Unsupervised Feature Learning through Divergent Discriminative Feature Accumulation

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Abstract

Unlike unsupervised approaches such as autoencoders that learn to reconstruct their inputs, this paper introduces an alternative approach to unsupervised feature learning called *divergent discriminative feature accumulation* (DDFA) that instead continually accumulates features that make novel discriminations among the training set. Thus DDFA features are inherently discriminative from the start even though they are trained without knowledge of the ultimate classification problem. Interestingly, DDFA also continues to add new features indefinitely (so it does not depend on a hidden layer size), is not based on minimizing error, and is inherently divergent instead of convergent, thereby providing a unique direction of research for unsupervised feature learning. In this paper the quality of its learned features is demonstrated on the MNIST dataset, where its performance confirms that indeed DDFA is a viable technique for learning useful features.

Introduction

The increasing realization in recent years that artificial neural networks (ANNs) can learn many layers of features (Bengio et al. 2007; Hinton, Osindero, and Teh 2006; Marc'Aurelio, Boureau, and LeCun 2007; Cireşan et al. 2010) has reinvigorated the study of representation learning in ANNs (Bengio, Courville, and Vincent 2013). While the beginning of this renaissance focused on the sequential unsupervised training of individual layers one upon another (Bengio et al. 2007; Hinton, Osindero, and Teh 2006), the number of approaches and variations that have proven effective at training in such *deep learning* has since exploded (Schmidhuber et al. 2011; Bengio, Courville, and Vincent 2013). This explosion has in turn raised the question of what makes a good representation, and how it is best learned (Bengio, Courville, and Vincent 2013). The main contribution of this paper is to advance our understanding of good representation learning by suggesting a new principle for obtaining useful representations that is accompanied by a practical algorithm embodying the principle.

The feature representation obtained through learning algorithms is often impacted by the nature of the training. For example, supervised approaches such as stochastic gradient descent (Cireşan et al. 2010) that aim to minimize the error in a classification problem in effect encourage the exclusive discovery of features that help to discriminate among the target classifications. In contrast, unsupervised approaches, which include both generative representations such as restricted Boltzmann machines (RBMs) (Hinton, Osindero, and Teh 2006) and autoencoders that are trained to reproduce their inputs (Bengio et al. 2007), yield a more general feature set that captures dimensions of variation that may or may not be essential to the classification objective. The hope of course is that such a set would nevertheless be useful for classification in any case, and the pros and cons of e.g. generative versus discriminative features have proven both subtle and complex (Ng and Jordan 2002; Jaakkola, Haussler, and others 1999). Nevertheless, one benefit of unsupervised training is that it does not require labeled data to gain traction.

An important insight in this paper is that there is an unrecognized option outside this usual unsupervised versus supervised (or generative versus discriminative) dichotomy. In particular, there is an alternative kind of discriminative learning that is unsupervised rather than supervised. In this proposed alternative approach, called *divergent discriminative feature accumulation* (DDFA), instead of searching for features constrained by the objective of solving the discriminative classification problem, a learning algorithm can instead attempt to *collect* as many features that discriminate strongly among training examples as possible, without regard to any particular classification problem.

The approach in such unsupervised discriminative learning is thus to search continually for novel features that discriminate among training examples in new ways. Interestingly, unlike conventional algorithms in deep learning, such a search is explicitly *divergent* (i.e. intentionally spreading out in the space rather than aiming for a specific point or area[1]) by design and therefore continues to accumulate new features without converging. In effect, a high-scoring feature is therefore relevant to discriminating among the examples, even though the ultimate discrimination problem is not known. A comprehensive set of such features that discriminate among the training set in fundamental ways is thereby suitable in principle for later supervised training

[1]This sense of divergence should not be confused with e.g. contrastive divergence (Hinton, Osindero, and Teh 2006).

from those collected features for any particular discrimination task. This idea is intuitive in the sense that even for humans, distinctions among experiences can be learned before we know how we will apply such distinctions.

In fact, this perspective on feature learning has the advantage over more conventional approaches in deep learning that learning does not depend on a fixed a priori number of features. Rather, it simply continues to accumulate new features as long as the algorithm is run. Furthermore, unlike in other unsupervised approaches, the accumulated features are known explicitly to be discriminative, suiting them well to later discriminative learning. Another potentially advantageous property of such a feature accumulator is its lack of convergence (thereby avoiding the problem of local optima), which stems from the fact that it is inherently divergent because it is not based on minimizing an error. In these ways DDFA is uniquely flexible and autonomous.

The driving force behind the feature accumulator is the imperative of finding novel features. Thus a well-suited algorithm for implementing this idea in practice is the recent *novelty search* algorithm (Lehman and Stanley 2011), which is a divergent evolutionary algorithm that is rewarded for moving *away* in the search space of candidate behaviors (such as discriminations) from where it has already visited to where it has not. By accumulating features that are themselves ANNs, novelty search in this paper enables DDFA. As with other unsupervised pretraining approaches such as autoencoders, once DDFA determines that sufficient features are collected, a classifier is trained above them for the classification task (through backpropagation in this paper). To demonstrate the potential of DDFA to collect useful features, it is tested in this paper by collecting single-layer features for the MNIST digital handwriting recognition benchmark (LeCun and Cortes 1998). Even with the consequent two-layer shallow classifier network, its testing performance rivals more conventional training techniques.

This initial proof of concept establishes the efficacy of accumulating features as a basis for representation learning. While the one-layer discriminative features from DDFA perform well, DDFA can conceivably improve further through layering (e.g. accumulating multilayer features or searching for novel features that are built above already-discovered features) and convolution (LeCun and Bengio 1995), just like other deep learning algorithms. Most importantly, based on the novel representational principle that discriminators make good features for classification problems, DDFA opens up a new class of learning approaches.

Background

This section reviews the two algorithms, novelty search and HyperNEAT, that underpin the DDFA approach.

Novelty Search

In just the last year, the idea that an evolutionary approach can help to collect a set of useful features has begun to attract significant interest. Researchers have proposed both to evolve a feature set all at once that is rewarded in aggregate for its diversity (Koutník, Schmidhuber, and Gomez 2014) and to evolve individual features that are collected for their contribution to ultimate classification performance (Auerbach, Fernando, and Floreano 2014; Knittel and Blair 2014). The novel direction in this paper is to collect individual features that are retained for their diversity rather than for their contribution to performance at a given problem, which also makes the proposed approach unsupervised.

The problem of *collecting* novel instances of a class is different from the more familiar problem of minimizing error. While error minimization aims at converging towards minima in the search space, collecting novelty requires diverging away from past discoveries that continue to accumulate. This divergent process is thus well-suited to a population-based approach that accumulates and remembers novel discoveries to help push the search continually to even more novelty as it progresses. The novelty search algorithm (Lehman and Stanley 2011) implements such a process in practice through an evolutionary approach.

The idea in novelty search is to reward candidates (by increasing their probability of reproduction) who are behaviorally novel. If the candidates are ANNs as in the present study, then the word "behaviorally" becomes critical because it refers to what the discovered ANNs *actually do* (e.g. how they discriminate) as opposed to just their underlying genetic representations (i.e. genomes), which may or may not do anything interesting. Thus discovering novel behaviors requires search (as opposed to just enumerating random sets of genes), thereby instantiating a nontrivial alternative to the traditional objective gradient.

This point is particularly important in the context of deep learning, where researchers have commented on the potential long-term limitations of optimization gradients and the need for a broader and less convergent approaches for learning representations. For example, when discussing the future of representation learning, Bengio (2013) notes:

> The basic idea is that humans (and current learning algorithms) are limited to "local descent" optimization methods, that make small changes in the parameter values with the effect of reducing the expected loss in average. This is clearly prone to the presence of local minima, while a more global search (in the spirit of both genetic and cultural evolution) could potentially reduce this difficulty.

Novelty search (Lehman and Stanley 2011) can be viewed as an embodiment of such a "genetic evolution" that is suited to accumulating discoveries free from the pitfalls of "local descent." In fact, while novelty search was originally shown sometimes to find the objective of an optimization problem more effectively than objective-based optimization (Lehman and Stanley 2011), Cully and Mouret (2013) recently raised the intriguing notion of novelty search as a *repertoire collector*. That is, instead of searching for a *solution* to a problem, novelty search can collect a set of novel skills (each a point in the search space) intended for later aggregation by a higher-level mechanism. This repertoire-collecting idea aligns elegantly with the problem of accumulating features for deep learning, wherein each feature detector is like a "skill" within the repertoire of a classifier.

In practice, novelty search maintains an *archive* of previously novel discoveries as part of the algorithm. Future candidates are then compared to the archive to determine whether they too are novel. A random sampling of candidates is entered into the archive, which implies that more frequently-visited areas will be more densely covered. Intuitively, if the average distance to the nearest neighbors of a given behavior b is large then it is in a sparse area; it is in a dense region if the average distance is small. The sparseness ρ at point b is given by

$$\rho(x) = \frac{1}{k}\sum_{i=0}^{k} \text{dist}(b, \mu_i), \quad (1)$$

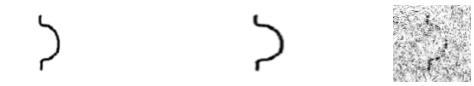
where μ_i is the ith-nearest neighbor of b with respect to the distance metric *dist*, which is a domain-dependent measure of behavioral difference between two individuals in the search space. The nearest neighbors calculation must take into consideration individuals from the current population and from the permanent archive of novel individuals. Candidates from more sparse regions of this behavioral search space then receive higher novelty scores, which lead to a higher chance of reproduction. Note that it is not known *a priori* how to enter areas of low density just as it is not known a priori how to construct a solution close to the objective. Thus, moving through the space of novel behaviors requires exploration.

Novelty search in effect runs as a regular evolutionary algorithm wherein novelty replaces fitness as the criterion for selection, and an expanding archive of past novel discoveries is maintained. This simple idea will empower DDFA in this paper to accumulate a collection of novel features.

HyperNEAT

The term for an evolutionary search for ANNs is *neuroevolution* (Stanley and Miikkulainen 2002; Floreano, Dürr, and Mattiussi 2008). This section is designed to introduce the particular neuroevolution algorithm (called HyperNEAT) that is combined with novelty search to search for features in this paper. Because neuroevolution is an independent field that may be unfamiliar to many in deep learning, this section is written to emphasize the main ideas that make it appealing for the purpose of feature learning, without including details that are unnecessary to understand the operation of the proposed DDFA algorithm. The complete details of HyperNEAT can be found in its primary sources (Stanley, D'Ambrosio, and Gauci 2009; Gauci and Stanley 2010; 2008; Verbancsics and Stanley 2010).

In a domain like visual recognition, the pattern of weights in useful features can be expected to exhibit a degree of contiguity and perhaps regularity. For example, it is unlikely that an entirely random pattern of largely unconnected pixels corresponds to a useful or interesting feature. It has accordingly long been recognized in neuroevolution that entirely random perturbations of weight patterns, which are likely to emerge for example from random mutations, are unlikely to maintain contiguity or regularity. While stochastic gradient descent (SGD) algorithms at least justify their trajectory through the search space through descent, a completely random perturbation of weights is arguably less principled and therefore perhaps less effective. Nevertheless, SGD still suffers to some extent from the same problem that even a step that reduces error may not maintain contiguity or regularity in the feature geometry. Neuroevolution algorithms have responded to this concern with a class of representations called *indirect encodings* (Stanley and Miikkulainen 2003), wherein the weight pattern is generated by an evolving genetic encoding that is biased towards contiguity and regularity by design. That way, when a mutation is applied to a feature, the feature deforms in a systematic though still randomized fashion (figure 1).



(a) Original Weight Pattern (b) HyperNEAT Mutation (c) Uniform Mutation

Figure 1: **Systematic Deformation in HyperNEAT-style Mutation.** Each image depicts the pattern of weights projecting from a single 28×28 input field to a single output node. The weight of a hypothetical feature (a) exhibits contiguity and some symmetry. The HyperNEAT style of mutation (b) perturbs the pattern of weights while still preserving the geometric regularities of the original feature. In contrast, simply randomly mutating weights with uniform probability (c) leads to an incoherent corruption of the original feature.

HyperNEAT, which stands for *Hypercube-based NeuroEvolution of Augmenting Topologies* (Stanley, D'Ambrosio, and Gauci 2009; Gauci and Stanley 2010; 2008; Verbancsics and Stanley 2010) is a contemporary neuroevolution algorithm based on such an indirect encoding. In short, HyperNEAT evolves an encoding network called a compositional pattern producing network (CPPN; Stanley 2007) that *describes* the pattern of connectivity within the ANN it encodes. Therefore, mutations in HyperNEAT happen to the *CPPN*, which then transfers their effects to the encoded ANN. In this way the CPPN is like DNA, which transfers the effects of its own mutations to the structures it encodes, such as the brain. Because the CPPN encoding is designed to describe patterns of weights across the geometry of the encoded network, the weights in HyperNEAT ANNs tend to deform in contiguity-preserving and regularity-preserving ways (as seen in figure 1), thereby providing a useful bias (Stanley, D'Ambrosio, and Gauci 2009; Gauci and Stanley 2010). Furthermore, CPPNs in HyperNEAT grow over evolution (i.e. their structure is augmented over learning), which means that the pattern of weights in the ANN they describe (which is fixed in size) can become more intricate and complex over time.

An important observation is that HyperNEAT's tendency to preserve geometric properties in its weights means that it is not invariant to permutations in the input vector. In effect (in e.g. the case of MNIST) it is exploiting the known two-dimensional geometry of the problem. However, at the same time, while it does exploit geometry, its use in this paper is not convolutional either: its input field is never broken into receptive fields and is rather projected in whole directly (without intervening layers) to a single-feature output

node. Thus the powerful advantage of convolution for visual problems is *not available in this investigation*, making the problem more challenging. As a consequence, the DDFA implementation in this paper does not fit neatly into the permutation-invariant-or-not dichotomy, and may be considered somewhere closer to typical permutation-invariant scenarios. Nevertheless, while not investigated in this study, it may be interesting in the future to compare the performance of DDFA with and without HyperNEAT to further isolate the advantage provided by indirect encoding.

This overview of HyperNEAT is left brief because its other details (which are widely disseminated in the venues above) are not essential to the main idea in this paper, which is to accumulate feature detectors through novelty search.

Approach: DDFA

Unsupervised pretraining in deep learning has historically focused on approaches such as autoencoders and RBMs (Bengio et al. 2007; Hinton, Osindero, and Teh 2006) that attempt to *reconstruct* training examples by first translating them into a basis of features different from the inputs, and then from those features regenerating the inputs. Of course, one potential problem with this approach is that there is no assurance that the learned features actually align with any particular classification or discrimination problem for which they might be used in the future. Yet this conventional approach to learning features also raises some interesting deeper questions. For example, is there any *other* way to extract meaningful features and thereby learn representations from a set of examples without explicit supervision?

There are some well-known simple alternatives, though they are not usually characterized as feature-learning algorithms. For example clustering algorithms such as k-means or Gaussian mixture models in effect extract structure from data that can then assist in classification; in fact at least one study has shown that such clustering algorithms can yield features as effective or more so for classification than autoencoders or RBMs (Coates, Ng, and Lee 2011). This result highlights that reconstruction is not the only effective incentive for extracting useful structure from the world.

The approach introduced here goes beyond simple clustering by emphasizing the general ability to learn diverse *distinctions*. That is, while one can learn how to *describe* the world, one can also learn how different aspects of the world *relate* to each other. Importantly, there is no single "correct" view of such relations. Rather, a rich set of learned relationships can support drawing important distinctions later. For example, in one view palm trees and "regular" trees share properties that distinguish them from other plants. However, in another view, palm trees are in fact distinct from regular trees. *Both* such views can be useful in understanding nature, and one can hold both simultaneously with no contradiction. When an appropriate question comes up, such as which plants are tall and decorative, the feature *tall* becomes available because it was learned to help make such general distinctions about the world in the past.

The idea in DDFA is to continually accumulate such distinctions systematically through novelty search, thereby building an increasingly rich repertoire of features that help divide and relate observations of the world. Why should accumulating a diverse set of features provide an advantage over optimization-based approaches? One reason is that searching for diversity is not susceptible in the same way to local optima: while e.g. an autoencoder or direct optimization on a classifier can converge to a local optimum, in contrast DDFA features are independently rewarded for diverging from other features, preventing such premature convergence. In addition, in principle, to discriminate one class from another a classifier must possess knowledge of every feature that might distinguish the two classes; DDFA is *explicitly* seeking all such possible distinctions while the objective of learning features that *reconstruct* the input in e.g. an autoencoder is not. Intuitively, DDFA can be interpreted as a formalization of *divergent thinking*, wherein the thinker achieves a novel insight by exploring many perspectives simultaneously and without prejudice.

More formally, suppose there are n training examples $\{x^{(1)}, ..., x^{(n)}\}$; whether or not they are labeled will not matter because feature learning will be unsupervised. Suppose also that any single *feature detector* h_i (i.e. a single hidden node that detects a particular feature) outputs a real number whose intensity represents the degree to which that feature is present in the input. It follows that h_i will assign a real number $h_i^{(t)}$ to every example $x^{(t)}$ depending on the degree to which $x^{(t)}$ contains the feature of interest for h_i. The output of h_i for all features $x^{(t)}$ where $t = 1, \ldots, n$ thereby forms a vector $\{h_i^{(1)}, \ldots, h_i^{(n)}\}$ that can be interpreted as the *signature* of feature detector h_i across the entire training set. In effect the aim is to continually discover new such signatures.

This problem of continually discovering novel signatures is naturally captured by novelty search, which can be set up explicitly to evolve feature detectors h_i, each of which takes a training example as input and returns a single output. The signature $\{h_i^{(1)}, ..., h_i^{(n)}\}$ of h_i over all training examples is then its *behavior characterization* for novelty search. The novelty of the signature is then measured by comparing it to the k-nearest signatures in the novelty archive, following equation 1. Novelty search then dictates that more novel features are more likely to reproduce, which means that gradients of novel signatures will be followed in parallel by the evolving population. Those features whose sparseness ρ (i.e. novelty) exceeds a minimum threshold ρ_{min} are stored in the growing novel feature collection for later classifier training. In summary, DDFA continually collects features that classify the examples in the training set differently from features that came before, thereby accumulating increasingly diverse means for distinguishing training examples from each other.

A likely source of confusion is the question of whether DDFA is a kind of exhaustive search over signatures, which would not tend to discover *useful* features in a reasonable runtime. After all, the number of theoretically possible distinctions is exponential in the number of training examples. However, a critical facet of novelty-based searches that are combined with HyperNEAT-based neuroevolution is that the complexity of features (and hence distinctions) tends to increase over the run (Lehman and Stanley 2011). As a result, the initial features discovered encompass simple principles

(e.g. is the left side of the image dark?) that gradually increase in complexity. For this reason, the most arbitrary and incoherent features (e.g. are there 17 particular dots at specific non-contiguous coordinates in the image?) are possible to discover only late in the search. Furthermore, because the novelty signature is measured over the training set, features that make broad separations *relevant* to the training set itself are more likely to be discovered early. In effect, over the course of DDFA, the feature discoveries increasingly shift from simple principles to intricate minutia. Somewhere along this road are likely diminishing returns, well before all possible signatures are discovered. Empirical results reported here support this point.

Interestingly, because DDFA does not depend on the minimization of error, in principle it can continue to collect features virtually indefinitely, but in practice at some point its features are fed into a classifier that is trained from the collected discriminative features.

Experiment

The key question addressed in this paper is whether a divergent discriminative feature accumulator can learn *useful* features, which means they should aid in effective generalization on the test set. If that is possible, the implication is that DDFA is a viable alternative to other kinds of unsupervised pretraining. To investigate this question DDFA is trained and tested on the MNIST handwritten digit recognition dataset (LeCun and Cortes 1998), which consists of 60,000 training images and 10,000 test images. Therefore, the signature of each candidate feature discovered by DDFA during training is a vector of 60,000 real values.

Because the structure of networks produced by HyperNEAT can include as many hidden layers as the user chooses, the question arises how many hidden layers should be allowed in *individual features* h_i learned by HyperNEAT. This consideration is substantive because in principle DDFA can learn arbitrarily-deep individual features all at once, which is unlike e.g. the layer-by-layer training of a deep stack of autoencoders. However, the explicit choice was made in this introductory experiment to limit DDFA to single-layer features (i.e. without hidden nodes) to disentangle the key question of whether the DDFA process represents a useful principle from other questions of representation such as the implications of greater depth. Therefore, feature quality is addressed straightforwardly in this study by observing the quality of classifier produced based only on single-layer DDFA features. As a result, the final classifier ANN has just two layers: the layer of collected features and the ten-unit output layer for classifying MNIST digits.

The single-layer DDFA approach with novelty search and HyperNEAT is difficult to align directly with common deep learning approaches in part because of its lack of permutation invariance even though it is not convolutional in any sense (thereby lacking the representational power of such networks), and its lack of depth in this initial test. Thus to get a fair sense of whether DDFA learns useful features it is most illuminating to contrast it with the leading result on an equivalently shallow two-layer architecture (which are rare in recent years) that similarly avoided special preprocessing like elastic distortions or deskewing. In particular, Simard, Steinkraus, and Platt (2003) obtained one of the best such results of 1.6% test error performance. Thus a significant improvement on that result would suggest that DDFA generates useful features that help to stretch the capacity of such a shallow network to generalize. DDFA's further ability to approach the performance of conventional vanilla deep networks, such as the original 1.2% result from Hinton, Osindero, and Teh (2006) on a four-layer network pretrained by a RBM, would hint at DDFA's potential utility in the future for pretraining deeper networks.

During the course of evolution, features are selected for reproduction based on their signature's novelty score (sparseness ρ) calculated as the sum of the distances to the k-nearest neighbors ($k = 20$), where neighbors include other members of the population as well as the historical novelty archive. At the end of each generation, each individual in the population (size $= 100$) has a 1% chance of being added to the novelty archive, resulting in an average of 1 individual added to the novelty archive on each generation. Separately, a list of individuals called the *feature list* is maintained. At the end of each generation, each member of the population is scored against the current feature list by finding the distance to the nearest neighbor ($k = 1$), where neighbors are members of the feature list. Those individuals that score above a threshold $\rho_{\text{min}} = 2{,}000$ are added to the feature list. In effect, the feature list is constructed in such a way that all collected features have signatures that differ by at least ρ_{min} from all others in the collection. This threshold-based collection process protects against collecting redundant features. A simple variant of HyperNEAT called HyperNEAT-LEO (Verbancsics and Stanley 2011) (which leads to less connectivity) was the main neuroevolution engine. The HyperNEAT setup and parameters can be easily reproduced in full because they are simply the default parameters of the SharpNEAT 2.0 publicly-available package (Green 2003–2014).

To observe the effect of collecting different numbers of features, DDFA was run separately until both 1,500 and 3,000 features were collected. After collection concludes, a set of ten classification nodes is added on top of the collected features, and simple backpropagation training commences. The training and validation procedure mirrors that followed by Hinton, Osindero, and Teh (2006): first training is run on 50,000 examples for 50 epochs to find the network that performs best on a 10,000-example validation set. Then training shifts to the full 60,000-example set, which is trained until it reaches the same training error as in the best validation epoch. The resulting network is finally tested on the full 10,000-example test set. This whole procedure is similar to how autoencoders are trained before gradient descent in deep learning (Bengio et al. 2007).

Results

The main results are shown in Table 1. DDFA was able to achieve test errors of 1.42% and 1.25% from collections of 1,500 and 3,000 features, respectively, which are both well below the 1.6% error of the similar shallow network trained without preprocessing from Simard, Steinkraus, and Platt (2003). In fact, the result for the 3,000-feature network

Features	DDFA Test Error	Random CPPNs Control	Random Weights Control
1,500	1.42%	1.63%	2.20%
3,000	**1.25%**	1.61%	2.00%

Table 1: **MNIST Testing Error Rates of DDFA and Controls.**

Figure 2: **Example Collected Features.** Each square is a weight pattern for an actual feature discovered by DDFA in which white is negative and black is positive. As these examples show, features range from simple line orientation detectors reminiscent of those found in the lower levels of conventional deep networks (towards left) to more complex shapes (towards right).

even approaches the 1.2% error of the significantly deeper network of Hinton, Osindero, and Teh (2006), showing that shallow networks can generalize surprisingly well by finding sufficiently high-quality feature sets, even despite a lack of exposure to distortions during training. It also appears that more collected features lead to better generalization, at least at these sizes. It took 338 and 676 generations of feature collection to obtain the 1,500 and 3,000 features, respectively. Collecting 3,000 features took about 36 hours of computation on 12 3.0 GHz cores.

Figure 2 shows a typical set of features collected by DDFA. Interestingly, unlike the bottom layer of deep learning networks that typically exhibit various line-orientation detectors, DDFA also collects more complex features because newer features of increasing complexity evolve from older features.

To rule out the possibility that the reason for the testing performance is simply the HyperNEAT-based encoding of features, a **random CPPNs control** was also run. It follows an identical procedure for training and testing, except that novelty scores and adding to the feature list during the feature accumulation phase are decided *randomly*, which means the final collection in effect contained random features with a range of CPPN complexity similar to the normal run. To further investigate the value of the HyperNEAT representation, an additional **random weights control** was tested whose weights were assigned from a uniform random distribution, bypassing HyperNEAT entirely. As the results in Table 1 show, the CPPN encoding in HyperNEAT provides a surprisingly good basis for training even when the features are entirely randomly-generated. However, they are still inferior to the features collected by normal DDFA. As shown in the last column, without HyperNEAT, testing performance with a collection of random features is unsurprisingly poor. In sum these controls show that the pretraining in DDFA is essential to priming the later classifier for the best possible performance.

Discussion and Future Work

The results suggest that DDFA can indeed collect useful features and thereby serve as an alternative unsupervised feature learner. While it may ultimately lead to better training performance in some cutting-edge problems, future work with more layers and on larger problems is clearly necessary to investigate its full potential for exceeding top results.

However, it is important to recognize that significantly more than performance is at stake in the dissemination of alternative unsupervised training techniques based on new principles. Deep learning faces several fundamental challenges that are not only about testing performance. For example, recent surprising results from Szegedy et al. (2013) show that very small yet anomalous perturbations of training images that are imperceptible to the human eye can fool several different kinds of deep networks that nevertheless ominously score well on the test set. The implications of these anomalies are not yet understood. At the same time, as Bengio (2013) points out, local descent on its own will not ultimately be enough to tackle the most challenging problems, suggesting the need for radical new kinds of optimization that are more global. These kinds of considerations suggest that simply scoring well on a test set in the short run may not necessarily foreshadow continuing success for the field in the long run, highlighting the need for new approaches.

By showing that unsupervised discriminative learning can be effective, DDFA brings several intriguing corollaries. Among those, it is possible to conceive training methods that act as continual feature accumulators that do not require a fixed "hidden layer size." Furthermore, it is possible to learn useful features without any kind of error minimization (which is even used in conventional unsupervised techniques). Relatedly, an interesting question is whether anomalous results are sometimes a side effect of the very idea that all useful knowledge ultimately must come from minimizing error. The divergent dynamics of novelty search also mean that the search is inherently more global than local descent for the very reason that it is continually diverging, thereby offering a hint of how more expansive feature sets can be collected. Thus, in addition to the many possibilities for training multilayer deep features in DDFA, another important path for future work is to investigate the long-term implications of these more subtle differences from conventional techniques, and to determine whether similar such unique properties can be introduced to deep learning through non-evolutionary techniques that also follow gradients of novelty instead of error.

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Addendum

This addendum contains data from additional runs that were performed after the initial publication to further validate the reported results. In these new results, each variant was tested in five separate runs of feature collection, and with a single run of backpropagation for each such feature collection. According to Student's t-test, The DDFA-generated feature sets are significantly better $(p < .001)$ than randomly generated CPPN-based feature sets based on the classification results they ultimately yield. Randomly generated CPPN-based feature sets are themselves significantly better $(p < .01)$ than completely random feature sets, regardless of whether sparse initialization (Martens, 2010) is used to generate the random feature sets.

Features	**DDFA**	**Random CPPN**	**Random***	**Random**
1,500	1.36 $\pm$ 0.08	1.56 $\pm$ 0.06	1.78 $\pm$ 0.12	2.08 $\pm$ 0.06
3,000	1.20** $\pm$ 0.03	1.53 $\pm$ 0.05	1.76 $\pm$ 0.13	1.80 $\pm$ 0.09

Table 1: Test error (%) with standard deviation on MNIST data set.
*Initialized using sparse initialization.
**Best = 1.16

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