Adversarial Active Learning for Deep Networks: a Margin Based Approach

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Abstract
We propose a new active learning strategy designed for deep neural networks. The goal is to minimize the number of data annotation queried from an oracle during training. Previous active learning strategies scalable for deep networks were mostly based on uncertain sample selection. In this work, we focus on examples lying close to the decision boundary. Based on theoretical works on margin theory for active learning, we know that such examples may help to considerably decrease the number of annotations. While measuring the exact distance to the decision boundaries is intractable, we propose to rely on adversarial examples. We do not consider anymore them as a threat instead we exploit the information they provide on the distribution of the input space in order to approximate the distance to decision boundaries. We demonstrate empirically that adversarial active queries yield faster convergence of CNNs trained on MNIST, the Shoe-Bag and the Quick-Draw datasets.

1. Introduction
The efficiency of deep networks is mainly known under typical training procedures and with large datasets. However, gathering and annotating huge dataset for supervised learning may prohibit the expansion of deep networks towards new fields such as chemistry or medicine (Smith et al., 2018; Hoi et al., 2006). A possible solution to build online an efficient but reduced training set is to rely on active learning. Active learning is a family of methods seeking to optimize automatically the training set for the task at hand in order to limit the need of human annotation. Active learning strategies are not only motivated by theoretical works demonstrating that one model may perform better using less labeled data if the data are model-crafted (Cohn et al., 1996), but also by its proven efficiency on a wide range of machine learning procedures: from preference rating information for a new user in a movie recommendation system (Sun et al., 2013) to classifying medical data that often requires very high cost labeling (Hoi et al., 2006). It is only recently that active learning has been investigated on deep networks, especially CNNs. The question to scale active learning on deep networks has been raised on a diverse range of topics: from image classification, to sentiment classification, or to VQA and dialogue generation (Gal et al., 2016; Zhou et al., 2010; Lin & Parikh, 2017; Asghar et al., 2017). All those works converge to a common assessment on the efficiency of active learning to reduce the need for a large labeled training set. Yet, transposing directly existing active learning on deep networks is not intuitive. First of all, scaling them to high dimensional parameters networks may turn out to be intractable: some classic active learning methods such as Optimal Experiment Design (Yu et al., 2006) require to inverse the Hessian matrix of the models at each iteration, which would be intractable for current standard CNNs. Secondly, one of the most standard active learning strategy is to rely on uncertainty measure. Uncertainty in deep networks is usually evaluated through the network’s output however this is known to be misleading. Indeed, the discovery of adversarial examples has demonstrated that the way we are measuring uncertainty may be overconfident. Adversarial examples are inputs modified with small (sometimes not perceptually distinguishable) but specific perturbations which result in an unexpected misclassification despite a strong confidence of the network in the predicted class(Szegedy et al., 2014). On one hand, the existence of such adversarial examples somehow discards uncertainty-based selection from being an efficient active learning criterion for deep networks. On the other hand, the magnitude of adversarial attacks does provide an information about how far a sample is from the decision boundaries of a deep network. This information is relevant in active learning and known as margin-based active learning. In a generic margin-based active learning, we assume that the decision boundaries evolve towards the optimal solution as the training set increases. Hence samples lying the farthest
2. Related Work

For a review of classic active learning methods and their applications, we refer the reader to Burr Settles (Settles, 2010). The main principle of active learning methods lies in iteratively building the training set: the iterative process alternates between training the classifier on the current labeled training set, and after convergence of the model, asks an oracle (usually a human annotator) to label a new set of points. Those new points are queried from a pool of unlabeled data given the heuristic in use. Several heuristics coexist as it is impossible to obtain a universal active learning strategy effective for any given task (Dasgupta, 2005). When it comes to deep learning, especially CNN, many existing active learning heuristics have proven to be not effective. For example, we empirically noticed in our experiments that uncertainty selection, or uncertainty sampling (Lewis & Gale, 1994), may perform worse than passive random selection. Since uncertainty selection consists in querying the annotations for the unlabeled samples which lead to predictions with lowest confidence, its cost is low and its setup simple. It has thus been used on deep networks for various tasks, ranging from sentiment classification to visual question answering and Named Entity Recognition (Zhou et al., 2010; Lin & Parikh, 2017; Yanyao Shen, 2018). Uncertainty selection has been improved in a pseudo-labeling method called CEAL (Wang et al., 2016): CEAL performs uncertainty selection, but also adds highly confident samples into the increased training set. The labels of these samples are not queried but inferred from the network’s predictions. In the case, one deal with a highly accurate network, CEAL will definitely improve the generalization accuracy. However, CEAL implies new hyperparameters to threshold the prediction’s confidence. If such a threshold is badly tuned, it will corrupt the training set with mistaken labels. Uncertainty selection may be also tailored to network ensemble, either by disagreement over the models (Query by committee, (Seung et al., 1992)) or by sampling through the distribution of the weights (Bayesian active learning, (Kapoor et al., 2007)). Recently, Gal et al. , in (Gal et al., 2016), demonstrated that dropout (and other stochastic regularization schemes) is equivalent to perform inference on the posterior distribution of the weights, enabling to leverage the cost of training and updating multiple models. Thus, dropout allows to sample an ensemble of models at test time: to perform Dropout Query By Committee (Ducoffe et al., (Ducoffe & Precioso, 2015)) or Bayesian Active Learning (Gal et al., (Gal et al., 2016)). Gal et al. proceeded with a comparison of several active learning heuristics: among all the metrics, BALD which maximizes the mutual information between predictions and model posterior consistently outperforms other metrics.

In the original problem, active learning only queries one sample at a time. However, such a strategy would not be stable considering deep networks. Since CNNs, and other
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deep learning algorithms, are trained with local optimization schemes, we need to add several sample at a time to have a consistent impact on the training. A possible solution is to select the samples with the top scores.

Sener et al. (Ozan Sener, 2018) define the batch active learning problem as a core set selection. They minimize the population risk of a model learned on a small labeled subset. To do so they propose an upper bound with a linear combination of the training error, the generalization error and a third term denoted as the core set loss. Due to the expressive power of CNNs, the authors argue that the first two terms (training and generalization error) are negligible. Therefore the population risk would mainly be controlled by the core set loss. The core set loss consists in the difference between the average empirical loss over the set of points which are already labeled, and the average empirical loss over the entire dataset including unlabeled points. If not considering the labels, the core set loss is equivalent to computing the covering radius over the network prediction. Finally, Sener et al. used a mixed integer programming heuristic to minimize at best the covering radius of the data. Thanks to their method, they achieve state-of-the-art performance in active learning for image classification.

Another direction, rarely explored for deep networks, is to rely on the distance to decision boundaries, namely margin-based active learning. Assuming that the problem is separable with a margin is a reasonable requirement assumed for many popular models such as SVM, Perceptron or AdaBoost. When positive and negative data are separable under SVM, Tong et al. have demonstrated the efficiency of picking the example which is the closest to the decision boundary (Tong & Koller, 2001). If, exploiting the geometric distances has been relevant for active learning on SVM (Tong & Koller, 2001; Brinker, 2003), it is not intuitive for CNNs since we do not know beforehand the geometrical shape of their decision boundaries. A first trial has been proposed in (Zhang et al., 2017). The Expected-Gradient-Length strategy (EGL ) consists in selecting instances with a high magnitude gradient. Not only such samples will have an impact on the current model parameter estimates but they will likely modify the shape of the decision boundaries. However, computing the true gradient for a given sample is intractable without its ground-truth label. In practice, they approximate the gradient with the expectation over the gradients conditioned on every possible class assignments.

3. Adversarial Active Learning with Deep-Fool attacks

In (Balcan et al., 2007), Balcan et al. demonstrated the significant benefit of margin-based approaches in reducing human annotations. We illustrate several margin-based active learning heuristics in figure 1: for each scenario, the data underlined in green will be queried. Especially, figure 1(d) describes our contribution. In the original case in figure 1(a), the projection of an unlabeled sample to the decision boundary determines whether or not it is worth to query its label, depending on the distance between the sample and the boundary. Margin-based strategies are effective but they require to know how to compute the distance to the decision boundary. When such a distance is intractable, a naive approximation consists in computing instead the distance between the sample of interest and its closest neighboring sample which has a different predicted class.

Figure 1. Illustration of different margin-based active learning scenarios in the binary case

Approximating the distance between a sample and the decision boundary, by the distance between this same sample and its closest neighboring sample from a different class, is coarse and computationally expensive. Instead, we propose DFAL , a Deep-Fool based Active Learning strategy which selects unlabeled samples with the smallest adversarial perturbation.

Indeed, adversarial attacks were originally designed to approximate the smallest perturbation to cross the decision boundary. Hence, in a binary case, the distance between a sample and its smallest adversarial example better approximates the original distance to the decision boundary than the
We have thus decided to use Deep-Fool algorithm to compute adversarial attacks for DFAL (Moosavi-Dezfooli et al., 2016). Indeed, Deep-Fool is an iterative procedure which alternates between a local linear approximation of the classifier around the source sample and an update of this sample so that it crosses the local linear decision. The algorithm stops when the updated source sample becomes effectively an adversarial sample regarding the initial class of the source sample. When it comes to DFAL, Deep-Fool holds three main advantages: (i) it is hyperparameter free (especially it does not need target labels which makes it more compliant with multi-class contexts); (ii) it runs fast as we empirically noticed in table 3; (iii) it is competitive with state-of-the-art adversarial attacks.

Moreover, DFAL is theoretically motivated by the robustness of neural networks: in (Tom Zahavy, 2018), Xu et al. used robustness to explain the generalization abilities of stochastic algorithms. They can generalize well as long as their sensitiveness to adversarial examples is bounded in average. Xu et al. explain that since deep learning methods, in the majority of cases, are involving stochastic optimization mechanisms due to the common schemes used in their training phase such as SGD or dropout, they can be considered as stochastic algorithms. Therefore, by adding samples sensitive to small perturbations, DFAL enforces the network to increase its ensemble robustness and generalization abilities.

In order to regularize the network and increase its robustness in DFAL, we add both the less robust unlabeled samples and their adversarial attacks. Thus, it is more likely that the network will regularize on the adversarial examples added to the training set and become less sensitive to small adversarial perturbations. Unlike CEAL, DFAL is hyperparameter-free and cannot corrupt the training set: from the basic definition of adversarial attacks, we know that a sample and its adversarial attack should share the same label.

Finally DFAL improves the robustness of the network by adding at each iteration unlabeled samples at half the cost of reading their true labels (one label amounts to two samples) as described in Algorithm 1.

### Algorithm 1 DFAL: DeepFool Active Learning

**Require:** $\mathcal{L}$ set of initial labeled training examples

**Require:** $\mathcal{U}$ set of initial unlabeled training examples

**Require:** $\mathcal{H}$ set of hyper-parameters to train the network

**Require:** $K$ the number of candidates

**Require:** $n_{\text{query}}$ the number of data to query

**Require:** $p$: the $L_p$ norm used ($p = 2$)

**Require:** $N$: the number of data to label

# init the training set

$k = 0$

$L_0 = \mathcal{L}$

$U_0 = \mathcal{U}$

while $k < N$ do

# Train the network $A_k$ given the current labeled training set

$A_k = \text{training}(\mathcal{H}, L_k)$

# Select randomly a pool of data $S_k$ of size $K$

$S_k \subseteq U_k; \ |S_k| = K$

for $x_i \in S_k$ do

# compute adversarial attacks with $L_p$ norms

$r_i \leftarrow \text{DeepFool}(x_i, A_k; p)$

end for

# query the labels of the $n_{\text{query}}$-th samples $Q_k$ owing the smallest $L_p$ norm perturbation

$index_k \leftarrow \text{argsort}(\langle r_i, r_i \rangle \mid i = 1..K)$

$Q_k \leftarrow \{x_j \mid j \in index_k[0 : n_{\text{query}}]\} \cup \{x_j + r_j \mid j \in index_k[0 : n_{\text{query}}]\}$

$L_{k+1} \leftarrow L_k \cup Q_k$

$U_{k+1} \leftarrow U_k \setminus Q_k$

end while

4. Experiments

4.1. Dataset and CNN

We tested our algorithms for fully supervised image classification on three datasets that have been considered in recent articles on active learning for Deep Learning (Huijser & van Gemert, 2017): MNIST, Shoe-Bag, and Quick-Draw:

- **MNIST**: 28x28 grayscale images from 10 digits classes.
  - The training and test set contains respectively 60,000 and 10,000 samples.
We compare the evolution of the test accuracy when querying data with DFAL against the following baselines:

1. BALD: we select on a random subset of the unlabeled training set, the first \( n_{\text{query}} \) samples which are expected to maximize the mutual information with the model parameters. In that order, we sample 10 networks from the approximate posterior of the weights by also applying dropout as test time.

2. CEAL: we select on the whole unlabeled training set, the first \( n_{\text{query}} \) samples with the highest entropy on their network’s prediction. We also label any unlabeled samples whose entropy is lower than a given threshold (which is set according to the authors’ guidelines: 0.05 for MNIST, 0.19 for Shoe-Bag and 0.08 for Quick-Draw). Their labels are not queried but estimated from the network’s predictions.

3. CORE-SET: we select on a random subset of the unlabeled training set, the \( n_{\text{query}} \) samples which cover best the training set (labeled and unlabeled data) based on the euclidean distance on the output of the last fully connected layer. To approximate the cover set problem, we follow the instructions prescribed in (Ozan Sener, 2018): we initialize the selection with the greedy algorithm, and iterate with their Mixed Integer Programming subroutine. We also handle the robustness as prescribed by the authors. We have used or-tools \(^1\) to reproduce the MIP subroutine.

4. EGL: we select from a random subset of the unlabeled training set, the first \( n_{\text{query}} \) samples whose gradients achieves the highest euclidean norm.

5. uncertainty: we select from the whole unlabeled training set, the first \( n_{\text{query}} \) samples with the highest entropy on their network’s prediction.

6. RANDOM: we select randomly from the whole unlabeled training set \( n_{\text{query}} \) samples.

We assess the efficiency of our method on two CNNs: LeNet5 and VGG8 (Adam, \( lr=0.001 \), \( batch=32 \)). We have used Keras and Theano (Chollet et al., 2015; Al-Rfou et al., 2016). Although we have only tested our methods for CNNs trained with cross-entropy, DFAL may be used on any architectures impaired by adversarial attacks.

### 4.2. Evaluation

We compare the evolution of the test accuracy when querying data with DFAL against the following baselines:

- **Shoe-Bag**: This dataset has been created in (Huijser & van Gemert, 2017) from the Handbags and the Shoes datasets. It contains RGB images of size 64x64: 184,792 for training along with 4,000 images for testing.
- **Quick-Draw**: 28x28 grayscale images from the Google Doodle dataset. We downloaded four classes: Cat, Face, Angel, and Dolphin. This lead us to a training set of 444,971 samples and a test set of size 111,246 samples.
- **Doodle dataset**: This dataset has been created in (Huijser et al., 2016). Although we have only tested our methods for CNNs trained with cross-entropy, DFAL may be used on any architectures impaired by adversarial attacks.

We observe that DFAL always remains in the top three of the best performing active learning methods. We define those methods based on the test error rate when the labeled training set reaches 1000 samples. When DFAL is outperformed, it is only by a really slight percentage, either by pseudo labeling method\(^2\) which contributes more to the training set, or by CORE-SET. Since CORE-SET is designed as a batch active learning strategy, it diminishes the correlations among the queries. In order to outperform CORE-SET, DFAL could be extended into a batch setting approach: instead of selecting the top score samples, one could increase the diversity using for example submodular heuristics (Wei et al., 2018).

First of all, an interesting observation is that, independently from networks or datasets, active learning methods originally designed for singleton query (BALD, CEAL, EGL, uncertainty) fail to always compete against random selection (fig 2). This may result from the correlations among the queries when using top score selection. When it comes to our method, DFAL tends to convergence faster than such methods and is always better than random selection, independently from the network or the dataset (table 1). Hence our method is more robust to the hyperparameters settings than other active learning methods, when considering top score selection.

On diverse configurations (Shoe-Bag with LeNet5 and Quick-Draw with VGG8), CEAL is worse than uncertainty selection, hence it selects samples with high entropy but mistaken predictions which adds noise into the training set. Unlike CEAL whose probability of acquiring extra samples depends on the efficiency of the network, DFAL holds a constant number of extra samples, depending only on the number of queries. Moreover DFAL creates artificial data which are not part of the pool of data. For example, in tables 2(a) and 1(c), CEAL used more than 20 % of the training set of MNIST and Shoe-Bag, while DFAL only used at most 2 %. Thus, DFAL allows more queries, and may also be combined with CEAL.

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Table 1. Test accuracy achieved by 7 active learning techniques (DFAL, BALD, CEAL, EGL, uncertainty and RANDOM) given the number of annotations on LeNet5 and VGG8.

| # annotations | 100 | 500 | 800 | 1000 | All |
|---------------|-----|-----|-----|------|-----|
| **MNIST (LeNet5)** | | | | | |
| Accuracy (%) | | | | | |
| # annotations | 100 | 500 | 800 | 1000 | All |
| Accuracy (%) | | | | | |
| **MNIST (VGG8)** | | | | | |
| Accuracy (%) | | | | | |
| # annotations | 100 | 500 | 800 | 1000 | All |
| Accuracy (%) | | | | | |
| **Shoe-Bag (LeNet5)** | | | | | |
| Accuracy (%) | | | | | |
| # annotations | 100 | 500 | 800 | 1000 | All |
| Accuracy (%) | | | | | |
| **Shoe-Bag (VGG8)** | | | | | |
| Accuracy (%) | | | | | |
| # annotations | 100 | 500 | 800 | 1000 | All |
| Accuracy (%) | | | | | |
| **Quick-Draw (LeNet5)** | | | | | |
| Accuracy (%) | | | | | |
| # annotations | 100 | 500 | 800 | 1000 | All |
| Accuracy (%) | | | | | |
| **Quick-Draw (VGG8)** | | | | | |
| Accuracy (%) | | | | | |
| # annotations | 100 | 500 | 800 | 1000 | All |

Figure 2. Evolution of the test accuracy achieved by 7 active learning techniques (DFAL, BALD, CEAL, EGL, uncertainty and RANDOM) given the number of annotations on LeNet5 and VGG8.
Table 2. Comparison of the number of annotations and effective data required to achieve the same test accuracy on LeNet5 and VGG8 as the accuracy obtained on the full training set (± 0.5). We considered DFAL against the active methods achieving best accuracy on 1000 samples.

| Method      | LeNet5  | VGG8   |
|-------------|---------|--------|
| DFAL        | 1210    | 2410   |
| CORE-SET    | 1810    | 1810   |
| CEAL        | 25000   | 5100   |
| # annotations | # labeled data | # annotations | # labeled data |

Table 3. Average runtime of DFAL and CORE-SET on MNIST: \( \mathcal{L} = 100, \mathcal{U} = 800, n_{query} = 10 \)

attributes scores to each unlabeled sample independently one from another. Hence DFAL can be easily parallelized to compute adversarial attacks for a large pool of unlabeled samples.

We demonstrate the computational time gap between our method, DFAL, and CORE-SET in Table 3: we have recorded the average runtime of selecting 10 queries on MNIST with a training set of 100 samples and an unlabeled pool of size 800. For a sake of fairness, we compare DFAL running time against the CORE-SET approach, with and without robustness. Notice that the runtime performance of DFAL is independent from the size of the labeled training set. While CORE-SET slows down while we add more and more data to the training set.

4.4. Transferability

Figure 3. Evolution of the test accuracy for (Shoe-Bag, VGG8) trained with different labeled training set: we compare the efficiency of DFAL and CORE-SET built on LeNet5 and transfered on VGG8. The data selected by DFAL for LeNet5 achieve better test accuracy than the data transfered from CORE-SET. At 1000 samples, they converge to similar test accuracy than the data transfered from CORE-SET.

In preliminary experiments to a new problem, we know in advance neither the model architecture nor the hyperparameters that are best suited for the problem. One can argue that a network with high capacity is likely to give high accuracy parameters that are best suited for the problem. One can argue that a network with high capacity is likely to give high accuracy
Table 4. Comparison of the transferability of DFAL and CORE-SET with 1000 annotations

| Dataset       | DFAL | CORE-SET | RANDOM |
|---------------|------|----------|--------|
| LeNet5 → VGG8 | 97.80| 96.90    | 94.46  |
| VGG8 → LeNet5 | 97.93| 97.40    | 95.31  |
(a) MNIST

| Dataset       | DFAL | CORE-SET | RANDOM |
|---------------|------|----------|--------|
| LeNet5 → VGG8 | 92.87| 91.06    | 89.94  |
| VGG8 → LeNet5 | 89.23| 89.41    | 89.42  |
(b) Quick-Draw

| Dataset       | DFAL | CORE-SET | RANDOM |
|---------------|------|----------|--------|
| LeNet5 → VGG8 | 99.40| 99.12    | 97.08  |
| VGG8 → LeNet5 | 98.75| 98.50    | 98.07  |
(c) Shoe-Bag

When it comes to the transferability, we empirically demonstrate DFAL’s potential on a baby task: in figure 3 we recorded Shoe-Bag adversarial queries for LeNet5 and use them for training VGG8. While the test accuracy achieved is lower than with the adversarial active queries designed for VGG8, the transferred training set achieves better accuracy than random selection, but also, when reaching 1000 annotated samples, it is also better than queries from other active criteria designed for VGG8. We go further and compare the test accuracy of DFAL and CORE-SET transferred dataset on 1000 samples in table 4. Surprisingly the transferred queries from CORE-SET perform better than random. However, in almost every case, the transferred queries from DFAL outperform CORE-SET and RANDOM. The only exception concerns the transferred queries from VGG8 to LeNet5: neither DFAL nor CORE-SET succeed in outperforming RANDOM. We believe that LeNet5 trained on Quick-Draw have a smoother decision boundary than VGG8 in our hyperparameter setting. Thus, it would result in VGG8 queries being useful for training LeNet5 while the opposite would not be true.

5. Conclusion

In this paper, we propose a new heuristic, DFAL, to perform margin based active learning for CNNs: we approximate the projection of a sample to the decision boundary by its smallest adversarial attack. We demonstrate empirically that our adversarial active learning strategy is highly efficient for CNNs trained on MNIST, Shoe-Bag, and Quick-Draw. Not only are we competitive with the state-of-the-art batch active learning method for CNNs, CORE-SET, but we also outperform CORE-SET for runtime performance. Thanks to the transferability of adversarial attacks, DFAL is a promising approach for combining active learning with model selection for deep networks.

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