OPTIMIZING CONNECTIVITY THROUGH NETWORK GRADIENTS FOR RESTRICTED BOLTZMANN MACHINES

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ABSTRACT

Leveraging sparse networks to connect successive layers in deep neural networks has recently been shown to provide benefits to large scale state-of-the-art models. However, network connectivity also plays a significant role on the learning performance of shallow networks, such as the classic Restricted Boltzmann Machines (RBM). Efficiently finding sparse connectivity patterns that improve the learning performance of shallow networks is a fundamental problem. While recent principled approaches explicitly include network connections as model parameters that must be optimized, they often rely on explicit penalization or have network sparsity as a hyperparameter. This work presents the Network Connectivity Gradients (NCG), a method to find optimal connectivity patterns for RBMs based on the idea of network gradients: computing the gradient of every possible connection, given a specific connection pattern, and using the gradient to drive a continuous connection strength parameter that in turn is used to determine the connection pattern. Thus, learning RBM parameters and learning network connections is truly jointly performed, albeit with different learning rates, and without changes to the model’s classic objective function. The method is applied to the MNIST and other data sets showing that better RBM models are found for the benchmark tasks of sample generation and input classification. Results also show that NCG is robust to network initialization, both adding and removing network connections while learning.

1 INTRODUCTION

While most neural network architectures adopt a fully connected network between units of successive layers, it has been long recognized that network connectivity plays a fundamental role in the model, not only reducing the number of parameters but also leading to a more accurate model or to faster learning Reed (1993); Blalock et al. (2020). This finding has recently reemerged in the context of deep neural networks, and while classic architectures such as ResNet He et al. (2016) and BERT Devlin et al. (2019) have millions of parameters that must be learned, recent works indicate that only a small fraction is necessary for the model to attain a similar performance under an equivalent training effort Blalock et al. (2020).

Most works on leveraging network connectivity to improve the model focus on deep neural networks or large scale networks. However, connectivity patterns play a fundamental role even on simple two-layer networks such as Restricted Boltzmann Machines (RBMs). While the reduction on the absolute number of parameters may be small, recent works observe that an effective connectivity pattern can still yield superior learning curves, learning faster and better Mocanu et al. (2018); de Oliveira & Figueiredo (2022). In fact, the connectivity of an RBM can be interpreted as a hyperparameter that influences its performance, just as the number of neurons (another hyperparameter) in its hidden layer Fischer & Igel (2014); Côté & Larochelle (2016).
Finding the best network connectivity for a given neural network is not a trivial problem, given its dependence on the input (training data), the discrete nature of the connections, and the exponentially large space of possible connection patterns (there are $2^{n^2}$ different networks between two layers with $n$ units each). A common approach to tackle this problem is to construct the connectivity pattern while training the network, starting with a dense network and using some pruning strategy to remove connections in a sequence of rounds (train and prune) Han et al. (2015); Frankle & Carbin (2019). A less explored yet more principled approach is to explicitly include the network connections as parameters that must be optimized in the model Savarese et al. (2020); Chen et al. (2021); Zhou et al. (2021). Intuitively, the model should jointly learn the optimal network weights and network connections during training.

However, the discrete nature of the network connections poses a challenge to widely used continuous optimization frameworks such as (stochastic) gradient descent, since discrete connection parameters have no derivatives (and thus, no gradient). To circumvent this problem, recent approaches adopt continuous variables and functions to represent network connections. Moreover, in order to drive the model towards sparse networks, many incorporate an explicit penalization term (representing the number of connections) into the objective function. Also, the discrete network connectivity is often only determined at the end of training (or a round), and does not evolve jointly with the optimization of other parameters. In contrast, this work proposes a novel method tailored to RBMs based on the notion of “network gradients”.

In a nutshell, the Network Connectivity Gradient (NCG) method computes the gradient for every possible network connection for any given connectivity pattern. Moreover, NCG uses a continuous parameter to represent the strength of every possible network connection which is updated according to the gradient as any other model parameter. Finally, the network strength is thresholded to yield a discrete connectivity pattern during optimization (i.e., at each training iteration) which in turn determines how information (probabilities) and gradients flow on the model during training.

Intuitively, the network gradient indicates the relevance of each possible connection given the current connection pattern. This gradient drives the connection strength parameter which in turn determines if a connection should be present or absent, effectively adjusting the connection pattern as the model is trained. Thus, if the initial connectivity pattern is too sparse or too dense, NCG will enable or disable connections early during training, respectively. In essence, NCG truly learns the network connectivity jointly with other RBM parameters, albeit with possibly different learning rates. Note that no changes are required to the objective function of the RBM.

Beyond proposing NCG, this work evaluates the method using the MNIST data set on two orthogonal tasks often used to assess RBMs: sample generation (average NLL is the performance metric) and input classification (accuracy is the performance metric). For the classification task, two other data sets from the UCI Evaluation Suite Dua & Graff (2017) are considered (Mushrooms and Connect-4). In both tasks NCG shows a superior learning curve, both learning faster and more accurately than a classic fully connected RBM. The evaluation also shows that NCG removes and adds network connections during training, indicating its effectiveness in searching for optimal network patterns and robustness to initialization. Comparison with static patterns and the SET method Mocanu et al. (2018) (also designed for optimizing the network connectivity of RBMs) indicate the superiority of NCG, especially during the early phases of training.

The remainder of this work is organized as follows: Section 2 has a cursory discussion of related works; Section 3 imparts a brief explanation of the RBM; Section 4 presents the NCG method proposed in this work; Section 5 shows the experimental results; and Section 6 has the concluding remarks.

2 RELATED WORK

Recent developments in Neural Architecture Search (NAS) focus on the design of effective network architectures for deep neural networks targeted to solve a given task. The design spaces often consider the structure of layers through which information flows as well as the type of operation (aggregation/activation) applied by each layer Elsken et al. (2019). Optimization problems that consider different design spaces for the network can be formulated and solved using different...
techniques Liu et al. (2019); Fang et al. (2020); Gao et al. (2022). However, due to extremely large search spaces such approaches focus on the macro scale organization of the network, and not on the fine connectivity pattern of consecutive layers (other than a small set of pre-defined connectivity patterns, such as different convolutions).

Independently of NAS, the idea of removing (pruning) connections between two adjacent network layers has recently reemerged in the context of deep neural networks. Pruning can improve the model’s learning curve (learning faster or better) and drastically reduce the number of model parameters Reed (1993); Blalock et al. (2020); Liang et al. (2021); Lin et al. (2021); Zhang et al. (2022). Finding the optimal connectivity pattern for two adjacent layers is not a trivial task. Most pruning approaches start with dense networks and iterate in rounds of training the model parameters and using the parameter values (and the input samples) to prune network connections, however pruning can also be performed before training starts Lee et al. (2019); de Jorge et al. (2021). In these approaches different heuristics are often used to determine which connections should be removed.

A more principled yet less explored approach explicitly includes the network connectivity as a parameter of the model, making the network connectivity a part of the optimization problem. This often requires increasing the number of parameters and modifying the objective function to induce pruning. A prominent example is Continuous Sparsification Savarese et al. (2020), that uses continuous parameters and continuous functions to approximate the discrete nature of network connections, and adds a penalization term to the objective function. The discrete network connectivity is determined at the end of training rounds. UGS Chen et al. (2021) deploys a similar approach tailored to Graph Neural Networks (GNN). Similar to this present work, DNW Wortsman et al. (2019) does not add penalization to the objective function, but keeps a constant number of edges (a hyperparameter) with the largest weight magnitude, discovering good sparse subnetworks in predefined network architectures. Another recent approach is SR-STE Zhou et al. (2021) where the (discrete) connectivity pattern is updated at each training iteration. However, the method assumes that each input unit is connected to a fixed number of output units and thus sparsity is predefined (a hyperparameter).

All prior works above focus on deep neural networks. However, network connectivity also plays a fundamental role on simple two-layer networks, including the Restricted Boltzmann Machine (RBM), a principled and probabilistic model that has been widely explored and applied in literature Fischer & Igel (2014); Decelle & Furtlehner (2021). RBMs’ hyperparameters have a significant impact on the model’s performance which has prompted different methods that choose adequate hyperparameters for a given task and input data Côté & Larochelle (2016); Hinton (2012); Papa et al. (2015). A prominent example is the infinite RBM Côté & Larochelle (2016), a variation where the number of hidden units (a hyperparameter in the classic model) is an explicit model parameter that is determined during training.

The connectivity between layers have also been investigated for RBMs. For example, recent work has shown that crafted connectivity patterns can yield significantly better learning performance on RBMs de Oliveira & Figueiredo (2022), and that sparse representations of RBMs can lead to more accurate and faster learning for Deep Belief Models (DBN) Wang et al. (2020). Moreover, the Sparse Boltzmann Machines (SBM) is a model where the connectivity is a sparse two-layer tree-like network Chen et al. (2017). Different tree-like networks can be learned from data and then used as hyperparameters when training the RBM, generating models that are less likely to over fit and that have better interpretability with respect to the dense RBM. In a more recent work, the network connectivity of the RBM is learned during training along with other model parameters. Their approach (called SET method) removes connections with the smallest weights and adds the same number of randomly chosen new connections at each training round Mocanu et al. (2018). Thus, network sparsity is predefined (a hyperparameter). In contrast, NCG (to be presented) learns the connectivity and sparseness during training using the gradients of the unmodified objective function of the model.

3 The Restricted Boltzmann Machine

The Restricted Boltzmann Machine (RBM), first proposed under the name Harmonium Smolensky (1986), is an energy-based model for unsupervised learning. It is a classic neural network model that has been applied to a number of different tasks. While initially designed for sample generation Decelle & Furtlehner (2021); Roux et al. (2011); Tang et al. (2012), it has been used for classification
While there are other methods that yield better approximations by changing how the approximation is marginal to main theme of this work.

An RBM is a probabilistic model composed of two layers of binary units: one visible $x$ of size $X$, representing the data, and one hidden (or latent) $h$ of size $H$, that extracts characteristics and increases learning ability. The two layers are fully connected through undirected weighted connections in a bipartite network. Figure 1 shows the example of an RBM network with $X = 4$ and $H = 5$.

Each configuration $(x, h)$ has the following associated energy: $E(x, h) = -h^T W x - x^T d - h^T b$, where $W \in \mathbb{R}^{H \times X}$ is the weight matrix of the layers’ connections ($w_{ij}$ is the weight between visible unit $x_j$ and hidden unit $h_i$), $d \in \mathbb{R}^X$ is the visible units’ bias vector ($d_j$ is the bias for $x_j$) and $b \in \mathbb{R}^H$ is the hidden units’ bias vector ($b_i$ is the bias for $h_i$). $W$, $d$ and $b$ are the model parameters, subsequently denoted by $\theta = (W, d, b)$. The probability distribution of the RBM is defined as $P_{\theta}(x, h) = Z^{-1} e^{-E(x, h)}$, with $Z$ being the normalization constant (or partition function). Note that this equation is in general not tractable due to the very large number of configurations ($2^{X+H}$, since all units are binary), and therefore for the most part one cannot know the exact probability of a given $(x, h)$ configuration.

### 3.1 Training the Restricted Boltzmann Machine

The RBM is typically trained to minimize the Negative Log-Likelihood (NLL) of the available data set, which is equivalent to maximizing the Log-Likelihood. In this case, the average NLL is often adopted in order to simplify the learning procedure. Given a data set $\{x^{(t)}\}_{t=1,...,T}$ with $T$ samples, the average NLL of the model is simply $\frac{1}{T} \sum_{t=1}^{T} - \ln P_{\theta}(x^{(t)})$. Note that the probability $P_{\theta}(x^{(t)})$ depends on the model parameters, $\theta$.

The RBM is trained by applying Stochastic Gradient Descent (SGD) Bottou (2010). Due to the intractability of the normalization constant, training methods such as Contrastive Divergence (CD) Hinton (2002) approximate the gradient with the following expression:

$$
\frac{1}{|B|} \sum_{t \in B} E_h \left[ \nabla_\theta E(x, h) \bigg| x = x^{(t)} \right] - \frac{1}{|B|} \sum_{t \in B} E_h \left[ \nabla_\theta E(x, h) \bigg| x = \tilde{x}^{(t)} \right],
$$

where $B$ corresponds to a batch of samples randomly chosen from the data, since Hinton (2012) has shown that computing the gradients using batches rather than the full data often leads to better learning curves; and $\tilde{x}^{(t)}$ is a random sample of the RBM given its parameters. Note that equation 1 requires generating a random sample from the RBM distribution for each data sample $x^{(t)}$, which is done applying $k$ steps of Gibbs Sampling on the model, starting from the data sample $x^{(t)}$.

While there are other methods that yield better approximations by changing how $\tilde{x}^{(t)}$ is generated Fischer & Igel (2014), this work focuses on the traditional CD method since improving such approximation is marginal to main theme of this work.

Calculating the corresponding expectations for each model parameter $w_{ij}, b_i, d_j$, the resulting parameter update rules are given by:

$$
W \leftarrow W + \alpha \frac{1}{|B|} \sum_{t \in B} \left( \hat{h}(x^{(t)}) x^{(t)T} - \hat{h}(\tilde{x}^{(t)}) x^{(t)T} \right)
$$
The classic RBM considers a fully connected network between its input and hidden layers. However, this is not necessarily the best connectivity pattern for learning a model for a particular task, prompting the investigation of other patterns.

Let \( A \in \mathbb{B}^{H \times X} \) denote a binary matrix that represents a given connectivity pattern for the RBM, in the sense that \( a_{ij} = A[i, j] = 1 \) if hidden unit \( h_i \) is connected to input unit \( x_j \), or \( a_{ij} = A[i, j] = 0 \) otherwise. Figure 2 shows examples of the adjacency matrix \( A \) for two connectivity patterns. Note that it is generally intractable to enumerate them even in the case of small models (\( 2^{H \times X} \) possibilities of \( A \)). In order to incorporate \( A \) into the model, the weights in matrix \( W \) must be zero on entries where a connection is not present. Thus, let \( C = W \odot A \) denote the acting weights of the model where \( \odot \) is the element-wise matrix product such that \( c_{ij} = C[i, j] = w_{ij}a_{ij} \). The classic model parameters can be learned as before by using matrix \( C \) instead of \( W \) to compute the gradients.

The novelty of the proposed method lies on computing a gradient for each possible element (connection) of \( A \). This can be analytically derived as with the other RBM parameters, where \( \theta \) in equation 1 also includes \( A \). In particular, the expectation over the energy gradient is given by

\[
\mathbb{E}_h [\nabla_{a_{ij}} E(x, h) | x] = \mathbb{E}_h \left[ \nabla_{a_{ij}} (-h_ia_{ij}w_{ij}x_j) | x \right] = -P_h(h_i = 1 | x) w_{ij}x_j = -\sigma(C_i, x + b_i) w_{ij}x_j = -\hat{h}_i(x) w_{ij}x_j
\]

where \( C_i \) is the \( i \)-th row in matrix \( C \). This expectation is used to calculate the gradient (Equation 1). Note that the gradient for a connection \((x_i, h_j)\) can be non-zero even when \( a_{ij} = 0 \). This is a key aspect in the methodology here proposed, since it provides a gradient for absent connections and consequently the possibility for them to be enabled (or permanently disabled).

However \( a_{ij} \) is binary, and thus the usual continuous optimization framework that leverages the gradient to update its value does not apply. To circumvent this limitation, a continuous parameter denoting the connectivity strength is introduced in the model, and represented by \( \alpha' \in [0, 1]^{H \times X} \) such that \( 0 \leq \alpha'_{ij} = A'[i, j] \leq 1 \). Thus, the connection strength can be updated using the corresponding gradient (but saturating at 0 or 1), and the binary connection becomes a function of the connection strength. In particular, a simple threshold (step) function is used to determine the presence or absence
of a connection. This idea leads to the following two-step update rule for the connection parameters:

\[
\begin{align*}
    a_{ij}' &\leftarrow a_{ij}' + \alpha_a \left[ \frac{1}{|B|} \sum_{t \in B} \left[ \hat{h}_i(x^{(t)}) w_{ij} x_j^{(t)} - \hat{h}_i(\tilde{x}^{(t)}) w_{ij} \tilde{x}_j^{(t)} \right] \right] \\
    a_{ij} &\leftarrow \mathbb{I}[a_{ij}' \geq \gamma]
\end{align*}
\]  

(6)

where \( \gamma \) is the hyperparameter that denotes the threshold for enabling/disabling a connection based on the connections strength, \( \mathbb{I}[\cdot] \) corresponds to the indicator/step function, and \( \alpha_a \) to the connectivity learning rate. The method is called Network Connectivity Gradient (NCG) and jointly learns the connectivity pattern and classic model parameters for the RBM. Note that \( \alpha_a \) allows to decouple the learning rate of model parameters from the connectivity pattern, which can lead to better learning curves, as shown in Section 5.3, which has empirically shown to bring advantages to the learning curves (discussed in the appendix).

4.1 Connectivity initialization

A fundamental aspect in continuous optimization frameworks such as SGD is the initialization of the parameters that must be optimized. Being parameters, the connectivity pattern and the connection strength must also be initialized. While the fully connected network is a possible initialization, intuitively it may not be the best pattern to start the optimization since it may take too many iterations to remove connections. A common initialization method in the context of RBM (and other models) is choosing random (and small) values for the parameters. Thus, by following this method each possible connection is initialized as active \((a_{ij} = 1)\) with probability \( p \) or inactive \((a_{ij} = 0)\) with probability \( 1 - p \). Intuitively, \( p \) will influence the learning performance of the RBM, since large/small \( p \) can lead to dense/sparse networks that may require many iterations to evolve. Thus, \( p \) is a hyperparameter of the initialization procedure.

Once the initial connection pattern has been determined, the connection strengths must also be defined. While initializing \( a_{ij}' = a_{ij} \) is a possible initialization, this leads to connection strengths that are either 0 or 1 which may require too many iterations in order to cross the threshold to enable or disable the connection, respectively. To avoid this cold start, connection strengths are randomly initialized as follows:

\[
    a_{ij}' = U(0, \gamma) \cdot \mathbb{I}[a_{ij} = 0] + U(\gamma, 1) \cdot \mathbb{I}[a_{ij} = 1],
\]  

(7)

where \( U(a, b) \) is the continuous uniform random value in the interval \([a, b]\). Note that the random value of the connection strength depends on the threshold \( \gamma \) for enabling/disabling the connection. Intuitively, a random value is chosen in the segment corresponding to the connection being absent (range \([0, \gamma]\)) or present (range \([\gamma, 1]\)).

5 Empirical Evaluation

Two tasks will be considered to evaluate the learning performance of the RBM under the NCG methodology: sample generation (average NLL is the performance metric) and sample classification (accuracy is the performance metric). The main data set used is MNIST, a frequently used benchmark in computer vision and the RBM literature Fischer & Igel (2014). Also, two data sets from the UCI Evaluation Suite Dua & Graff (2017) are used for the classification task: Mushrooms and Connect-4.

The MNIST data set consists of gray-scale square images of 28 × 28 pixels. It has two separate sets of data: a train set, with 60 k samples; and a test set, which has 10 k samples. The images were converted into black and white in order to be directly used as input to the RBM. The conversion was probabilistic such that each pixel was assigned a black color with probability proportional to its darkness (gray-scale) in the original image, a methodology commonly adopted Salakhutdinov & Murray (2008); Côté & Larochelle (2016). Some examples of the resulting data are shown in figure 3.

For MNIST, each image in the data set has 784 pixels, each of which corresponds to a visible unit of the RBM. The experiments use 500 hidden units, and training was achieved using CD with 10

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1 Data set available at [http://yann.lecun.com/exdb/mnist/](http://yann.lecun.com/exdb/mnist/).

2 Data sets available at [https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/](https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/)
The learning rate for the model parameters was set to $\alpha = 0.1$ and mini batches of 50 random samples. The connectivity learning rate was $\alpha_A = 0.5$, unless otherwise specified. No momentum or weight decay were used. The RBM weight parameters were initialized with null biases and small random weights, uniformly distributed in the interval $[-1, 1]$. For the connection threshold in NCG, $\gamma = 0.5$ was adopted as this is the midpoint value in the possible range for the connection strengths, not favoring either a more sparse ($\gamma > 0.5$) or dense network ($\gamma < 0.5$).

During training, one epoch corresponds to one iteration over the entire training data set with the model’s parameters being updated at every batch. Since the batch size was 50 data samples, an epoch corresponds to 1200 parameter updates necessary to iterate over the 60 k samples in this data set. Batch elements are randomly determined for every epoch.

Besides MNIST, two other data sets were used. The Mushrooms data set contains characteristics of different types of mushrooms, subdivided into edible and poisonous categories. There are 21 attributes, converted into 112 binary features, and 8124 samples (subdivided into 2 k for training the rest for testing). Lastly, the Connect-4 data set contains board situations for the game of Connect-4, labeled by whether the first player wins, loses, or there is a draw. There are 67557 samples (with 16 k separated for training), each with 42 board spaces, converted into 126 binary features.

Experiments for the UCI Evaluation Suite data sets used 100 hidden neurons, batch of 10 random samples, $\alpha = 0.01$ and $\alpha_A = 0.05$, unless otherwise specified. Other hyperparameters were kept the same as specified for MNIST.

Although fine-tuning these parameters could improve the learning performance of the RBM, the goal of this work is to compare NCG with other connectivity patterns, and not necessarily obtain the best model across different hyperparameters.

5.1 Generative Results

In the sample generation task, a classic generative RBM is trained as to generate random samples similar to the input examples. The performance is assessed using the average NLL across the training set. Since the exact average NLL cannot be computed due to intractability of the normalization constant, the Annealed Importance Sampling (AIS) method is used as an approximation Salakhutdinov & Murray (2008), with 100 runs and 14.5 k intermediate distributions. Note that all experiments on this task are evaluated using the MNIST data set.

Figure 4 shows the learning curve (evolution of the average NLL over the epochs) for the classic fully connected RBM and three initializations of the NCG method. Clearly, the fully connected network exhibits a significantly worse learning curve, both in terms of sample mean and variance. Interestingly, the three different initializations for NCG exhibit a very similar performance (with the exception of a few outliers for the case $p = 1$).\footnote{While training NCG with $p = 1$, two of the 10 runs exhibited much higher than average NLL at epoch 120 and one of the 10 runs at epoch 200.} While the mean performance for $p = 0.1$ could be said to be slightly better, the overlapping quartiles show that the sparsity of the random initialization is not particularly important in this scenario. Indeed, the similar learning curves indicate that NCG can find effective networks independently of the (random) initial connectivity, and is therefore robust to connectivity initialization.

Despite the similar learning curves, the evolution of the network degrees is very different across the different initializations. Figure 5 shows the evolution of the maximum, minimum and average degree of the hidden units for the three initializations. For $p = 1$ a sharp decrease is observed in all three statistics in the first 10 epochs, with the curves indicating a slight decay even over 200 epochs, while for $p = 0.5$, the initial decrease is not as strong and the curves seem closer to convergence. Interestingly, the case $p = 0.1$ shows an increase in all three statistics in the first 10 epochs and...
convergence after 200 epochs. This shows that NCG can not only prune connections but also add connections when the network is too sparse. The similar learning curves but different network patterns indicate that the joint optimization of model parameters and network connectivity can compensate for one another, leading to similar performance even when the connectivity pattern is different. Indeed, the literature of network pruning suggests that different network patterns can often achieve similar performance Blalock et al. (2020).

Further insight is provided by figure 6 which shows that NCG tends to increase the number of connections when the initial network is too sparse (up to 30% of connections initially activated) and decrease the number of connections when the initial network is too dense (40% or more connections). Note that randomness of the final density (vertical bars) is much larger than that of initial density (horizontal bars), as the final density depends on the optimization.

Despite the good performance, it is known that sparse networks can outperform their dense counterparts. Indeed, even simple patterns such as the line pattern (connecting each hidden unit to $v$ consecutive visible units) can achieve better learning curves de Oliveira & Figueiredo (2022), which prompts the need to compare NCG with connectivity baselines. Figure 7 shows the learning curves of NCG together with both the line pattern and a random pattern (corresponding to a bipartite Erdős-Rényi random graph). For fairness of comparison, RBMs with the same (average) number of initial connections are created for all patterns: 50% and 10% densities. Note that NCG shows
better performance than any other pattern after 50 training epochs (for both initializations) while also showing less noisy learning curves. Interestingly, all patterns outperformed the fully connected RBM.

Lastly, Figure 8 shows a direct comparison between NCG and SET, trained with 2500 hidden units, sparsity parameter $\epsilon = 11$ and fraction of removed edges $\zeta = 0.3$ (parameters reported in the original
paper, using the publicly available code). For the learning rate, experiments were performed with both 0.1 and 0.01 values. The first allows for a direct comparison with the NCG experiments (same learning rate) and the second reduces the fluctuations during learning. However, note that SET did not outperform the fully connected network (on this task), and was thus significantly outperformed by NCG.

5.2 Classification Results

In the classification task, the RBM is trained to classify the given input (the digit in the image, for MNIST). The RBM is expanded to have additional visible (input) units in order to encode the label of the image during training Fischer & Igel (2014); Larochelle et al. (2012). There is one extra unit per class, and only one is activated for each input sample, the one corresponding to the sample class (the image digit, from 0 to 9, for MNIST). The connections between hidden units and the label units are fixed and not subjected to optimization, as they are crucial for the classification task. Moreover, the RBM is trained using Contrastive Divergence as in the generative task, and is not a priori aware of the classification task (no changes to the objective function).

While the generative task relied on the approximate NLL to measure the learning performance of the RBM, the classification task uses the accuracy as performance, given by the fraction of images correctly classified. Classification is performed by presenting the image to the RBM, setting each label units to 0.5, calculating the probabilities of each hidden unit being activated, and finally selecting the label unit (digit) with the higher probability of being activated. This digit is the predicted label for the image.

Figure 9 shows the evolution of the classification accuracy over the epochs for different NCG initializations for the train and test sets. Note that all three initializations generate models that are consistently better than the fully connected RBM in the early stages of training. Moreover, the performance between training and test sets are qualitative and quantitatively similar, indicating there is likely no overfitting.

Interestingly, figure 9 shows that accuracy is inversely proportional to the initial density during the first epochs of training: initializing the network with fewer connections yields superior accuracy in early stages of training. However, as the number of epochs increase, the accuracy between the NCG
models becomes more similar. This indicates that NCG is capable of overcoming a poorly initialized connectivity pattern by adjusting both the connections and model weights. Note that the degrees of the hidden units of different initializations are still very different after 10 epochs, as shown in figure 6, despite the similar accuracy performances.

As with the generative task, NCG was also compared with the line and random patterns in the classification task. Figure 10 shows the accuracy of these different models for the first 10 epochs.
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![Graphs showing classification accuracy over training epochs for different data sets and network configurations.](image)

Figure 11: Classification accuracy over the training epochs of NCG for the test and train sets of the MNIST, Mushrooms, and Connect-4 data sets with $\alpha_A = \alpha$ (0.1 for MNIST and 0.01 for the other data sets); lines correspond to the sample mean over 25 experimental runs.

...connection pattern fast enough and the connectivity gradient becomes subdued by other model parameters. This example highlights the importance of decoupling the learning rates when jointly optimizing network connectivity and other model parameters.

5.3 Learning Rate Analysis

Empirical results showed that adopting a higher learning rate for the connectivity parameters allows the network connectivity to evolve fast in the early stages of training. Intuitively, this allows NCG to quickly adjust for poor initial network patterns before other model parameters start to converge. As discussed below, this decoupling of the learning rates (and being faster for network connectivity) is crucial for NCG.

Figure 11 shows the accuracy when using the same learning rate for both the connectivity and the other model parameters, $\alpha_A = 0.1$ for MNIST and $\alpha_A = 0.01$ for the Mushrooms and the Connect-4 data sets. In comparison to figures 9 and 10, note the significant decrease in accuracy for all three initialization and all epochs of training. Moreover, only the networks initialized with all connections activated ($p = 1$) manages to achieve a higher mean accuracy than the traditional RBM (fully connected network) for all three data sets. This is in marked contrast to the previous results, for which NCG shows better performance than the traditional RBM even for initializations with 50% and 10% of the connections activated.

Interestingly, the initialization with 10% of the connections activated ($p = 0.1$) often shows superior performance after the first epoch of training, having the best mean performance for both the MNIST and Mushrooms data sets. However, the model fails to continue improving its accuracy and falls behind the other models, including the fully connected network. Intuitively, the model cannot adjust its connection pattern fast enough and the connectivity gradient becomes subdued by other model parameters. This example highlights the importance of decoupling the learning rates when jointly optimizing network connectivity and other model parameters.
6 CONCLUSION

This work presented Network Connectivity Gradient (NCG), a method tailored to RBMs that learns the optimal connectivity network jointly with other model parameters (weights and biases). NCG computes gradients for each possible network connection given a connectivity pattern. The gradients are used to drive the continuous connectivity strength parameter that in turn determines to maintain, add or remove the connection in each training epoch. NCG requires no change in RBM’s objective function nor its classic optimization framework. Evaluation of NCG on generative and classification tasks using the MNIST and other data sets demonstrated its effectiveness in learning better models (learning faster and better) than the dense RBM, other static patterns, and the SET method, as well as robustness with respect to its initialization.

However, recent works on pruning at initialization Lee et al. (2019); de Jorge et al. (2021) might be leverage to design more effective initial networks for NCG. Last, while NCG has been designed for RBMs, future work will reveal if its core ideas can be applied to other neural network models.

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A Classification Degree Statistics

Figure 12 portrays the degree statistics (minimum, average, and maximum) of the network’s hidden units over the epochs for the NCG classification experiments in the MNIST data set (Figure 9 shows the accuracy). Note that for $p = 1$ all degrees are 784 at time zero, and NCG significantly reduces the degrees of the network; the average degree is reduced by 30% after 10 epochs. On the other hand, for $p = 0.1$, NCG significantly increases the degrees of the network; the average degree is 2.5 times larger after 10 epochs. Finally, for $p = 0.5$ NCG shows a relatively small change in the degrees. Moreover, while the degrees change and converge over the epochs, the initialization density has a strong influence: the average degree of the three models after 10 epochs reflects their initial density.

![Figure 12](image1)

Figure 12: Degree statistics (minimum, average, maximum) of the hidden units over the training epochs for the MNIST data set – lines correspond to the sample mean and shades to the sample quartiles over 25 experimental runs.

Furthermore, figure 13 shows the degree statistics of the networks trained for the Mushrooms data set, and figure 14 for the Connect-4 data set. These experiments pertain to the accuracy performances

![Figure 13](image2)

Figure 13: Degree statistics (minimum, average, maximum) of the hidden units over the training epochs for the Mushrooms data set – lines correspond to the sample mean and shades to the sample quartiles over 25 experimental runs.

![Figure 14](image3)

Figure 14: Degree statistics (minimum, average, maximum) of the hidden units over the training epochs for the Connect-4 data set – lines correspond to the sample mean and shades to the sample quartiles over 25 experimental runs.
portrayed in figure 10. Once again, one can see that the final sparsity reflects the initial sparsity, and the networks end training with very different connectivity patterns after 10 epochs, despite the similar accuracy performances.

Lastly, figures 15, 16 and 17 show the degree statistics for training experiments with a lower connectivity learning rate. The plots correspond, respectively, to experiments performed with the MNIST, Mushrooms and Connect-4 data sets, and pertain to the accuracy results presented in figure 11. As expected, one can see much less change in the connectivity with regards to the previous experiments, which use a higher learning rate. This is especially notable for the MNIST $p = 1$ experiments.

Figure 15: Degree statistics (minimum, average, maximum) of the hidden units over the training epochs for the MNIST data set trained with $\alpha_A = \alpha = 0.1$ – lines correspond to the sample mean and shades to the sample quartiles over 25 experimental runs.

Figure 16: Degree statistics (minimum, average, maximum) of the hidden units over the training epochs for the Mushrooms data set trained with $\alpha_A = \alpha = 0.01$ – lines correspond to the sample mean and shades to the sample quartiles over 25 experimental runs.

Figure 17: Degree statistics (minimum, average, maximum) of the hidden units over the training epochs for the Mushrooms data set trained with $\alpha_A = \alpha = 0.01$ – lines correspond to the sample mean and shades to the sample quartiles over 25 experimental runs.
B QUARTILE FIGURES

Some plots in the main body had their uncertainties removed to avoid clutter. The plots with quartile representing the uncertainty are shown here. Figure 18 shows the learning curves of NCG and the classic RBM compared to the line and random patterns, as in Figure 7, and figure 19 shows the comparison with the SET method, as in figure 8, for the generative task.

Figure 18: (Regarding figure 7) Average NLL over the training epochs – lines are the mean values and shades are the quartiles over 10 experiments. Comparison of NCG with the Line and Random patterns.

Figure 19: (Regarding figure 8) Average NLL over the training epochs – lines are the mean values and shades are the quartiles over 10 experiments. Comparison of NCG with the SET method Mocanu et al. (2018).

Meanwhile, Figure 20 presents the classification results for training of NCG compared with the fully connected RBM, the line and the random patterns, for data sets MNIST, Mushrooms and Connect-4, as in Figure 10. Lastly, figure 21 shows the classification performances of NCG for training with lower connectivity learning rate (same learning rate as the other model parameters, $\alpha_A = \alpha$), as in figure 11.
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Figure 20: (Regarding figure 10) Classification accuracy for NCG, the classical RBM, and the Line and Random patterns for the test and train sets of MNIST, Mushrooms and Connect-4 data sets; lines are the sample means and shades are the quartiles over 25 runs.

Figure 21: (Regarding figure 11) Classification accuracy over the training epochs of NCG, for the test and training sets of MNIST, Mushrooms and Connect-4 data sets with $\alpha_A = \alpha$; lines are the sample means and shades are the quartiles over 25 runs.
C \textbf{CONTRASTIVE DIVERGENCE APPROXIMATION}

The experiments on this article applied Contrastive Divergence training using 10 steps of Gibbs Sampling (CD-10). However, changing the number of steps (and the way of obtaining the sample \( \tilde{x} \) entirely) can deeply affect results. To exemplify this, some evaluations using CD-1 (only one step of Gibbs Sampling) were performed. This creates a poorer gradient approximation, which usually affects training negatively.

\textbf{Generative Results} Figure 22 portrays the learning curves for dense RBM and NCG, and Figure 23 the corresponding degree statistics. It is clear that CD-1 causes a major performance drop for all models considered: by the end of training the fully connected RBM has the average NLL around 290 in comparison to the 150 seen in Figure 4, and the models trained with the NCG method reach at most 150, when before the worse average did not surpass 120. The degree statistics for \( p = 1 \) and \( p = 0.5 \) appear to show less change along the epochs than what was observed for CD-10, but the differences do not appear to be significant.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure22.png}
\caption{Average NLL over the training epochs for the MNIST dataset with CD-1 – lines correspond to the sample mean and shades to the sample quartiles over 10 experimental runs.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure23.png}
\caption{(a) \( p = 1 \) \hspace{2cm} (b) \( p = 0.5 \) \hspace{2cm} (c) \( p = 0.1 \)}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure23.png}
\caption{Degree statistics (minimum, average, maximum) of the hidden units over the training epochs. Generative results on MNIST, trained using CD-1. Lines correspond to the sample mean and shade corresponds to the sample quartiles over 10 experimental runs.}
\end{figure}

Interestingly, the NCG models’ NLL increase less than the classical RBM, for which the final NLL is double the value when considering CD-10, and the relative increase in performance derived from optimizing the connectivity (NCG) is much larger.

\textbf{Classification Results} While the goal in the classification task is to maximize accuracy, the objective function used during training with aims to minimize the NLL, using CD as an approximation to

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the gradient. Therefore NCG trains the connectivity network for a slightly inaccurate objective, as well as all the other parameters that the traditional network trains. It stands to reason, therefore, that in worsening the approximation for the gradients, its performance will suffer.

Figure 24 shows the evolution of the accuracy over epochs for the dense RBM as well as three initializations for the NCG model, for both the train and test sets. Figure 25 presents the corresponding degree statistics evolution, giving an idea of how the connectivity changes with training. Once again, the degree statistics do not show much difference from their CD-10 counterparts, except that they suffer less change throughout training.

Figure 24: Classification accuracy over the training epochs for the train (a) and test (b) sets of the MNIST data set. Trained with CD-1. Lines correspond to the sample mean and shades to the sample quartiles over 25 experimental runs.

Figure 25: Degree statistics (minimum, average, maximum) of the hidden units over the training epochs. Classification results on MNIST, trained with CD-1. Lines correspond to the sample mean and shades to the sample quartiles over 25 experimental runs.

Although all RBMs have a worse accuracy when training with CD-1, it is clear from the results that the relative performance between NCG and the fully connected model diminishes. In these circumstances, only NCG initializing with all connections activated ($p = 1$) manages to surpass the traditional RBM, and even then they have very close results. It is not clear that the difference is statistically significant. The $p = 0.1$ training seems to suffer the most, not showing a better accuracy even in the first epoch of training. Overall, the results indicate a very different scenario in comparison to the one observed in the generative task, for which the addition of connectivity optimization resulted only in positive results, regardless of the CD approximation used.

### D SET TRAINING

As mentioned in Section 5.1, the learning curves reported for the SET method used the hyperparameters mentioned by Mocanu et al. (2018). Figure 26 shows the comparison of NCG with SET, in which SET was trained with the same parameters as the previous experiments. Note that the sparsity
parameter $\epsilon$ was chosen so as to create SET networks with nominal sparsity of 50% and 10% of all possible connections activated, which corresponds to values used for NCG initialization.

![Graph showing average NLL over training epochs](image)

Figure 26: Average NLL over the training epochs – lines are the mean values and shades are the quartiles over 10 experiments. Comparison of NCG with the SET method.

This choice of hyperparameters for the SET method did not yield good performance, which shows noisy learning curves without apparent convergence. Since this scenario did show good results for SET, experiments with other hyperparameters were performed and reported in Figure 8. In any case, NCG showed significantly superior and more robust performance (less noisy learning curves).