

# Accelerating Deep Learning with Memcomputing

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## Abstract

Restricted Boltzmann machines (RBMs) and their extensions, often called “deep-belief networks”, are very powerful neural networks that have found widespread applicability in the fields of machine learning and big data. The standard way to training these models resorts to an iterative unsupervised procedure based on Gibbs sampling, called “contrastive divergence”, and additional supervised tuning via back-propagation. However, this procedure has been shown not to follow any gradient and can lead to suboptimal solutions. In this paper, we show a very efficient alternative to contrastive divergence by means of simulations of digital memcomputing machines (DMMs). We test our approach on pattern recognition using the standard MNIST data set of hand-written numbers. DMMs sample very effectively the vast phase space defined by the probability distribution of RBMs over the test sample inputs, and provide a very good approximation close to the optimum. This efficient search significantly reduces the number of generative pre-training iterations necessary to achieve a given level of accuracy in the MNIST data set, as well as a total performance gain over the traditional approaches. In fact, the acceleration of the pre-training achieved by *simulating* DMMs is comparable to, in number of iterations, the recently reported *hardware* application of the quantum annealing method on the same network and data set. Notably, however, DMMs perform far better than the reported quantum annealing results in terms of *quality* of the training. Our approach is agnostic about the connectivity of the network. Therefore, it can be extended to train full Boltzmann machines, and even deep networks at once.

**Keywords:** Deep Learning, Restricted Boltzmann Machines, Memcomputing

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## 1. Introduction

The progress in machine learning and big data driven by successes in deep learning is difficult to overstate. Deep learning models (a subset of which are called “deep-belief networks”) are neural networks with a certain amount of layers,  $n$ , with  $n > 2$  [1]. They have proven themselves to be very useful in a variety of applications, from computer vision [2] and speech recognition [3] to super-human performance in complex games[4], to name just a few. While some of these models have existed for some time [5], the dramatic increases in computational power combined with advances in effective training methods have pushed forward these fields considerably [6].

Successful training of deep-belief models relies heavily on some variant of an iterative gradient-descent procedure, called back-propagation, through the layers of the network [7]. Since this optimization method uses only gradient information, and the error landscapes of deep networks are highly non-convex [8], one would at best hope to find an appropriate local minimum.

However, there is evidence that not even this is sufficient. In these high-dimensional non-convex settings, the issue is not getting stuck in some local minima but rather

at saddle points, where the gradient also vanishes [9], hence making the gradient-descent procedure of limited use. A takeaway from this is that a “good” initialization procedure for assigning the weights of the network, known as *pre-training*, can then be highly advantageous.

One such deep-learning framework that can utilize this pre-training procedure is the Restricted Boltzmann Machine (RBM) [5], and its extension, the Deep Belief Network (DBN) [10]. These machines are a class of neural network models capable of unsupervised learning of a parametrized probability distribution over inputs. They can also be easily extended to the supervised learning case by training an output layer using back-propagation or other standard methods [1].

Training RBMs usually distinguishes between an unsupervised pre-training, whose purpose is to initialize a good set of weights, and the supervised procedure. The current most effective technique for pre-training RBMs utilizes an iterative sampling technique called *contrastive divergence* (CD) [11]. Computing the exact gradient of the log-likelihood is exponentially hard in the size of the RBM, and so CD approximates it with a computationally friendly sampling procedure. While this procedure has brought RBMs most of their success, CD suffers from the slow mixing of Gibbs sampling, and is known not to follow the gradient of any function [12].

The unexplored potential of RBMs has been approached from many angles, including variations of CD [13], CD

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done on memristive hardware [14], and more recently, approaches based on quantum annealing that try to recover the exact gradient [15]. Some of these methods are classical algorithms simulating quantum sampling [16], and still others attempt to use a *hardware* quantum device in contact with an environment to take independent samples from its Boltzmann distribution for a more accurate gradient computation. For instance, in a recent work, the state of the RBM has been mapped onto a commercial quantum annealing processor (a D-Wave machine), the latter used as a sampler of the model distribution [17]. The results reported on a reduced version of the well-known MNIST data set look promising as compared to CD [17]. However, these approaches require expensive hardware, and cannot be scaled to larger problems as of yet.

In the present paper, inspired by the theoretical underpinnings [18, 19] and recent empirical demonstrations [20, 21] of the advantages of a new computing paradigm –*memcomputing* [22]– on a variety of combinatorial/optimization problems, we seek to test its power toward the computationally demanding problems in deep learning.

Memcomputing [22] is a novel computing paradigm that solves complex computational problems using processing embedded in memory. It has been formalized by two of us (FLT and MD) by introducing the concept of universal memcomputing machines [18]. In short, to perform a computation, the task at hand is mapped to a continuous dynamical system that employs highly-correlated states [23] (in both space and time) of the machine to navigate the phase space efficiently and find the solution of a given problem as mapped into the equilibrium states of the dynamical system.

In this paper, we employ a subset of these machines called *digital memcomputing machines* (DMMs) and, more specifically, their self-organizing circuit realizations [19]. The distinctive feature of DMMs is their ability to read and write the initial and final states of the machine *digitally*, namely requiring only *finite* precision. This feature makes them easily *scalable* as our modern computers.

From a practical point of view DMMs can be built with standard circuit elements with and without memory [19]. These elements, however, are *non-quantum*. Therefore, the ordinary differential equations of the corresponding circuits can be efficiently simulated on our present computers. Here, we will indeed employ only *simulations* of DMMs on a single Xeon processor to train RBMs. These simulations show already substantial advantages with respect to CD and even quantum annealing, despite the latter is executed on hardware. Of course, the hardware implementation of DMMs applied to these problems would offer even more advantages since the simulation times will be replaced by the actual physical time of the circuits to reach equilibrium. This would then offer a realistic path to real-time pre-training of deep-belief networks.

In order to compare directly with quantum annealing results recently reported [17], we demonstrate the advan-

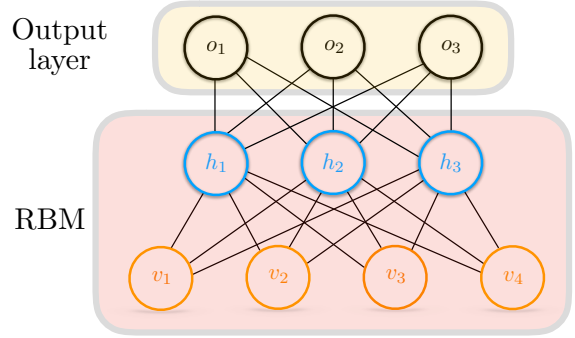


Figure 1: A sketch of an RBM with four visible nodes, three hidden nodes, and an output layer with three nodes. The value of each stochastic binary node is represented by  $v_i, h_i \in \{0, 1\}$ , which are sampled from the probabilities in Eqs. (5), (6). The connections between the layers represent the weights,  $w_{ij} \in \mathbb{R}$  (biases not shown). Note the lack of connections between nodes in the same layer, which distinguishes the RBM from a Boltzmann machine. The RBM weights are trained separately from the output layer with generative pre-training, then tuned together via back-propagation (just as in a feed-forward neural network).

tage of our memcomputing approach by first training on a reduced MNIST data set as that used in Ref [17]. We show that our method requires far less pre-training iterations to achieve the same accuracy as CD, as well as an overall accuracy gain over both CD and quantum annealing. We finally train the RBMs on the full MNIST data set where the quantum annealing results are not available. Also in this case, we find both a substantial reduction in pre-training iterations needed as well a higher level of accuracy of the memcomputing approach over the traditional CD.

Our approach then seems to offer many of the advantages of quantum approaches. However, since it is based on a completely classical system, it can be efficiently deployed in software (as we demonstrate in this paper) as well as easily implemented in hardware, and can be scaled to full-size problems.

## 2. RBMs and Contrastive Divergence

An RBM consists of  $m$  visible units,  $v_j, j = 1 \dots m$ , each fully connected to a layer of  $n$  hidden units,  $h_i, i = 1 \dots n$ , both usually taken to be binary variables. In the restricted model, no intra-layer connection are allowed, see Fig. 1.

The connectivity structure of the RBM implies that, given the hidden variables, each input node is conditionally independent of all the others:

$$p(v_i, v_j | \mathbf{h}) = p(v_i | \mathbf{h}) p(v_j | \mathbf{h}). \quad (1)$$

The joint probability is given by the Gibbs distribution,

$$p(\mathbf{v}, \mathbf{h}) = \frac{1}{Z} e^{-E(\mathbf{v}, \mathbf{h})}, \quad (2)$$

with an energy function

$$E(\mathbf{v}, \mathbf{h}) = - \sum_i \sum_j w_{ij} h_i v_j - \sum_j b_j v_j - \sum_i c_i h_i, \quad (3)$$

where  $w_{ij}$  is the weight between the  $i$ -th hidden neuron and the  $j$ -th visible neuron, and  $b_j$ ,  $c_i$  are real numbers indicating the “biases” of the neurons. The value,  $Z$ , is a normalization constant, and is known in statistical mechanics as the partition function. Training an RBM then amounts to finding a set of weights and biases that maximizes the likelihood (or equivalently minimizes the energy) of the observed data.

A common approach to training RBMs for a supervised task is to first perform generative unsupervised learning (pre-training) to initialize the weights and biases, then run back-propagation over input-label pairs to fine tune the parameters of the network. The pre-training is framed as a gradient ascent over the log-likelihood of the observed data, which gives a particularly tidy analytic form for the weight updates:

$$\Delta w_{ij} = \epsilon [\langle v_i h_j \rangle_{\text{DATA}} - \langle v_i h_j \rangle_{\text{MODEL}}]. \quad (4)$$

The first expectation value on the rhs of Eq. (4) is taken with respect to the conditional probability distribution with the data fixed at the visible layer. This is relatively easy to compute. Evaluation of the second expectation on the rhs of Eq. (4) is exponentially hard in the size of the network, since obtaining independent samples from a high-dimensional model distribution easily becomes prohibitive with increasing size [11]. This is the term that CD attempts to approximate.

The CD approach attempts to reconstruct the difficult expectation term with iterative Gibbs sampling. This works by sequentially sampling each layer given the sigmoidal conditional probabilities, namely

$$p(h_i = 1 | \mathbf{v}) = \sigma \left( \sum_j w_{ij} v_j + c_i \right), \quad (5)$$

for the visible layer, and similarly for the hidden layer

$$p(v_j = 1 | \mathbf{h}) = \sigma \left( \sum_i w_{ij} h_i + b_j \right), \quad (6)$$

with  $\sigma(x) = (1 + e^{-x})^{-1}$ . The required expectation values are calculated with the resulting samples. In the limit of infinite sampling iterations, the expectation value is recovered. However, this convergence is slow and in practice usually only one iteration, referred to CD-1, is used [24].

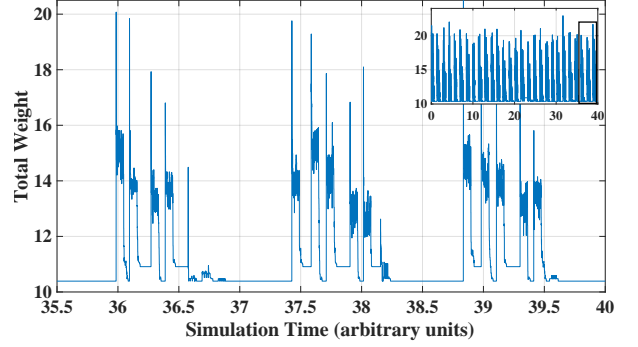


Figure 2: Plot of the total weight of a MAX-SAT clause as a function of simulation time (in arbitrary units) of a DMM. A lower weight variable assignment corresponds directly to a higher probability assignment of the nodes of an RBM. If the simulation has not changed assignments in some time, we restart with another random (independent) initial condition. The inset shows the full simulation, with all restarts. The main figure focuses on the last three restarts, signified by the black box in the inset.

### 3. Efficient Sampling with Memcomputing

We replace the CD reconstruction with our approach that utilizes memcomputing to compute a much better approximation to the model expectation than CD. More specifically, we map the RBM pre-training problem onto DMMs realized by self-organizing logic circuits (SOLCs) [19]. These electrical circuits define a set of coupled differential equations which are set to random initial conditions and integrated forward toward the global solution of the given problem [19, 20, 21]. The ordinary differential equations we solve can be found in Ref. [19] appropriately adapted to deal with the particular problem discussed in this paper.

Within this memcomputing context, we construct a reinterpretation of the RBM pre-training that explicitly shows how it corresponds to an NP-hard optimization problem, which we then tackle using DMMs. We first observe that to obtain a sample near most of the probability mass of the joint distribution,  $p(v, h) \propto e^{-E(v, h)}$ , one must find the minimum of the energy of the form Eq. 3, which constitutes a *quadratic unconstrained binary optimization* (QUBO) problem [25].

We can see this directly by considering the visible and hidden nodes as one vector  $\mathbf{x} = (\mathbf{v}, \mathbf{h})$  and re-writing the energy of an RBM configuration as

$$E = -\mathbf{x}^T Q \mathbf{x}, \quad (7)$$

where  $Q$  is the matrix

$$Q = \begin{bmatrix} B & W \\ 0 & C \end{bmatrix}, \quad (8)$$

with  $B$  and  $C$  being the diagonal matrices representing the biases  $b_j$  and  $c_i$ , respectively, while the matrix  $W$  contains the weights.

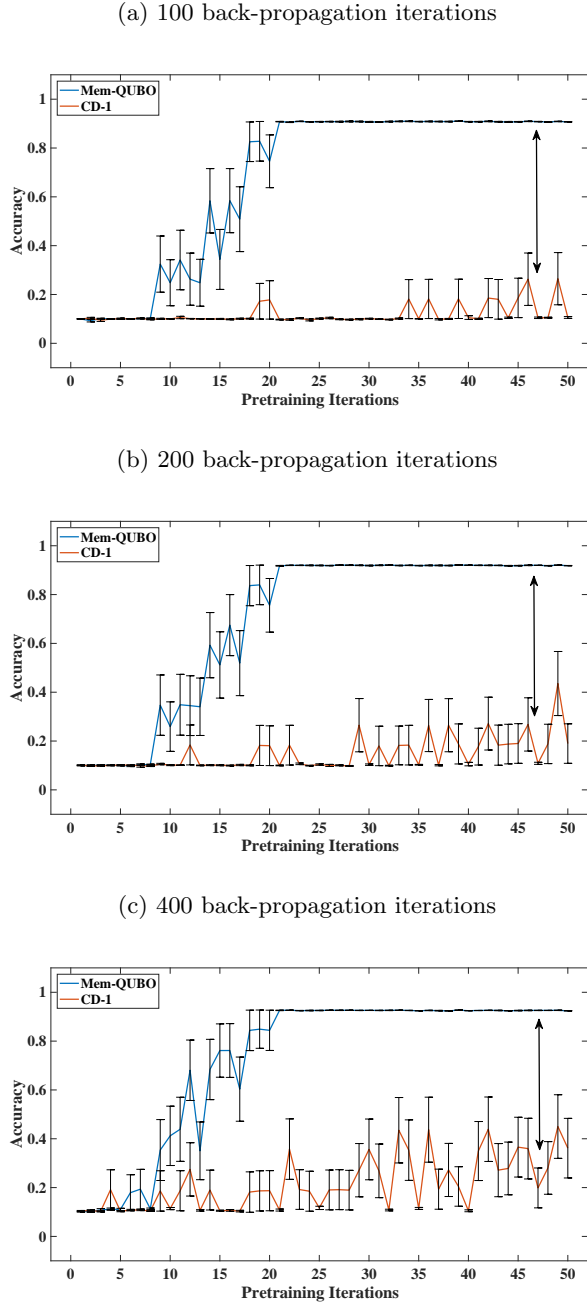


Figure 3: Memcomputing (Mem-QUBO) accuracy on the test set of the reduced MNIST problem versus contrastive divergence for  $n = 100$ (a),  $200$ (b),  $400$ (c) iterations of back-propagation with mini-batches of 100. The plots show average accuracy with  $\pm \sigma/\sqrt{N}$  error bars calculated across 10 DBNs trained on  $N = 10$  different partitions of the training set. One can see a dramatic acceleration with the memcomputing approach needing far less iterations to achieve the same accuracy, as well as an overall performance gap (indicated by a black arrow) that back-propagation cannot seem to overcome. Note that some of the error bars for both Mem-QUBO and CD-1 are very small on the reported scale for a number of pretraining iterations larger than about 20.

We then employ a mapping from a general QUBO problem to a *weighted maximum satisfiability* (weighted MAX-SAT) problem, similar to [26], which is directly solved by

the DMM. The weighted MAX-SAT problem is to find an assignment of boolean variables that minimizes the total weight of a given boolean expression written in conjunctive normal form [25].

This problem is a well-known problem in the NP-hard complexity class [25]. However, it was recently shown in Ref. [20], that simulations of DMMs show dramatic (exponential) speed-up over the state-of-the-art solvers [20], when attempting to find better approximations to hard MAX-SAT instances beyond the inapproximability limit [27].

The approximation to the global optimum of the weighted MAX-SAT problem given by memcomputing is then mapped back to the original variables that represent the states of the RBM nodes. Finally, we obtain an approximation to the “ground state” (lowest energy state) of the RBM as a variable assignment,  $\mathbf{x}^*$ , close to the peak of the probability distribution, where  $\nabla P(\mathbf{x}^*) = 0$ . This assignment is obtained by integration of the ordinary differential equations that define the SOLCs dynamics. In doing so we collect an entire trajectory,  $\mathbf{x}(t)$ , that begins at a random initial condition in the phase space of the problem, and ends at the lowest energy configuration of the variables (see Fig. 2).

Since the problem we are tackling here is an optimization one, we do not have any guarantee of finding the *global* optimum. (This is in contract to a SAT problem where we can guarantee DMMs *do* find the solutions of the problem corresponding to equilibrium points, if these exist [19, 28, 29].) Therefore, there is an ambiguity about what exactly constitutes the stopping time of the simulation, since *a priori*, one cannot know that the simulation has reached the *global* minimum.

We then perform a few “restarts” of the simulation (that effectively correspond to a change of the initial conditions) and stop the simulation when the machine has not found any better configuration within that number of restarts. The restarts are clearly seen in Fig. 2 as spikes in the total weight of the boolean expression. In this work we have employed 28 restarts, which is an over-kill since a much smaller number would have given similar results.

The full trajectory,  $\mathbf{x}(t)$ , together with the above “restarts” is plotted in Fig. 2. It is seen that this trajectory, in between restarts, spends most of its time in “low-energy regions,” or equivalently areas of high probability. A time average,  $\langle \mathbf{x}(t) \rangle$ , gives a good approximation to the required expectations in the gradient calculation in Eq. 4. In practice, even using the best assignment found,  $\mathbf{x}^*$ , shows a great improvement over CD in our experience. This is what we report in this paper. Note also that a full trajectory, as the one shown in Fig. 2, takes about 0.5 seconds on a single Xeon processor.

As a testbed for the memcomputing advantage in deep learning, and as a direct comparison to the quantum annealing hardware approaches, we first looked to the reduced MNIST data set as reported in [17] for quantum annealing using a D-wave machine. Therefore, we have

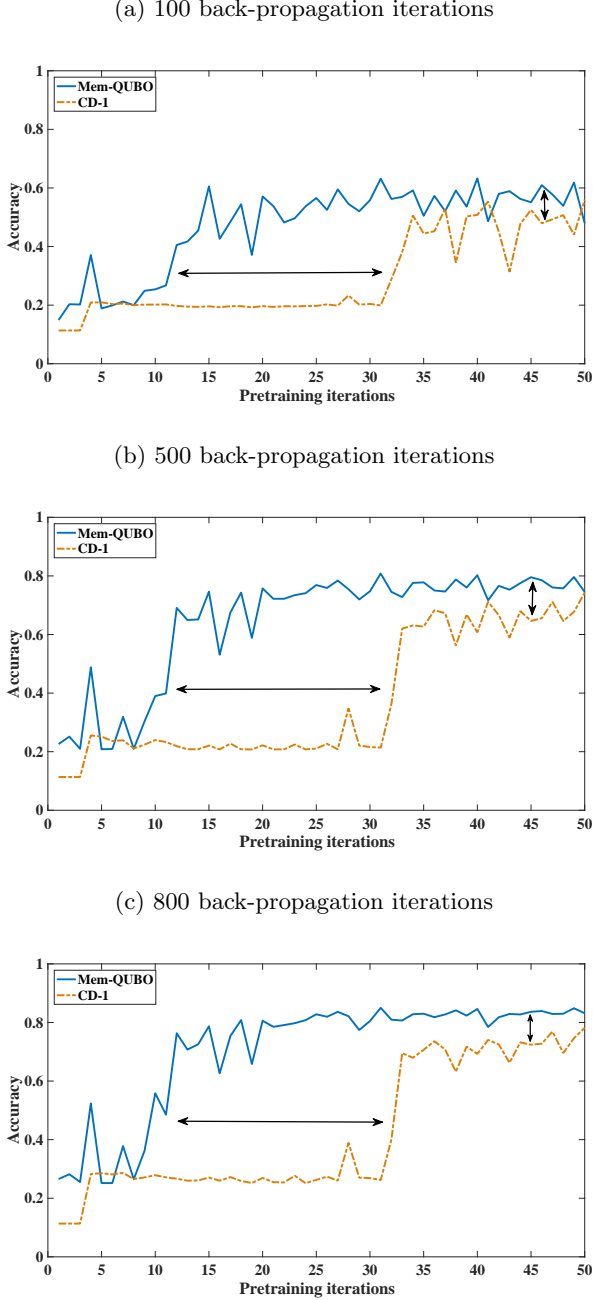


Figure 4: Mem-QUBO accuracy on the full MNIST test set vs. CD-1 after  $n = 100$ (a),  $500$ (b),  $800$ (c) iterations of back-propagation with no mini-batching. The resulting pre-training acceleration shown by the memcomputing approach is denoted by the horizontal arrow. A performance gap also appears, emphasized by the vertical arrow, with Mem-QUBO obtaining a higher level of accuracy than CD-1, even for the highest number of back-propagation iterations. No error bars appear here since we have trained the full test set.

first applied the same reduction to the full MNIST problem as given in that work, which consists of removing two pixels around all  $28 \times 28$  grayscale values in both the test and training sets. Then each  $4 \times 4$  block of pixels is replaced by their average values to give a  $6 \times 6$  reduced image. Finally, the four corner pixels are discarded resulting in a

total of 32 pixels representing each image.

We also trained the same-size DBN consisting of two stacked RBMs each with 32 visible and hidden nodes, training each RBM one at a time. We put both the CD-1 and our Memcomputing-QUBO (Mem-Qubo) approach through  $N = 1, \dots, 50$  generative pre-training iterations using no mini-batching.

For the memcomputing approach, we solve one QUBO problem per pre-training iteration to compute the model expectation value in Eq. (4). We pick out the best variable assignment,  $\mathbf{x}^*$ , which gives the ground state of Eq. (3) as an effective approximation of the required expectation. After generative training, an output classification layer with 10 nodes was added to the network (see Fig. 1) and 1000 back-propagation iterations were applied in both approaches using mini-batches of 100 samples to generate Fig. 3. For both pre-training and back-propagation, our learning rate was set to  $\epsilon = 0.1$  and momentum parameters were  $\alpha = 0.1$  for the first 5 iterations, and  $\alpha = 0.5$  for the rest, same as in [17].

Accuracy on the test set versus CD-1 as a function of the number of pre-training iterations is seen in Fig. 3. The memcomputing method reaches a far better solution faster, and maintains an advantage over CD even after hundreds of back-propagation iterations. Interestingly, our *software* approach is even competitive with the quantum annealing method done in *hardware* [17] (cf. Fig. 3 with Figs. 7, 8, and 9 in Ref. [17]). This is quite a remarkable result, since we integrate a set of differential equations of a *classical* system, in a scalable way, with comparable sampling power to a physically-realized system that takes advantage of *quantum* effects to improve on CD.

Finally, we also trained the RBM on the full MNIST data set. We are not aware of quantum-annealing results for the full data set, but we can still compare with the CD approach. We follow a similar procedure as discussed above. In this case, however, no mini-batching was used for a more direct comparison between the Gibbs sampling of CD and our memcomputing approach. The results are shown in Fig. 4 for different numbers of back-propagation iterations. Even on the full MNIST set our memcomputing approach requires a substantially lower number of pre-training iterations to achieve a high accuracy and, additionally, shows a higher level of accuracy over the traditional CD, even after 800 back-propagation iterations.

## 4. Conclusions

In this paper we have demonstrated how the memcomputing paradigm can be applied toward the chief bottlenecks in deep learning today. In this paper, we directly assisted a popular algorithm to pre-train RBMs and DBNs, which consists of gradient ascent on the log-likelihood. We have shown that memcomputing can accelerate considerably the pre-training of these networks far better than what is currently done.



In fact, *simulations* of digital memcomputing machines achieve accelerations of pre-training comparable to, in number of iterations, the *hardware* application of the quantum annealing method, but with better quality. In addition, unlike quantum computers, our approach can be easily scaled on classical hardware to full size problems. Even further, the form of the energy in Eq. 3 is quite general and encompasses full DBNs. In this way, our method can also be applied to pre-training *entire* deep-learning models at once, potentially exploring parameter spaces that are inaccessible by any other classical or quantum methods. We leave this interesting line of research for future studies.

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