

Technical document

1. Current Status

The library implementations are at a point such that an end-to-end process can be run: data with training parameters are specified, and a CSCV based PBO is output.

A full list of implementations is as follows:

- Network Types
 - Feedforward Network
 - Restricted Boltzmann Machine
 - Stacked Auto Encoder
- Learning Algorithms
 - Contrastive Divergence-1 for RBM pre-training
 - Online Gradient Descent
 - Stochastic Gradient Descent
- Validation Algorithms
 - CSCV
 - PBO
- Data Processes
 - Log fluctuation implementation to format dataset with rolling windows
 - Library to generate synthetic data
- Optimizations
 - SGD: L1 & L2 Regularizations
- Neural Network Configurations
 - Activations: Sigmoid, ReLU, Softmax
 - Initialisations: Normal, Hinton, Xavier, He (Normal & Uniform variations)
 - Cost Functions: MSE, CE, Loglikelihood
- Output Library
 - Effective graphing of training logs (epoch based performance, weight update rates, output reconstructions etc.)
- Technical Testing
 - Basic hyperparameter search method & outputs
 - Automated Unit Tests for CD1, OGD and

2. Future Status

There's a fair amount to do before starting tests on the actual dataset, from software engineering tasks to algorithm optimizations to more critical experiment implementation details. The to-do lists below have been split up into critical and non-critical tasks(or tasks which might not be necessary)

Critical

- Database work: MongoDB/SQL implementation to record parameters and results
- Learning Optimizations: Variable learning rate (AdaGrad/ADAM/ADA)
- Trading Strategy: Decide on the basic strategy used to derive returns
- Synthetic Tests: Run tests on synthetic data to inform experiment design and parameter choices
- Finalise Dataset: Need to properly account for survivorship bias, and decide which data to use
- SAE updates: Decide whether the SAE should be updated periodically or not
- Literature Review: There are various inclusions and amendments to be made here

Non-Critical/Maybe

- Better hyper-parameter search technique, e.g. Random Search
- Parallelization of training tasks
- Denoising SAEs
- Learning Optimization: Momentum
- Weight monitoring visualizations

3. Milestones & Deliverables

Finish Date	Item
Done	1 Literature Review
In Progress	2 Data Collection
Done	3 Data Log Fluctuation Processing
Done	4 SAE Implementation
Done	5 Online FFN/LSTM Implementation
Done	6 CSCV Implementation
Done	7 Synthetic Data Generation
30/11	8 Finalise Implementation Process
30/11	9 Database Implementation
30/11	10 Learning Optimizations
14/12	11 Test full implementation on synthetic data
14/01	12 Test full implementation on actual dataset
31/01	13 Statistical Analysis (incl. profitability of trading strategy)
28/02	14 Write up & Revisions

4. Process Implementation

The steps below indicate how everything is expected to fit together at a high level perspective:

1 Data preparation

- The data is processed into day to day log fluctuations
- At each time point, rolling historic summations are calculated (e.g. the past 1, 7 and 30 days)
- At each time point, rolling future summations are calculated (e.g. the next 10 days)

2 Data Segregation

- The processed dataset is split into 3 parts, to be used for the following processes: SAE/SGD training, OGD training, hold-out validation (e.g. 60%, 20%, 20%)

3 SAE Training

- The dataset defined for SAE/SGD is used to train the auto-encoder network (using either RBM pretraining/weight initialization algorithms + SGD)
- Notably, this SAE/SGD dataset will itself be split into training & testing portions in order to train and validate the SAE network
- Once the SAE network has been defined, it can be used to reprocess the datasets such that the input is now encoded, and the output is as before. These encoded datasets will be used for all following steps.

4 FFN/SGD Training

- The same SAE/SGD portion of the data will then be used to train the FFN network to predict future prices, using the implemented SGD algorithm & optimizations.

5 OGD Training

- The second portion of data will be used to train and optimize the FNN from 4 for OGD. The purpose of this will be to optimize the OGD parameters

6 Holdout Validation

- The third and last portion of data will be used to obtain results for the model. Predictions will be made on the relevant stock price log fluctuations

7 Returns generations

- A basic trading strategy will be used to generate returns from the predicted and actual prices in the holdout dataset. These returns for each time period and each configuration of the model defined by steps 3-5 will form the M matrix for the CSCV process.

8 CSCV & PBO

- Using the M matrix from 7, the CSCV process will be run which will then allow a calculation of PBO.

5. Points of concern

There are several issues which are still undecided/uncertain or which could use further refinement:

- End to end process: Should the FFN network be trained with SGD prior to OGD, or should the first dataset just be used for OGD training on the FFN after pre-training/weight initialization has taken place?
- Predictions attempted: How many steps and stocks should be attempted in the prediction process?
- Trading strategy: The CSCV method requires returns to be used, which can then be assessed with something like the Sharpe Ratio. Should an actual trading strategy be used for each configuration here, or just a representation of accuracy which can be calculated as a single figure for each time period (such as MSE)? If a trading strategy is used, what should it be?
- SAE Updating: The current implementation does not have any SAE updates taking place as more data is observed. While easy to change, I'm not sure if or when the SAE network should be updated
- Denoising SAE: The initial proposal was to use denoising autoencoders. The implementation process is easy enough, but I'm unsure if denoising would be effective in a financial context (where data is already so noisy)
- Final Dataset: The current dataset doesn't account for survivorship bias, and I'm a little unsure of how best to pick the final stocks/indices etc. (the initial proposal was rather limited in comparison to what is now available)

6. Meeting Minutes

16th June 2018

- Literature Review Include: Wilcox & Debbie Hierarchical Paper; Crutchfield & Farmer: Geometry of Time Series; F Takens: Detecting strange attractors in turbulence; Reference Riaz
- Implementation
 - Key implementation point was the data segmentation choices
 - LSTM network would resolve this point for us (CNN convolution could also potentially work)
 - Non LSTM will run risk of correlating times with stocks
 - Representation needs a mixture of time scales as well as the features
 - Will be considering data for the entire index at any time point t
 - Will need to consider how to address the changing constituents
 - Aspect of how often the feature selection is updated (e.g. SDAE in online model)
 - Does it get updated in the online model ?
 - SDAE result should be similar to edge detection which will give set of predictions essentially
 - Use known test cases for CSCV method development
- Data
 - Use simple noise with Gaussian distribution & long trends to develop network models (6 variations of increasing, decreasing and flat with low or high variability)
 - Build backdated tests module with surrogate data afterwards
 - Not going to try intraday data due to different nature of problem
 - Implementation of either a flat file or MongoDB
 - Important to include Volume data
 - Volume time $-i$ might be far more predictable; volume and variance linked
- Other
 - Admin: Single document - table of contents (nice to have) with authors; sections etc. ; full doc with versioning; PDF + latex (always send both)
 - Further Correspondence: * Iterate over FFN/LSTM implementations rather than starting with LSTM * For the meantime, assume the models do not differ fundamentally enough to be considered as separate for the PBO calculations

Online non-linear prediction of financial time-series patterns

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1 Introduction

2 LiteratureReview

2.1 Technical Analysis

Technical analysis is a financial analysis practice that makes use of past price data in order to identify market structures, as well as forecast future price movements. The techniques are typically objective methodologies which rely solely on past market data (price and volume). They stand in contrast to fundamental analysis, where experts will consider a companies operations, management and future prospects in order to arrive at an evaluation. The basis of much technical analysis, originally developed through Dow Theory, is the belief that stock market prices will move directionally (upwards, downwards or sideways), and that past movements can be used to determine these trends [62].

One of the primary methods in technical analysis is the use of charts in order to identify price patterns. These charts will be produced using the available market data and a known design, such as the popular candle-bar plot, which can then be compared to historical data to match it to a particular pattern. These patterns are thus indicative that the stock is likely to take on a particular price trend, or is in a particular state [62]. There is a certain amount of controversy around technical analysis, where many argue that it is contradictory to the random walk and weak form efficient market hypotheses, and as such is not valuable or useful [31]. The argument against this, is that technical analysis does not rely on past action to predict the future, but is rather a measure of current trading, and how the market has reacted after similar patterns have occurred in the past [47]. Further, even if the analysis is unable to effectively forecast future price trends, it can still be useful to exploit trading opportunities in the market [71].

With the advent of processing power becoming cheaply available, there has been an increase in research to adapt computing techniques to technical analysis. The breadth and superhuman speed in which systems are able to perform technical analysis far outstrips what was possible before, and as such they have become the focus of competitive performance for many market participants [46]. To this end, there has been much research to apply machine learning algorithms to perform pattern recognition on stock price movements.

Financial markets have been shown to be complex and adaptive systems, where the effects of interaction between participants can be highly non-linear [3]. Complex and dynamic systems such as these may often exist at the 'order-disorder border' - they will generate certain non-random patterned and internal organisation, which can be assessed and identified, however they will also exhibit a certain amount of randomness in their behaviours, or 'chaos' [18]. As a result, trying to identify these patterns and structures is a simultaneously reasonable and notoriously difficult goal. While it is often clear in hindsight that the patterns exist, the amount of noise and nonlinearity in the system can make prediction challenging. Fittingly then, neural networks have become a popular choice for modelling within the financial markets. Due to their structure, they are able to learn non-linear interactions between their inputs and outputs, with even early research showing their ability to achieve statistically significant results, which lends weight to the argument against the efficient market hypothesis [75].

2.2 Neural Networks

A Neural Network (NN) is a learning model which was originally inspired by the biological mechanisms of neurons in brains. The structure is essentially that of a network system, with connected nodes and edges, or neurons and weights in context. The neurons are based on the same idea as synapses as seen in the brain - where a buildup of input results in a firing of output. The input here is determined by the models input (real numbers typically), and processed through the weights and activation functions of the neuron, which then results in an output value either at an intermediate level, or as the models final output. The system learns by considering input samples sequentially, and adjusting the weights between edges to result in more accurate outputs, which may either be classification or regression values.

Structured neural networks that learn to some extent have been around since the second half of the 21st century [69], though have been through several cycles of popularity. The first versions tended to be very simple with one one layer of hidden neurons [43]. It was only later, through the application of the backpropagation algorithm, that they started to become more practical and popular [85].

With the rise in popularity, many different network formations were developed and suggested. One of the initial suggestions was the conceptually simple Feedforward Neural Network (FNN) as described above - an acyclic graph where inputs are processed in a single direction until the output is reached. The other notable earlier model was the Recurrent Neural Network (RNN), which has a cyclic graph instead - this results in a more powerful computational system than the standard FNN, which was shown to be effective quite early on [74]. The Long Short-Term Memory (LSTM) network was another that used recurrent dynamics, though at a neuron level, in that the neuron is responsible for remembering values for an arbitrary time period [40]. Convolutional Neural Networks (CNN) have a non-recurrent structure, but implement separate pooling layers of neurons which consider the adjacent input values for each feature (e.g. pixels next

to each other). These have been shown to be incredibly effective at tasks such as image recognition, as elaborated on later.

There are three primary learning paradigms used in neural network training - Supervised Learning (SL), where the network is trained on inputs with known outputs; Unsupervised Learning (UL), where the network is trained to identify unknown structures as an output; and Reinforcement Learning (RL), where environmental reactions are used as inputs to train a network for certain outputs [69]. While all of these configurations and paradigms have their benefits and uses, this paper will largely focus on FNN and RNNs, trained through SL and UL.

2.2.1 Training and Backpropagation

Historically, the crux of neural networks popularity has often been based on the development of novel training methodologies, and how they have increased performance. In line with this, the Backpropagation (BP) algorithm (as defined in 3.2.3) has played a pivotal part: while neural network (or perceptron) models were around long before NN popularity, they were largely deemed ineffective, at least in comparison to other available models of the time [61]. It was only during the 1980s that the BP algorithm was applied to NNs, and the field started to gain in popularity again [52, 86].

Rumelhart et al. showed that the BP algorithm as applied in NNs resulted in useful feature representations occurring in hidden layers and the empirical success that resulted thereof [67]. Shortly after, LeCun et al. applied the BP algorithm to CNNs with adaptive connections. They were able to show impressive performance for the time in classifying handwritten images, with the images as a direct input (rather than a feature vector) [53].

While many improvements were made during this time via gradient descent modifications (as expanded on in section 2.5), the models were typically of a shallow nature due to problems encountered trying to train deeper networks. Early experiments with deep networks resulted in poor performance due to what is now widely known as the problem of either vanishing or exploding gradients [63]. Essentially, as more layers are added to the network, the backpropagation algorithm (with typical activation function neurons), results in error signals that either shrink or grow out of bounds at an exponential rate. One of first suggested and primary solutions to the problem is to perform pre-training on the network through unsupervised learning [69], which is discussed more fully in 2.3.2.

There were also initial concern that the BP algorithm as applied to high dimensional neural networks would result in the network weights being trapped in local minima if a simple gradient descent was used (e.g. where no small changes to the configuration would reduce the average error rate) [54]. However, empirically, this tends not to so problematic, and large networks usually reach solutions of equitable performance. More recent research has shown that the solution spaces largely consist of many saddle points, each with varying gradients of the features, but which also tend to have similar values of the objective function [19]. Ge et al. have also shown that it is possible to escape saddle points and offer a guaranteed global convergence in certain non-convex problems [27].

2.2.2 Activation Functions

One of the upfront configuration choices necessary is the activation function, which allows the mapping of input to output at the neuron level. There have been many suggestions and experiments with different functions, though there are some common features amongst functions which might make them appropriate: Non-linearity allows for neural networks to operate as universal approximators, as shown in [41], continuous differentiability allows for the use of gradient descent and whether the function is monotonic has been shown to indicate whether the solution can be guaranteed to have a unique periodic solution [87]. Lastly, the range of the function (infinite or finite) can impact both the stability and efficiency of the training.

Some of the most popular functions that have been used are the Sigmoid, TanH, ReLU and Softsign. There have been various studies showing the effectiveness of the different activations under varying initialization (or pre-training) for weights. Glorot and Bengio noted that the typical Sigmoid and TanH functions performed poorly with standard minimization, and result in slower convergence and worse minima, and showed that Softsign with a non-standard initialization resulted in quicker convergence [29]. Further research with Bordes & Bengio found that the rectifier (ReLU) functions were more effective in deep sparse networks compared to the TanH function [30].

2.2.3 Deep Learning

As noted above, most of the earlier work using neural networks relied on shallow models with few layers. However, a resurgence in interest occurred in 2006 after several papers demonstrated the efficacy of unsupervised pre-training of networks prior to supervised training. The effect was substantial enough to allow much deeper layered networks to be

trained than before [10, 35].

The essential point behind the unsupervised learning was to initialize the weights in the network to sensible values in light of the problem context. The methods used trained each layer to be able to reconstruct the model of the features in the layer below (to a varying degree of accuracy). Sequentially pre-training and combining layers like this, the process generated a deep neural network with appropriate weights. Once done, a final output layer was added and the entire network could then be fine-tuned through backpropagation, without suffering such performance degradation through vanishing or exploding gradients [35, 66, 36]. This is expanded up further in 2.3.2. Le Roux and Bengio were able to show that within the DBNs produced by Hinton [35], adding hidden nodes resulted in strictly improved modelling capabilities, and they suggested that increasing the number of layers is likely to result in increased representational ability (subject to efficacy of previous layers), thus establishing the argument for deep networks in theory as well as practice [55].

FNNs had been shown to be effective in modelling high dimensional data even prior to the breakthroughs in deep networks [11], so it fits that the deep networks were shown to be extremely effective in high dimensional data classification. Early implementations shown increased efficacy in handwriting recognition, as well as pedestrian recognition [72]. When it came to data types such as sound and images, CNNs were implemented on several occasions with record breaking model performances in recognition, notably in ImageNet and WaveNet [44, 83].

As more research into deep networks was conducted, it became apparent that with large enough datasets, the layerwise pretraining of networks was not actually necessary to achieve high performance standards [44, 30, 15]. When training for long enough, it was reported that the pre-training offered little to no benefit, though these models were typically using datasets far larger than were attempted before (as a result of hardware improvements enabling as much). While these results did require certain attention was paid to the initialization, as well as the use of nonlinear activation units, it did suggest that pre-training largely acted as a prior which may not be necessary if large enough labelled datasets are available [12]. Naturally, pre-training was still implemented to prevent overfitting in smaller datasets.

2.2.4 Backpropagation Improvements

One of the instrumental improvements which aided the above achievements, was to modify the backpropagation algorithm using the dropout technique, as suggested by Hinton et al [38]. When training of large networks is attempted on small datasets, it often results in overfitting and poor results on out of sample data. Dropout helps resolve this by randomly excluding a certain percentage (usually 0.5) of feature detectors on each training iteration. The effect is to stop co-adaptations of feature detectors, and by rather training each neuron in a wide variety of internal configurations, it forces them to take on more usefully generalizable characteristics (it was noted that this is not a dissimilar technique to ensemble methods, or bagging). The authors were able to show that the method resulting in significant improvements on benchmark data sets (e.g. MNIST, CIFAR-10), and that a simpler model using dropout was able to achieve near comparable performance for the ImageNet dataset.

Goodfellow et al. used the dropout technique as the basis for their maxout activation function technique, which leverages and improves on dropouts fast optimisation and accuracy through averaging characteristics. The maxout model was shown to achieve state of the art performance on benchmark datasets, as well as have a strong theoretical grounding [28]. Further work was done by Wang et al., which improved on the dropout (and potentially maxout) techniques through fast sampling, resulting in an order of magnitude speedup in training [82].

2.3 Stacked Autoencoders

2.3.1 High Dimensional Data Reduction

As noted, machine learning techniques have been shown to be extremely effective at modelling non-linear inputs to outputs - neural networks have even been shown to be universal function approximators in this regard [41]. More traditional statistical models will typically process the available feature data to select the most significant features to be used in the model once its defined - evident in a processes such as subset selection [68]. Machine learning techniques are no different in this regard, and feature data will typically be transformed to smaller observations of more significance prior to being used as input to a model, such as the neural networks described above.

Financial data, in line with the complex and dynamic system that it represents, is often of a very high dimensional nature, which offers opportunities through more sophisticated analysis, but also introduces the curses of dimensionality [21]. The increased dimensionality can result in higher processing complexities when needing to do basic tasks such as estimating a covariance matrix (a commonplace necessity in finance), as well as increase the risk of incorrect assumptions based on spurious variable collinearity [25]. Noise accumulation in high dimensional data can create further problems, resulting

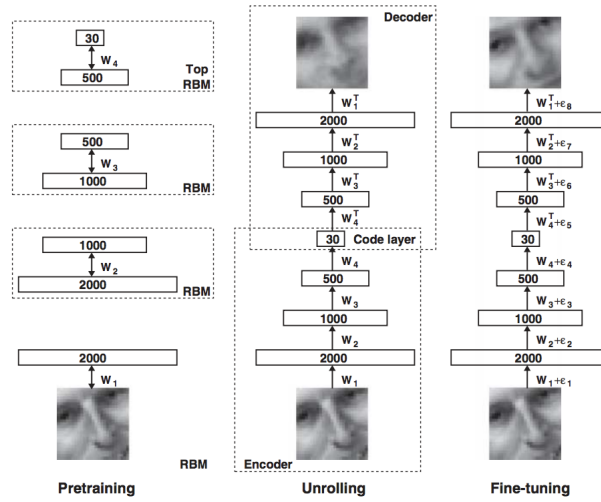


Fig. 1: The Autoencoder training steps [36]

in problems performing variable selection and ultimately having a large impact on classification and regression models [26].

Time series data can introduce its own set of challenges - there is often not enough data available to understand and predict the process [24], the time variable dependence creates complexity in how much past data to consider at any point, and the data is typically non-stationary [50]. Thus, high dimensional time series data (which many financial problems focus on), require careful consideration on how to handle their inputs and analysis.

Deep learning techniques are a natural choice in this context, and much research has been done to show their (varying) efficacy on time series data. The most successful of these models have been ones which modify deep learning techniques to incorporate the temporal aspect of the data (e.g. Conditional Restricted Boltzmann Machines or Recurrent Neural Networks), rather than static, and those which have performed feature selection processes rather than operating on the raw data (e.g. Auto-encoders) [50].

Two of the seminal pieces of research that have lead to the resurgence in machine learning and deep learning were the algorithms for training deep belief networks [35], as well as the usage of stacked auto-encoders [66, 10].

2.3.2 Deep Belief Networks

Autoencoders were suggested by Hinton et. al as a method of transforming high dimensional data to lower dimensional input vectors, in order to alleviate some of the problems detailed above, and increase performance of deep belief networks [36].

One of the more prominent classical techniques for dimension reduction is principal components analysis (PCA), which uses linear algebra to find the directions of greatest variance, and represent the observation samples features along each of these directions, thus maximising the variational representation. Hinton et al. show that autoencoders are a nonlinear generalization of PCA. The structure and training algorithms of the autoencoder show it to be a specialised neural network - there is a multilayer encoder network which is able to transform to a lower dimension, and a symmetrical decoder network to recover the data from the code as represented in Figure 1. As with neural networks, the gradient weights can be trained through the feedforward and backpropagation algorithms.

The primary challenge presented here is the initial weighting of the networks - with large initial weights the autoencoder will often find a poor local minima, and with small initial weights the gradients are too small to effectively train deep layered networks. The critical suggestion by Hinton et al. was to used layered Restricted Boltzmann Machines (RBM) in order to initialise the weights. For each layer of the desired autoencoder, a RBM is formed and trained with the previous layer (or RBM) [37]. Once all the layers have been trained in this way, they are mirrored to form the decoder network. This then forms the initial weights to be fine tuned further, as per the Fine-tuning step in 1. They showed the deep autoencoder networks were significantly more effective than PCA or shallow autoencoders on multiple dataset types.

2.3.3 Stacked Denoising Autoencoders

The second important piece of work was the development of a denoising autoencoder (DAE), by Vincent et al. [79]. One of the problems identified in the DBN model (and those similar), is that if the encoder dimensions were too high, it is likely that the encoder would learn a trivial encoding - essentially creating a copy the input model. The one way of tackling this issue is to constrain the representation with bottlenecks and sparse autoencoder layers, which can be seen in figure 1.

Vincent et al. explore a very different approach to the problem, which was to develop an implementation of autoencoder which focused on partially corrupting the input, and so force the network to denoise it. The theory here is based on two ideas - the first, is that a higher dimensional representation should be robust to partial corruption of the input data; and the second is that the denoising process will force model focus to shift to extracting useful features from the input.

The algorithms and structures are largely the same as described for DBNs above, with the key difference being that the model is trained to reconstruct the original input, but only using a corrupted version of the input (where noise has been added to it), and so is forced to learn smarter feature mappings and extractions. The DAE suggested then is a stochastic variant of the autoencoder, which has the benefit of being able to implement higher dimensional representations without risking training of a trivial identity mapping. Notably, in the Stacked Denoising Autoencoder (SDAE) formation, only the initial input is corrupted (as opposed to the input from layer to layer). It was shown that the SDAE model outperformed previous AE and DBN networks on numerous benchmark datasets [79].

2.3.4 Pre-training

The methods described above follow a similar approach: greedy layer-wise unsupervised pre-training in order to determine initial weights, followed by supervised fine tuning to arrive at the final model. It is shown numerous times, that the pretraining process results in significant performance gains [79]. However it is not immediately apparent, given the nature of backpropagation algorithms and the like, why this is the case. Erhan et al. performed extensive empirical simulations in order to suggest an explanation to the mechanism of pre-training [23].

While their results were not entirely conclusive, they did lend themselves to a reasonable hypothesis: the unsupervised pre-training results in a form of regularization on the model - variance is minimized, and the bias introduced acts as a prior to direct the model configuration towards a sample space that is effective for the unsupervised learning generalization optimisations.

2.3.5 Time Series Applications

The autoencoder papers reviewed so far in this section derive their results primarily from classification problems, and so do not necessarily account for the problems involved with time series as described in 2.3.1. Due to the inherent difficulties with predictions in the financial system, it can sometimes be unclear if the shortcoming in results is due to this system complexity or if the methodologies used are unsuited for the purpose. In light of this it is worth pointing out that Stacked Autoencoder (SAE) implementations have been shown to be effective in many time series systems.

Lv et al. implemented a deep learning SAE model using the methods described in 2.3.3 in order to predict traffic flow at various time intervals (15, 30, 45 and 60 minutes) - a problem not so structurally dissimilar from what will be presented in this paper [58]. They were able to show that the deep SAE was able to offer prediction results which were both objectively good and also persistently outperformed the comparison models used (backpropagation neural network, random walk forecast, support vector machine and a radial basis function neural network).

In a review of unsupervised feature learning and deep learning methods on time series, Langkvist et al. noted that the use of autoencoders, either as a technique in themselves, or as an auxiliary technique to models such as convolutional neural networks, were able to offer performance increases in areas such as video analysis, motion capture data and bacteria identification [50].

2.3.6 Financial Applications

There have of course also been successful applications of stacked autoencoders and deep learning models in finance as well. Takeuchi et al. performed some earlier work showing the use of autoencoders when applied to a momentum trading strategy. They implemented an RBM pre-trained DBN as per 2.3.2, and assessed the networks classification performance for ordinary shares on NYSE, AMEX and Nasdaq. This showed that using a DBN network resulted in significant performance increases compared to the standard momentum strategy [76].

Zhao et al. used SDAEs and combined them with the bootstrap aggregation ensemble method (bagging) in a study of predicting the crude oil price. They compared the proposed model to a variety of benchmarks, including standard SAE, bagged and standard feedforward networks and SVRs. The results indicated that the SAE models were more accurate,

with the bagged SAE model performing the best, though at a significant increase in computational costs in comparison to standard SAE [91].

While much of the financial literature has focused on the use of RBM based models, Autoencoders and SAEs have recently been gaining popularity in performing feature reduction. Troiano et al. specifically investigate the use of different feature reduction models for trend prediction in finance [77]. In line with being primarily interested in the effect of feature reduction techniques, rather than the classification performance itself, only an SVM model was used to test results. Using various periods from historical S&P 500 data, they were able to show that AE outperformed the RBM model significantly in numerous accuracy measures, and was able to do so at a fraction of the training time.

Bao et al. note that the research has been lacking with regards to whether SAEs should be used for financial prediction models or not [8]. They suggest a novel model which combines Wavelet Transformation, SAEs and a Long Short Term Memory (LSTM) network. Using data from several financial exchanges (considering a range of developed and undeveloped markets), they assess the models applicability to OHLC prediction. Comparing the model to configurations without the SAE layers, and a RNN model as benchmark, they showed that the inclusion of SAEs resulted in less volatility and greater accuracy, which in turn offered higher profitabilities in a buy-and-hold trading strategy.

More novel autoencoder applications have also been attempted, with Hsu suggesting the use of a Recurrent Autoencoder for multidimensional time series prediction [42]. There is a clear pattern through the literature that the use of AEs and SAEs both by themselves and when used as an assisting technique result in more accurate prediction results and less computationally expensive training.

2.4 Data Segmentation

One of the aspects of time series not yet discussed is how the data might be segmented for analysis. Financial pattern matching, as discussed in 2.1, requires methodologies to decide the length of data to consider when determining whether a subset of data matches a pattern or not.

There are numerous classical approaches to this problem, which were widely applied in machine learning prior to the resurgence in deep learning. One of the earliest and more common approaches was the Sliding Window, where each the model input for each observation is padded by a predetermined number of observations that occurred both prior and after the one in question. This has the advantage of being fairly model agnostic, but fails to capture any correlations in the dependent variable values [16]. The Recurrent Sliding Window method aims to resolve this by including the same number of prior predictions made as part of the input. In this case, input would be $\langle x_{t-d}, \dots, x_t, x_{t+d} \rangle$ and $\langle y_{t-d}, \dots, y_t \rangle$. This was shown to be significantly more effective than the plain sliding window method [7]. Notably, the sliding window approach can only be implemented in an offline model.

These methods can be adapted to take on online formats, as well as incorporate data reduction benefits through algorithms such as Piecewise Linear Approximation (PLA), which adapts a linear representation to the leading portion of the window. Some novel approaches (Feasible Space Window and its stepwise adaption) were suggested by Liu et al. in order to compensate for the computational requirements of reprocessing the entire window at each step for online models [56].

Window based methods represent a fairly static and unsophisticated approach to data segmentation. A suggested solution to this is to segment the data by dynamically identifying significant partition points, known as perceptual important points (PIP) [17]. The computational cost of identifying PIPs was initially rather large, making them unsuitable for quickly changing and dynamic environments such as finance. However, Zhou et al. suggested a novel approach which reduced computational costs through intelligent binary tree traversal. They were able to show this approach was effective in identifying traditional financial stock patterns with the use of a layered neural network [93]. In a similar fashion, input data turning points (TP) were shown to potentially offer lower error rates than PIPs by Yin et al. [88].

More recently, Wan et al. conducted a review on the effect of segmentation on financial time series pattern matching, comparing perceptual important points, piecewise aggregate approximations, piecewise linear approximations and turning point based methods [80]. They use several pattern matching algorithms (template-based, rule-based, hybrid, decision tree, and symbolic aggregate approximation) for each of the segmentation methods in order to determine their effect on a broader level. The analysis was performed on real stock market data, as well as synthetic data generated to display common patterns such as positive/negative head and shoulders (H&S). Measuring accuracy, precision and recall, they showed that PIP based segmentation generally offered superior results to the others (though it is worth noting that there were various performance differences within the segmentation methods depending on the matching algorithm used).

2.5 Online Learning Algorithms and Gradient Descent

Most classic machine learning algorithms operate under the assumption that, for all intents and purposes, the full dataset has been collected and that the amount of training data for the model is both finite and immediately available. However, as the growth of information grows in an exponential fashion, there are numerous areas where the expected training data for the model will continue to grow. In these cases it would be disadvantageous to go through the full training and validation process again in order to incorporate the newly available data.

Online algorithms are designed to offset these issues by adjusting the batch training technique to rather repetitively draw on single samples from the data on which the models parameters can be adjusted. The benefit is that they are able to quickly process a large number of observations and readjust the model, though the downfall is that they are not always able to optimize the cost function to the same extent as offline batch algorithms [1].

Bottou and Cun argue that as the size of the dataset grows significantly, online algorithms advantages result in them outperforming offline models, despite any initial drawbacks [13]. Previous research had shown that online algorithms typically perform as fast as batch algorithms during the search phase of parameter optimization, but that final phase convergence tended to fluctuate around the optima due to the noise present in single sample gradients [51, 14]. Bottou and Cun showed in fact, that it is more practical to consider the convergence towards the parameters of the optima, rather than the optima itself (as defined by the cost function) - the difference between the learning speed and optimization speed, respectively [13]. Theoretical and empirical findings were presented to show that a stochastic online gradient descent (SGD) algorithm [referenceappendix] was able to outperform the batch model for parameter estimation, and was able to asymptotically outperform in the number of samples processed in a time period. The stochastic aspect of the algorithm is related to random observations from batch sample groups being used as the gradient basis. Theoretically, this slows down the convergence, but speeds up the processing speed of each batch - a technique which has later been shown to be generally successful [73, 92].

The SGD algorithm has resulted in a fair amount of further research due to its applicability to machine learning and the online benefit, which can largely be group into two categories: improvements affecting gradient learning and convergence rates, and processing improvements through parallelization.

One of the earlier improvements to convergence rates was the Momentum algorithm, as developed by Tseng [78]. As noted, stochastic descent often introduces significant oscillation around an optima, which slows down convergence. Momentum reduces this by decreasing movement in directions of high curvature, and increasing increasing movement towards directions consistent with previous gradients (this is achieved through combining gradient movements in opposite directions) .

There have also been several attempts to introduce effective regularization into the SGD process. Bartlett et al. presented Adaptive Online Gradient Descent, which implements an adaptive step size through a λ penalty on the learning rate, which was shown to be nearly optimal in a strong sense [9]. Langford et al. demonstrated a variation named Truncated Gradient, which introduced an enforced weight sparsity parameter. The weight sparsity is able to achieve equitable effects to L_1 regularization (similar to Lasso Regression). They were able to show that implementation performed effective feature reduction, while having little effect on performance [49]. Other approaches, such as AdaGrad, aim to improve the robustness of gradient training by adjusting the updates to parameters according to frequency - e.g. larger updates to infrequent parameters, and smaller updates to frequent parameters [22, 89].

A parallel implementation of SGD largely rests on the idea of splitting up data to be processed in individual runs of the gradient descent. The results are periodically aggregated, and the new model parameters are distributed to processing nodes for further training [90]. Depending on the configuration, the variance within results can result in poor convergence rates [59]. Mahajan et al. suggest a novel implementation which improves the distribution impacts through the use of better approximating functions in the processing nodes, which in turn improves the efficacy of the algorithms convergence [59]. Povey et al. presented a Natural Gradient SGD, which improves the learning rates through the use of a factor matrix used on the new gradients. They were able to show empirical evidence of this improving performance issues introduced from the parameter averaging typically used in parallelization [65].

There have been some more recent improvements focusing on making the SGD algorithm more dynamic, including the Inconsistent SGD (ISGD) and AdaBatch adaptations. The idea behind ISGD is to treat the training on a particular batch as a stochastic process, and adjust it according to the expected loss identified. Gradient updates from small loss batches are relatively small compared to large loss batches, and so by focusing efforts here ISGD is able to optimize performance. Wang et al. performed careful testing of SGD vs. ISGD and found inconsistent training to consistently outperform in terms of convergence speed and results [81]. It is worth noting that due to its nature, ISGD can be effectively combined with other SGD improvements (e.g. Momentum, as per the authors experiments). AdaBatch, as presented

by Devarakonda et al., introduces dynamism through the adjustment of batch sizes. Small batch sizes in SGD offer the benefit of faster convergence in fewer training epochs, however larger batch sizes are more computationally efficient due to their applicability to parallelization. The algorithm uses a monotonically increasing batch size, which is started small to gain traction in convergence, and later increased to allow the benefits of data parallelism. The effect, as shown, is to offer improvements in training performance of up to 6x, with less than 1% of accuracy when compared to the fixed batch baselines [20]. Both of these algorithms have been shown to be effective and applicable in the context of online neural network training.

2.6 Backtesting and Model Validation

Much of financial academic literature is currently facing a problem in terms of validation and verification of results. The primary method of going about these ends in the past has been to perform historical simulations, or backtests, in order to prove profitability of a trading strategy. The recent advances in both technology and the algorithms available to construct these strategies has resulted in researchers being able to run so many iterations of a model or strategy configuration through these backtests, that its become increasingly difficult to control for spurious results, with some papers suggesting that most published research findings are false [45].

The standard way of implementing backtests is to split the data into two portions: an In Sample (IS) portion which is used to train the model, and an Out of Sample (OOS) portion which is used to test the model and validate results. The problem lies in that millions of different model configurations might be tested, and if more sophisticated test measures are not in place (i.e. not just the standard Neyman-Pearson hypothesis testing framework is implemented), then it is only a matter of time before a false positive result occurs which shows high performance both IS and OOS (i.e. overfitting). The nature of financial data, where there is a low signal-to-noise ratio in a dynamic and adaptive system, and where there is only one true data sequence, makes it difficult to resolve these issues effectively [4, 60].

Overfitting is not a novel issue, and has of course been tackled in various literature areas, including machine learning. However, in that context, the frameworks are often not suited to the buy/sell with random frequency structure of investment strategies. They also do not account for overfitting outside of the output parameters, or take into consideration the number of trials attempted. Other methods, such as hold-out, are arguably still faulty due to researcher knowledge while constructing models [70]. One of the downfalls of the typical IS-OOS set up in the financial context is also that the most recent (and relevant) data will not be able to be used for the model training.

There have been some suggestions to resolve the problem that is occurring in the literature as a result of this - some work suggesting new frameworks, which this section will cover, and others which focus on the review process or how data and replication procedures are made available [64]. While the points made with regard to the review process and so on are certainly important, they don't aid with more effective model training for the researcher up front, and so will not be covered here.

2.6.1 Testing Methodologies

Considering the issues laid out above, there has been much work to develop alternative approaches to backtesting. One of the common approaches to avoid backtest overfitting is the hold-out strategy, where a certain portion of the dataset is reserved for testing true OOS performance. Numerous problems have been pointed out with this approach, including that the data is often used regardless, or that awareness of the movements in the data may, consciously or otherwise, influence strategy and test design by the researchers [70]. For small samples, a hold-out strategy may be too short to be conclusive [84], and even for large samples it results in the most recent data (which is arguably the most pertinent) not being used for model selection [34, 4].

There has been work by several authors to try and lay out techniques to try and avert backtest overfitting. The Model Confidence Set (MCS), as developed by Hansen et al. [32], starts with a collection of models or configurations, and remove models iteratively according to a defined loss function. The confidence set is defined by the remaining models once a non-rejection takes place within the process, and these models are considered to be statistically similar within a certain confidence range. MCS is thus able to facilitate equitable model selection. However, Aparicio et al. [2], showed that while MCS is a potential strategy, in practice is ineffective due to the inordinate requirement of signal-to-noise necessary to identify true superior models, as well as a lack of penalization over the number of trials attempted.

Bailey et al. [4] have developed a more robust approach to backtesting and how overfitting during strategy selection might be avoided. Their research defines backtest overfitting as having occurred when the strategy selection which maximizes IS performance systematically underperforms median OOS in comparison to the remaining configurations. They use this definition to develop a framework which measures the probability of such an event occurring, where the sample

space is the combined pairs of IS and OOS performance of the available configurations. The probability of backtest overfitting (PBO) is then established as the likelihood of a configuration underperforming the median IS while outperforming IS.

Formulaically, the definition of backtest overfitting is given by

$$\sum_{n=1}^N E[\bar{r}_n | r \in \Omega_n^*] Prob[r \in \Omega_n^*] \leq N/2 \quad (1)$$

Where the search space Ω consists of the N ranked strategies, and their ranked IS performance r and OOS performance \bar{r} . This allows the PBO, using the bayesian formula, to be defined as

$$PBO = \sum_{n=1}^N Prob[\bar{r} < N/2 | r \in \Omega_n^*] Prob[r \in \Omega_n^*] \quad (2)$$

Notably, the above definitions consider IS as the data made available to the strategy selection, rather than the models calibration (e.g. the full IS dataset, rather than, by way of example, the number of days used in a moving average). This allows the model-free and non-parametric nature of the definition.

They further developed the combinatorially symmetric cross-validation (CSCV) framework as a methodology to reliably estimate the probability used in PBO, which allows a concrete application of the concept. The CSCV framework does not require using the typical hold-out strategy (and thus avoids credibility issues), and is ultimately able to provide a bootstrapped distribution of OOS performance.

The methodology can be briefly summarised (skipping some details and nuances) as the following steps:

- 1 Generate a TxN performance series matrix, M , representing the profits and losses by the N trials over T time periods
- 2 Partition the M matrix into S submatrices
- 3 Generate the combination set C of all combinations of the S submatrices
- 4 For each combination in C :
 - a Form the training set by joining the 2 combination sets, and testing set as the rest of the combinations (all in order)
 - b Determine the ranked in-order IS and OOS performance for the sets
 - c Determine n^* as the best performing IS strategy
 - d Determine the relative rank of the n^* strategies OOS performance, where we should observe that \bar{r}^* systematically outperforms OOS as well. Define logit $\lambda = \frac{\bar{w}_c}{(1-\bar{w}_c)}$, where a high value implies consistency between IS and OOS performance, and thus a low level of backtest overfitting
- 5 The λ values can then be collected and used to define the relative frequency at which λ occurs across all combination sets in C , signified by $f(\lambda)$.

The CSCV framework and results thus allows the consideration of several notable statistics. First and foremost, the PBO may now be estimated using the CSCV method and using an integral over the $f(\lambda)$ function as defined above which offers a rate at which the best IS strategies underperform the median of OOS trials. If $\varphi \approx 0$, it is evidence of no significant overfitting (inversely, $\varphi \approx 1$ would be a sign of probable overfitting). Critically then, a PBO measure may be used in a standard hypothesis test to determine if a model should be rejected or not. This can be extended, as shown by Bailey et al., to show the relationship between overfitting and performance degradation of a strategy. It becomes clear that with models overfitting to backtest data noise, there comes a point where seeking increased IS performance is detrimental to the goal of improving OOS performance.

The CSCV methodology provides several important benefits (some already mentioned) over traditional testing frameworks, including the usual K-fold cross validation used in machine learning. By recombining the slices of available data, both the training and testing sets are of equal size, which is particularly advantageous when comparing financial statistics such as the Sharpe Ratio (SR), which are susceptible to sample size. Additionally, the symmetry of the set combinations in CSCV ensure that performance degradation is only as a result of overfitting, and not arbitrary differences in data sets. It is pointed out that while CSCV and PBO should be used to evaluate the quality of a strategy, they should not be the function on which strategy selection relies, which in itself would result in overfitting.

2.6.2 Test Data Length

The CSCV methodology offers an important but highly generalised framework to assess models and backtest overfitting. It doesn't however indicate which metrics should be used to assess the IS and OOS performance, nor any indication on the amount of data needed to do so effectively. One of the noted limitations of the framework is that a high PBO indicates overfitting within the group of N strategies, which is not necessarily indicative that none of the strategies are skillful - it could be that all of them are. Also, as pointed out, it should not be used as an objective function to avoid overfitting, but rather as an evaluation tool. To this end it helps assess overfitting, but not necessarily avoid it.

A typical measure of evaluation used for financial models is the Sharpe Ratio (SR), which is the ratio of between average excess returns and the returns standard deviation - a measure of the return on risk. In the context of comparing models, SR is typically expressed annually to allow models with different frequencies to be compared. Lo et al. [57] show that annulaized SR can be expressed as

$$SR = \frac{\mu}{\sigma} \sqrt{q} \quad (3)$$

Using sample means and deviations, $\hat{\mu}$ and $\hat{\sigma}$, SR can be shown to converge as follows (as $y \rightarrow \infty$)

$$\hat{SR} \rightarrow \mathcal{N}[SR, \frac{1 + \frac{SR^2}{2q}}{y}] \quad (4)$$

Thus, when using SR estimations, which follow a Normal distribution, it is possible that where the true SR mean is zero we may still (with enough configurations attempted) find an SR measurement which optimises IS performance. This is shown by Bailey et al. [5], who propose the non-null probability of selecting an IS strategy with null expected performance OOS. Notably, typical methods such as hold-out once again fail, as the number of configurations attempted are not recorded. They add a further derivation, which is the Minimum Backtest Length (MinBTL), ultimately showing that

$$MinBTL \approx \left(\frac{(1 - \gamma)Z^{-1}[1 - \frac{1}{N}] + \gamma Z^{-1}[1 - \frac{1}{N}e^{-1}]}{E[max_N]} \right)^2 < \frac{2\ln[N]}{E[max_N]} \quad (5)$$

The statistic highlights the relationships between: selecting a strategy with a higher IS SR than expected OOS, the number of strategies tested (N), and the number of years tested (y). The equation shows that as the number of strategies tested increases, the minimum back test length much also increase in order to contain the likelihood of overfitting to IS SR.

As shown extensively throughout ML literature, increased model complexity and number of parameters is one of the primary causes of overfitting. In context of the MinBTL formula, model complexity affects the number of configurations that are available and which may be tested, which in turn will increase likelihood of overfitting. A lack of consideration, or reporting, of the number of trials makes the potential for overfitting impossible to assess.

Bailey et al. expanded on this view with assessing the impact of presenting overfit models as correct. They were able to show that in lieu of any compensation effects (i.e. a series following a Gaussian random walk), there is no reason for overfitting to result in negative performance. However, where compensation effects apply (e.g. economic/investment cycles, bubble bursts, major corrections etc.), then the inclusion of memory in a strategy is likely to be detrimental to OOS performance if overfitting isn't controlled for [5].

2.6.3 Sharpe Ratio

The use of the Sharpe Ratio in financial backtesting is not just an arbitrary or persistent literature choice. The statistic offers two benefits: the effectively strategy-agnostic financial information contained, as well as being relatable to the t-statistic, and so simple to perform hypothesis testing. The SR ratio (estimate from sample as \hat{SR}) is defined as

$$SR = \frac{\mu}{\sigma} \quad (6)$$

The t-ratio is defined as

$$t - ratio = \frac{\hat{\mu}}{\hat{\sigma}/\sqrt{T}} \quad (7)$$

Evidently, the link heree ratio (though it can be generalized to another statistic with a probabilistic interpretation). Additionally, PBO is generally more in line with machine learning literature with the cross validation like approach on time series data.

It should be noted, that the literature detailing usage of the Sharpe ratio for strategy comparison is extensive, with numerous variations and methodologies offered [6]. However, the crux of this paper lies in whether an online neural network is able to make effective enough predictions that a strategy might use the predictions to be profitable. The subtlety here is that we will consider the usage of such forecasting *within* a strategy, rather than *as* a strategy itself. In line with this, statistics such as the Sharpe ratio will be used, but not form a critical consideration of the research here as the comparison of strategies used will be a secondary concern.

3 Implementation

3.1 Process Overview

The implementation focuses on bringing together several ideas: data reduction, deep learning with pre-training/weight initialization, online learning and backtest overfitting validation for the purposes of stock price prediction. To this end, the full process was implemented with the following steps:

- 1 The dataset was split into 3 subsets: the SAE/FFN portion, the OGD portion and the hold-out set for validation
- 2 The first subset was used to train the SAE and deep FFN using the SGD algorithm. These networks were implemented with pre-training and weight initialization techniques
- 3 The second subset of data was used to continue training the network in an online manner using OGD
- 4 The third and last 'hold-out' subset was used to generate log fluctuation prediction
- 5 The predictions from 5 were used in a simple trading strategy to generate returns
- 6 These returns were then used as an input for the CSCV process, and so obtain a PBO calculation for the implementation as a whole

3.2 Feedforward Neural Networks

Feedforward Neural Networks (FFN) in the form of multilayer perceptrons is a well established network technique, providing effective nonlinear representations for both shallow and deep structures [69]. Specifically, a FFN is made up of several non-cyclical layers: the first and last are the input and output layers, respectively, and any inbetween are referred to as 'hidden' layers. Each layer is made up of nodes which are fully connected to the nodes in the previous and following layers, but does not have connections to nodes within the layer - information only travels forward. Each node has an activation function, which acts on the weighted input from the previous layers' nodes.

3.2.1 Notation and Network Representation

- The weights from the j^{th} node in the l^{th} layer from the k^{th} node in the $(l-1)^{th}$ layer are represented by w_{jk}^l
- The bias for the j^{th} node in layer l is represented by w_{0j}^l
- The output for the j^{th} node is defined as $o(z_j)$, for an activation function o and weighted input z
- The weighted input for the j^{th} neuron in a layer is $z_j^l = \sum_{n=i} a_i^{l-1} w_{ij} + w_{0j}$

These definitions allow an input into the network to be propagated through it, having the original values processed through the weights and activations functions, and have an output in the form of the network's last layer.

3.2.2 Activation Functions

As noted in 2.2.2, there are 3 primary characteristics of concern for activation functions: non-linearity, continuous differentiability and monotonicity. While many different functions have been suggested and used, 2 of the most used were implemented here.

Sigmoid The sigmoid, or logistic, function is one of the most popular and widely used activation functions historically, and is defined as

$$f(x) = \frac{1}{1 + e^{-x}} \quad (8)$$

The Sigmoid function is in the range $[0,1]$, making it a suitable choice for problems requiring a probabilistic output. The slope of the function curve is both a boon and a drawback: it allows for fast learning initially, but results in learning slowdown later (often causing what is referred to as node 'saturation'). The exponent calculation is also computationally expensive, relatively speaking.

ReLU The Rectified Linuear Unit (ReLU) is, as discussed in [, a newer activation function which has been shown to](#) be effective in deep learning networks. It is defined as

$$f(x) = \max(0, x) \quad (9)$$

The function has the benefits of quick learning which doesn't saturate, as well as being computationally cheap. The downside is that the non-gradient for the negative range of the function can result in 'dead' nodes, which stop updating with the learning process (though 'Leaky ReLUs' can be used to help resolve this)

3.2.3 Backpropagation

The backpropagation algorithm, as discussed in [2.2.1](#), has allowed for effective training of FNNs for given data. The algorithm relies on incremental improvements of the model, as defined by decreasing the cost function. A common choice for cost is Mean Squared Errors (MSE):

$$C = \frac{1}{2} \|y - a^L\|^2 \quad (10)$$

This allows the backpropagation algorithm to implemented as follows:

- Let N be a neural network of weights w , inputs x and outputs y , where the weights are (naively) initialized to random values
- The algorithm then iterates through the following:
 - 1 Select a set of m samples x_s
 - 2 Forward Pass:
 - i Propagate the samples through the network using the functions defined in [3.2.1](#) to generate out output y_s
 - ii Calculate the error term (aka cost), as

$$\lambda_x^L = \nabla_a C \otimes o'(z^L) = (a^L - y) \otimes o'(z^L) \quad (11)$$

- 3 Backward Pass:
 - i Propagate activation value back through the network to calculate the delta values (the difference between the network outputs and desired output values at each layer)

$$\lambda_x^l = ((w^{l+1})^T \lambda^{l+1}) \otimes o'(z^l) \quad (12)$$

- ii Each weights output delta and input activation are multiplied to find the weights gradient and this gradient is reduced by a factor of the learning rate η , and the mean of this is subtracted from the network weights

$$w^l \rightarrow w^l - \frac{\eta}{m} \sum_x \lambda^{x,l} (a^{x,l-1})^T \quad (13)$$

- 4 Repeat from step 1, unless a minima or other stopping criterion is reached

3.2.4 Gradient Descent Algorithms

Stochastic Gradient Descent (SGD), as discussed in [2.5](#), has been shown to increase the speed at which the backpropagation algorithm can converge a minima in terms of cost. The algorithm runs backpropagation over the entire dataset for a number of 'epochs', and updates the network incrementally through the epoch. The stopping condition for the algorithm is usually defined as either a particular number of epochs being reached, or cost no longer decreasing for some number of epochs (i.e. a minima has been reached).

- For each epoch:
 - 1 Select k samples at random from the data which have not yet been sampled in this epoch
 - 2 Use backpropagation on the network using the k samples to update the weights
 - 3 Repeat 1-2 until all samples from the dataset have been sampled
 - 4 Start a new epoch, or finish if a stopping condition has been reached

Where SGD is appropriate and effective for scenarios where the entire dataset is available, Online Gradient Descent (OGD) is applicable for when the model is learning in an online fashion. In this case, the backpropagation is run as defined above, but for only one sample at a time (i.e. $m = 1$)

3.2.5 Gradient Descent Improvements

This section will detail and improvements that are used in the project - i.e. L1 and L2 regularization, or the learning rate schedule

3.3 Restricted Boltzmann Machines

Restricted Boltzmann Machines (RBM) are generative networks which can be trained to learn probability distributions over a dataset. They are structurally different from a FFN in that they have a recurrent weight function - a typical RBM has one visible layer (input/output), and one hidden layer. A sample will be processed from the input layer to the hidden layer, and the activation values from the hidden layer will be used by the input layer to provide a reconstruction. The hidden units thus correspond to feature detection of the visible unit data structures, and the learning process of the network results in effective parameter estimation.

One of the primary differences from an FFN lies in the stochastic unit determination - the values in a hidden layer will typically be implemented such that they take on a binary value with a probabilistic likelihood. Thus, the input and output have the same structure, and the processing from the hidden layer creates the generative process learned by the RBM. The joint configuration (v, h) of the visible and hidden units has an energy given by:

$$E(v, h) = - \sum_{i \in \text{visible}} a_i v_i - \sum_{j \in \text{hidden}} b_j h_j - \sum_{i,j} v_i h_j w_{ij} \quad (14)$$

where v, h correspond to the binary states of the visible and hidden units, with biases a, b , and weights w . It can be shown that network weights can be adjusted to change the probabilities assigned to a particular training sample. The derivations of 14 show that performing a stochastic ascent for the log probability of the data can be implemented through the following weight adjustment:

$$\Delta w_{ij} = \eta (\langle v_i h_j \rangle_{\text{data}} - \langle v_i h_j \rangle_{\text{model}}) \quad (15)$$

The angular brackets here indicate expectations under the distribution specified by the following subscript. Due to the probabilistic nature of RBMs, the [0,1] ranged Sigmoid activation function is typically used. Thus, for hidden nodes and a data sample v , it is easy to get unbiased sampling of $\langle v_i h_j \rangle_{\text{data}}$

$$p(h_j = 1) = \sigma(w_{0j} + \sum_{i=1} v_i w_{ij}) \quad (16)$$

Similarly, the visible states (or reconstruction), can then be calculated as

$$p(v_i = 1) = \sigma(w_{0i} + \sum_{j=1} h_j w_{ij}) \quad (17)$$

Getting an unbiased sample of $\langle v_i h_j \rangle$ proves more problematic, and so the model reconstructions via Gibbs sampling are used instead (this is explained below), resulting in the weight updates of

$$\Delta w_{ij} = \eta (\langle v_i h_j \rangle_{\text{data}} - \langle v_i h_j \rangle_{\text{reconstruction}}) \quad (18)$$

While it's important for the hidden units to take on a binary value (and so avoid communicating real values rather than learning structure), the visible units may be chosen to take on the probability values, rather than the stochastic samples, particularly if real valued output is necessary.

3.3.1 Contrastive Divergence

The process of sampling and resampling may be run for many iterations between the two layers before finishing on an output - this potentially long running and stochastic process results in the generative aspect of the network, and constitutes a Gibbs sampling chain. Multiple sampling steps in this chain is known as Contrastive Divergence, or CD- n , where n represents the number of steps, and which allows for effective parameter estimation. Thus, CD-1 is the following:

- For a random training sample V' , sample H' from $P(V|H)$
- Sample V from $P(V|H')$
- Sample H from $P(H|V)$
- Return $(V, H) \sim R$, where R is the reconstructed distribution for $\langle vh \rangle$

Using the reconstructed distribution $R(V, H)$, the weight update for CD-1 is, as above, then

$$\Delta CD(W) = \eta(E_{P(H|V)D(V)}[VH^T] - E_{R(V,H)}[VH^T]) \quad (19)$$

There's no upper bound on the iterations used for CD, and running for many can prove more effective for certain purposes. In this case however, where RBMs are used for the purposes of weight initialization, CD-1 is usually deemed sufficient.

3.3.2 CD-1 and SGD

In the same way that the backpropagation learning algorithm in 3.2.3 can be implemented in an SGD process for FFNs, so can the CD learning algorithm for RBMs. The framework is kept the same, with the implementation of epochs and weight updates based on stochastically chosen minibatches, but the calculation used to update the weights is CD-1 instead.

3.4 Stacked Autoencoders

As noted in 2.3, the use of Stacked Autoencoders (SAE) have resulted in significant improvements in deep learning networks, and allowed effective reduction of high dimensional data. A single autoencoder is a specialized type of FNN with 3 layers: one input, one hidden, and one output. The network is trained (using backpropagation as per 3.2.3) to reconstruct the input, so the input and output layers have the same structure, and the hidden layer needs to have fewer nodes than the input. This forces the hidden layer to learn effective features of the data, and reduce the dimensional representation.

Stacked autoencoders follow a similar structure, but with multiple hidden layers. The only strict requirement of the hidden layers is that the middle one, which will be used as the encoder layer, still has fewer nodes than the input. This structure can still be trained using backpropagation, but with more layers, it is likely to begin suffering from the vanishing or exploding gradient problem. As noted, the work by Hinton et al. for initialization of weights helps resolve this.

3.4.1 Greedy Layerwise SAE Training

The algorithm for implementing the SAE training suggested by Hinton et al is as follows

- 1 Define a network structure which conforms to the requirements of an SAE, with L layers
- 2 For the first hidden layer, train as you would for an RBM with 2 layers - with the input layer, and the first layer as the hidden layer, using CD-1 and SGD
- 3 For each layer l in $(2, L/2)$:
 - Process the data through the previously trained layers using the forward propagation as defined in 3.2.1
 - This processed data then forms the input to the l^{th} layer, which can be trained once again using CD-1 and SGD as if it were two layers
- 4 Once all the layers up until the encoder layer have been trained in this greedy layerwise fashion, mirror the weights and layers structures after the encoder to create a fully L layered FNN with pre-trained weights
- 5 This network can then be trained using the backpropagation and SGD algorithms, where cost of reproducing the network input is minimised
- 6 Once a minima or acceptable level of reconstruction has been reached, the network can be truncated as the encoder layer, and so the first $L/2$ layers are used as the SAE

Notably, this weight initialization will only be effective if the RBM and SAE networks use the same activation function, which due to the RBM implementation, needs to be a function that can output a probabilistic value in $[0,1]$.

3.4.2 Denoising Autoencoders

If denoising is implemented (presumably Gaussian denoising), then this section will detail the implementation.

decide

3.5 Deep Network Weight Initializations

As noted in 2.2.1, one of the primary barriers to effective deep learning networks was weight initializations: backpropagated gradient values from SGD would either vanish or explode after multiple layers if the initial weights were too small or too large. The effect of which was to either reduce or completely halt the networks learning process. The first breakthrough, as per 2.3.2, was to initialize the weights through greedy layerwise pretraining of Restricted Boltzmann Machines. Later research, as per ??, has shown that weights can be initialized to maintain expected variance between the input and output layers. Both methods have been implemented and tested for the purposes of SAE and FNN training.

3.5.1 Deep Belief Network Training

4 Data

5 Results

6 Conclusion

7 References

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