann, Mo Yu, and Hinrich Schütze. Comparative study of cnn and rnn for natural language processing. arXiv preprint arXiv:1702.01923, 2017.
- [22] Y-T Zhou, Rama Chellappa, Aseem Vaid, and B Keith Jenkins. Image restoration using a neural network. *IEEE Transactions on Acoustics, Speech, and Signal Processing*, 36(7):1141–1151, 1988.

Curriculum Vitae