A Geometric Approach to Active Learning for Convolutional Neural Networks

Ozan Sener
Department of Computer Science
Stanford University
ozansener@cs.stanford.edu

Silvio Savarese
Department of Computer Science
Stanford University
ssilvio@stanford.edu

Abstract
Convolutional neural networks (CNNs) have been successfully applied to many recognition and learning tasks using a universal recipe; training a deep model on a very large dataset of supervised examples. However, this approach is rather restrictive in practice since collecting a large set of labeled images is very expensive. One way to ease this problem is coming up with smart ways for choosing images to be labelled from a very large collection (i.e. active learning).

In this paper, we first show that existing active learning heuristics are not effective for CNNs even in an oracle setting. Our counterintuitive empirical results make us question these heuristics and inspire us to come up with a simple but effective method, choosing a set of images to label such that they cover the set of unlabeled images as closely as possible. We further present a theoretical justification for this geometric heuristic by giving a bound over the generalization error of CNNs. Our experiments show that the proposed method significantly outperforms existing approaches in image classification experiments by a large margin.

1 Introduction
Deep convolutional neural networks (CNNs) have shown unprecedented success in many areas of research in computer vision and pattern recognition, like image classification, object detection, and scene segmentation. Although CNNs are universally successful in many tasks, they have a major drawback: they need a very large amount of labeled data to be able to learn their millions of parameters. More importantly, it is almost always better to have more data since the accuracy of CNNs is often not saturated with increasing dataset size. Hence, there is a constant desire to collect more and more data. Although this is the behavior you want from an algorithmic perspective (higher representative power is typically better), labeling a dataset is a time consuming and an expensive task. These practical considerations raise a critical question: “what is the optimal way to choose data points to label such that the highest accuracy can be obtained given a fixed labeling budget.” Active learning is one of the common paradigms to address this question.

The goal of active learning is to find effective ways to choose data points to label, from a pool of unlabeled data points, in order to maximize the accuracy. Although it is not possible to obtain a universally good active learning strategy [5], there exist many heuristics [29] which have been proven to be effective in practice. To the best of our knowledge, most of these heuristics are typically not effective for CNNs. The prevalent belief for explaining this behavior is CNNs’ tendency to make very confident mistakes. It is empirically observed that when CNNs make mistakes, they can assign arbitrary confidence values to their decisions. In other words, it is typically not possible to deduce that a CNN is uncertain solely by looking at its outputs. Although we agree with this observation, our empirical analysis suggests that this is not the main reason behind the ineffectiveness of active learning for CNNs.
Following our empirical study, we decided not to adopt an uncertainty based method, and approach the problem from a geometric perspective. We hypothesize that given a large dataset, the desired property of the set of labeled points is to cover the set of unlabelled ones as closely as possible (See Figure 1 for a visualization). In other words, we find a set of points to label such that when they are labeled, every remaining unlabelled point in the dataset will have a close labeled neighbor. We formulate this space-covering property as an optimization problem and present an efficient solution.

We carry out an in-depth analysis of our algorithm both theoretically and empirically. We study the generalization error of CNNs in a realistic setting and present a bound on the difference between the population risk and the empirical risk. We further consider the active learning case and present a bound over the risk of the unlabelled data points in terms of the maximum distance between unlabelled points and their labeled nearest neighbors. We further study the behavior of our proposed algorithm empirically for the problem of image classification using three different datasets. Our empirical analysis demonstrates state-of-the-art performance by a large margin.

2 Related Work

We discuss the related work in the following categories separately. Briefly, our work is different from existing approaches since i) it specifically targets CNNs, ii) we consider both fully supervised and weakly supervised cases, and iii) we theoretically analyze our algorithm.

Active Learning

Active learning has been widely studied and most of the early work can be found in the classical survey [29]. It discusses most query strategies such as information theoretical methods [22], ensemble approaches [24, 9] and uncertainty based methods [32, 19, 16, 20].

Bayesian active learning methods typically use a non-parametric model like Gaussian process to estimate the expected improvement by each query [17] or expected error after a set of queries [27]. These approaches are not applicable to deep learning scenarios since they do not scale to large-scale datasets. Ensemble methods are also not applicable to deep learning due to the large parameter space of neural networks. Such ensemble methods require an intractable number of networks to be trained.

One important class is that of uncertainty based methods, which try to find hard examples using heuristics like highest entropy [16], and geometric distance to decision boundaries [32, 3]. We present an empirical result in Section 4.1 which motivated us to move away from such techniques. We empirically demonstrate that even in the oracle case, such algorithms are not effective for CNNs.

There are recent optimization based approaches which can trade-off uncertainty and diversity to obtain a diverse set of hard examples. Elhamifar et al. [8] design a discrete optimization problem for this purpose and use its convex surrogate. However, the algorithm uses \( n^2 \) variables where \( n \) is the number of data points. Hence, it does not scale to the deep learning case. There are also many discrete optimization based active learning algorithms designed for the specific class of machine learning algorithms like k-nearest neighbors and naive Bayes [36]. Even in the algorithm agnostic case, one can design a set-cover algorithm to cover the hypothesis space using sub-modularity [13, 10]. Our algorithm can be considered to be in this class; however, we do not use any uncertainty information. Our algorithm is also the first one which applies to the CNNs.

Recently, a discrete optimization based method [2] which is similar to ours has been presented for k-NN type algorithms in the domain shift setting. Although our theoretical analysis borrows many techniques from [2], their results are only valid for k-NN and are not applicable to CNNs.

To the best-of-our-knowledge, the only active learning algorithm for CNNs is presented in [35]. It is a heuristic based algorithm which directly assigns labels to the data points with high confidence and queries labels for the ones with low confidence. We discuss its limitations in Section 6.

Unsupervised Subset Selection

The closest literature to our work is the problem of unsupervised subset selection. This problem considers a fully labeled dataset and tries to choose a subset of it such that the model trained on the selected subset will perform as closely as possible to the model trained on the entire dataset. For specific learning algorithms, there are methods like core-sets for SVM [33] and core-sets for k-Means and k-Medians [15].

The most similar algorithm to ours is the unsupervised subset selection algorithm described in [37]. It uses a facility location problem to find a diverse cover for the dataset. Our algorithm differs in that it uses a slightly different formulation of facility location problem. Instead of the min-sum, we use
Our paper is also related to semi-supervised deep learning. When there is no direct measure of uncertainty over the hypothesis class, the active learning problem is not well defined. However, we have seen adversarial methods which can learn a data distribution as a result of a two-player non-cooperative game. These methods are further extended to feature learning.

We consider a large collection of data points which are sampled i.i.d. over the space $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ as $\mathbf{x}_i, y_i \sim p_{\mathcal{Z}}$ where $|n| = \{1, \ldots, n\}$. We further consider an initial pool of data points chosen uniformly at random as $s^0 = \{s^0(j) \in [n] \}_{j \in [n]}$.

An active learning algorithm only has access to $\mathbf{x}_i, y_i$ and $\{y_{s(j)}\}_{j \in [m]}$. In other words, it can only see the labels of the points in the initial sub-sampled pool. It is also given a budget $B$ of queries to ask an oracle, and a learning algorithm $A_{w}$ which outputs a set of parameters $w$ given a labelled set $s$. The active learning with a pool problem can simply be defined as

$$\min_{s^1:|s^1| \leq B} E_{x,y \sim p_{\mathcal{Z}}}[l((x, y; A_{w_{0∪s^1}}))]$$  

In other words, an active learning algorithm can choose $b$ extra points and get them labelled by an oracle to minimize the future expected loss. There are a few differences between our formulation and the classical definition of active learning. Classical methods consider the case in which the budget is $1$ ($b = 1$) but a single point has negligible effect in a deep learning regime hence we consider the batch case. It is also very common to consider multiple rounds of this game. We also follow the multiple round formulation with a myopic approach by solving the single round of labelling as;

$$\min_{s^{k+1}:|s^{k+1}| \leq B} E_{x,y \sim p_{\mathcal{Z}}}[l((x, y; A_{w_{0∪\ldots∪s^{k+1}}}))]$$

We only discuss the first iteration where $k = 0$ for brevity although we apply it over multiple rounds. At each iteration, an active learning algorithm has two stages: 1. identifying a set of data points and presenting them to an oracle to be labelled, and 2. training a classifier using both the new and the previously labeled data points. The second stage (training the classifier) can be done in a fully or weakly-supervised manner. Fully-supervised is the case where training the classifier is done using only the labeled data points. Weakly-supervised is the case where training also utilizes the points which are not labelled yet. Although the existing literature only focuses on the active learning for fully-supervised models, we considered both cases and experimented on both.

4 Active Learning as a Set Cover

When there is no direct measure of uncertainty over the hypothesis class, the active learning problem is typically considered as refining decision boundaries by querying hard examples. Hence, using uncertainty is an empirically proven heuristic. However, this heuristic has very limited success in CNNs. This is widely attributed to the fact that the CNNs typically make very confident mistakes and the confidence values computed via soft-max outputs do not correspond to the true confidence of the model. Here, we focus on the following more fundamental question: would classical query methods work for CNNs if CNNs had an accurate uncertainty estimate? Although the common sense answer is affirmative, our empirical analysis shows that this is typically not the case. We describe this experiment in detail in Section 4.1.
Inspired by the empirical observation on the ineffectiveness of uncertainty based approaches, we propose not using uncertainty information, and instead approach the problem from a purely geometric perspective. We design an algorithm based on the heuristic of covering the set of unlabeled data points as closely as possible. We explain this algorithm in detail in Section 4.2 and further analyze it empirically in Section 6 and theoretically in Section 5.

4.1 Ineffectiveness of Uncertainty based Methods

It is common to attribute the ineffectiveness of uncertainty based methods in CNNs to the inaccuracy of the uncertainty estimates based on soft-max outputs. The common hypothesis is the following: Deep learning algorithms lead to an inaccurate estimate of uncertainty, hence the uncertainty based active learning methods fail. Although this hypothesis is intuitive considering the many confident mistakes CNNs make, it is not enough to answer more fundamental question: If CNNs produced accurate estimates of uncertainty, would uncertainty based active learning methods work for CNNs?

We can answer this question by simply replacing the uncertainty estimate in active learning with oracle ground truth loss. In other words, we replace the uncertainty with \( l(x_i, y_i, A^o) \) for all unlabeled examples \( x_i \). Since this is the oracle for the estimation of the uncertainty, in practice the uncertainty based methods are expected to be upper bounded by this oracle. We sample the queries from the normalized form of this function by setting the probability of choosing the \( i^{th} \) point to be queried as \( p_i = \frac{l(x_i, y_i, A^o)}{\sum_j l(x_j, y_j, A^o)} \). We use two loss functions, classification accuracy (\( \mathbb{I}[y_i = \arg \max_c h_c(x_i; A^o)] \)) and cross entropy (\( -\log h_c(x_i; A^o) - \sum_{c \in [C]} y_i \log(1 - h_c(x_i; A^o)) \)) where \( \mathbb{I} \) is the indicator function and \( h_c(\cdot, w) \) is the activation of \( c^{th} \) softmax output given network weights \( w \). As the oracle, we use the maximum accuracy obtained by querying based on either of these loss functions. We perform this experiment for the fully supervised and weakly supervised cases and plot the results in Figure 2. (See Section 4.3 for implementation details)

Results in Figure 2 suggest that even in the oracle case, uncertainty based methods are not effective for CNNs when compared with random sampling. We even observe that it causes the accuracy to drop in the weakly-supervised case. Hence, the aforementioned hypothesis is not entirely correct at least for the batch setting. Hence, we can conclude that inaccurate estimate of uncertainty does not explain the failure of uncertainty based active learning methods in CNNs in batch setting.

We believe this counterintuitive result is mostly due to the fact that we are sampling/labelling images in batches instead of querying one by one. The batch sampling of queried samples creates strong correlation among the chosen data points. On the other hand, querying images one by one is not desired since a single point has no significant effect in deep learning due to the SGD. In order to fix this, we perform the same experiment with exploration as sampling points from the oracle density with probability 0.8 and sampling uniformly with probability 0.2. We plot the oracle with exploration in the same figure. Although it helps, the oracle does not outperform random.

In order to visualize the correlation, consider an embedding of images computed using the tSNE[21] algorithm based on features learned after incorporating the entire dataset in learning. We plot the images in the initial pool (s0), chosen images for labelling (s1), and remaining images (\( |\mathcal{I}| \setminus (s0 \cup s1) \)) with separate colors in Figure 1. As shown in Figure 1a, the oracle algorithm fails to cover the space efficiently creating a bias. A successful set of queries must not only be hard-negatives but also cover the space efficiently. Hence, we believe covering the space effectively is very important for CNNs and we design an algorithm purely based on space covering in Section 4.2. We also show the tSNE plot for our algorithm in Figure 1b.

![Figure 1: tSNE embeddings of the CIFAR dataset and behavior of uncertainty oracle as well as our method. For both methods, the initial labeled pool of 1000 images are shown in blue, 1000 images chosen to be labeled in green and remaining ones in red. Our algorithm results in queries evenly covering the space. On the other hand, samples chosen by uncertainty oracle fails to cover the large portion of the space.](image)
Figure 2: Comparison of random sampling and active learning with oracle uncertainty. This figure suggests that even with oracle loss estimates, uncertainty based active learning algorithms are not effective for CNNs.

4.2 The Algorithm

We hypothesize that a good way to choose points to be labelled is to cover the unlabelled data points as closely as possible with labeled points. For example, consider a set of balls with radius $\delta$ centered at labelled points covering the entire unlabelled dataset. Intuitively, smaller $\delta$ should indicate a better performance. Hence, we try to choose a subset of points which can minimize $\delta$ as an active learning strategy.

Our algorithm is simply based on the $k$-Center problem (minimax facility location) which can intuitively be defined as follows: choose $k$ center points such that the largest distance between a data point and its nearest center is minimized. Formally, we are trying to solve:

$$\min_{s^1} \max_{i,j \in s^1 \cup s^0} \Delta(x_i, x_j)$$  \hspace{1cm} (3)

Unfortunately this problem is NP-Hard. However, it is possible to obtain a $2 - \text{OPT}$ solution efficiently using a greedy approach shown in Algorithm 1. If $\text{OPT} = \min_{s^1} \max_{i,j \in s^1 \cup s^0} \Delta(x_i, x_j)$, the greedy algorithm shown in Algorithm 1 is proven to have a solution ($s^1$) such that:

$$\max_{i,j} \min_{s^1 \cup s^0} \Delta(x_i, x_j) \leq 2 \times \text{OPT}.$$  

Although the greedy algorithm gives a good initialization, in practice we can improve the $2 - \text{OPT}$ solution by iteratively querying upper bounds on the optimal value. In other words, we can design an algorithm which decides if $\text{OPT} \leq \delta$. In order to do so, we define a mixed integer program (MIP) parametrized by $\delta$ such that its feasibility indicates $\min_{s^1} \max_{i,j \in s^1 \cup s^0} \Delta(x_i, x_j) \leq \delta$. A straight-forward algorithm is using this MIP as a sub-routine and performing a binary search between the result of the greedy algorithm and its half since the optimal solution is guaranteed to be included in that range. While constructing this MIP, we also try to handle one of the weaknesses of k-Center algorithm, namely robustness. To make the k-Center problem robust, we assume an upper limit on the number of outliers $\Xi$ such that our algorithm can choose not to cover at most $\Xi$ unsupervised data points. This mixed integer program can be written as:

$$\text{Feasible}(b, s^0, \delta, \Xi) : \sum_j u_j = |s^0| + b, \quad \sum_{i,j \in s^1 \cup s^0} \xi_{i,j} \leq \Xi$$

$$\sum_j \omega_{i,j} = 1 \quad \forall i,$$

$$\omega_{i,j} \leq u_j \quad \forall i, j$$

$$u_j = 1 \quad \forall j \in s^0,$$

$$\omega_{i,j} = \xi_{i,j} \quad \forall i, j \mid \Delta(x_i, x_j) > \delta.$$  \hspace{1cm} (4)

**Algorithm 1 k-Center-Greedy**

**Input:** data $x_i$, existing pool $s^0$ and a budget $b$

**Initialize** $s = s^0$

**repeat**

1. $u = \arg \max_{x_i \in [n]} \min_{j \in s} \Delta(x_i, x_j)$
2. $s = s \cup \{u\}$
3. until $|s| = b + |s^0|$

**return** $s \setminus s^0$

**Algorithm 2 Robust k-Center**

**Input:** data $x_i$, existing pool $s^0$, budget $b$ and outlier bound $\Xi$

**Initialize** $s_y = k$-Center-Greedy($x_i, s^0, b$)$\quad \delta_{2-OPT} = \max_j \min_{i \in s_y} \Delta(x_i, x_j)$

$$\text{lb} = \frac{\delta_{2-OPT}}{2}, \quad \text{ub} = \delta_{2-OPT}$$

**repeat**

1. if Feasible($b, s^0, \frac{\text{lb} + \text{ub}}{2}, \Xi$) then
2. $\text{ub} = \max_{i,j} \Delta(x_i, x_j) \leq \frac{\text{ub} + \text{lb}}{2}$
3. else
4. $\text{lb} = \min_{i,j} \Delta(x_i, x_j) \geq \frac{\text{ub} + \text{lb}}{2}$
5. end if

**until** $\text{ub} = \text{lb}$

**return** $\{i \ s.t. \ u_i = 1\}$
While implementing our algorithm, we used the Gurobi framework for checking feasibility of the MIP defined in (??). As an upper bound on number of outliers, we used Ξ = 1e−4 × n where n is the number of unlabelled points.

5 Analysis of the Algorithm

In this section, we analyze our algorithm in terms of generalization error. We are typically interested in the error in unseen images $E_{x,y\sim p_2}[l(x,y,A_n)]$ in terms of the empirical loss over the labelled images $\frac{1}{n} \sum_{i\in[n]} l(x_{s(i)}, y_{s(i)}, A_n)$. However, this analysis requires joint treatment of the generalization error and the effect of query selection. For simplicity, we divide this analysis into two parts. First, we analyze the relationship between expected loss in unseen images (generalization error) and the empirical loss over the entire dataset ($\frac{1}{n} \sum_{i\in[n]} l(x_i, y_i, A_n)$). Secondly, we analyze the relationship between the loss over the entire dataset and loss over the labelled samples. We study the first relationship by assuming a Lipschitz continuous loss function. We state the following proposition as direct result of one of the examples from [39] and defer its proof to the appendix.

**Proposition 1 ([39, Example 4]).** Given $n$ i.i.d. samples drawn from $p_2$ as $\{x_i, y_i\}_{i\in[n]}$. If loss function $l(\cdot, y, w)$ is $\lambda_1$-Lipschitz continuous for all $y, w$, bounded by $L$ and $X\mathcal{Y}$ has a covering number $N(\mathcal{X}, \mathcal{Y}, \cdot; [2]) = K$, with probability at least $1 - \gamma$,

$$E_{x,y\sim p_2}[l(x,y,A_n)] - \frac{1}{n} \sum_{i\in[n]} l(x_i, y_i, A_n) \leq \lambda_1\epsilon + L \sqrt{\frac{2K \log 2 + 2 \log(1/\gamma)}{n}}.$$

First of all, this proposition is applicable to any machine learning algorithm with a Lipschitz loss function and we further prove the Lipschitz-continuity of CNNs. It can clearly be seen that the empirical loss converges to the expected loss with large number of data points $n$ since $\lambda_1\epsilon$ term can be made arbitrarily small. In order to complete the study about the generalization performance of CNNs, we prove the Lipschitz-continuity of the loss function of a CNN with the following lemma where max-pool and restricted linear units are the non-linearities and the loss is defined as the $\ell_2$ distance between the desired probabilities and the softmax outputs.

**Lemma 1.** A convolutional neural network with $n_c$ convolutional (with max-pool and ReLU) and $n_{fc}$ fully connected layers defined over $C$ classes with loss function defined as the 2-norm between the softmax output and class probability is $\left(\sum_{c=1}^{C} \alpha^{n_c+n_{fc}}\right)$-Lipschitz.

Here, $\alpha$ is the maximum sum of input weights per neuron (see appendix for formal definition). Although it is in general unbounded, it can be made arbitrarily small without changing the loss function behavior (i.e. keeping the label of any data point $s$ unchanged). We can conclude that CNNs enjoy a 0 generalization error in the limiting case thanks to the Lipschitz property.
In order to complete the analysis, we need to study the behavior of the loss over the dataset in terms of the empirical loss over the selected (queried) samples. Here, we make a no training error assumption; in other words, we assume that the training error for labelled images is 0 at the end of the learning. This is clearly a restrictive assumption, however, it is very feasible due to the large parameter space of CNNs. Moreover, this can also be enforced by simply converting average loss into maximal loss \[30\]. Using this assumption, we show that the loss over the entire dataset can be bounded using the result of our discrete optimization problem.

**Theorem 1.** Given \(n\) i.i.d. samples drawn from \(p_Z\) as \(\{x_i, y_i\}_{i \in [n]}\), and \(m\) chosen points \(\{s(i) \in [N] \}_{i \in [m]}\). If loss function \(l(\cdot, y, w)\) is \(\lambda^L\)-Lipschitz continuous for all \(y, w\) and bounded by \(L\), regression function is \(\lambda^\mu\)-Lipschitz, \(\{s(i) \in [N] \}_{i \in [m]}\) is \(\delta\) cover of \(\{x_i, y_i \}_{i \in [n]}\), and \(l(x_{s(j)}, y_{s(j)}, A_S) = 0\) \(\forall j \in [m]\); with probability at least \(1 - \gamma\),

\[
\frac{1}{n} \sum_{i \in [n]} l(x_i, y_i) \leq \delta(\lambda^L + \lambda^\mu L C) + \sqrt{\frac{L^2 \log(1/\gamma)}{2n}}.
\]

It can easily be shown that in this setting, \(\lim_{m \to \infty} \frac{1}{n} \sum_{i \in [n]} l(x_i, y_i, A_S) = \delta(\lambda^L + \lambda^\mu L C)\). Clearly, \(\delta\) decreases when \(m\) increases; however, the rate is critical. To show that our algorithm has finite query, we need to show that \(\delta\) can be made arbitrarily small with finite \(m\) in the limiting behavior of number of unlabelled data points (i.e. \(n \to \infty\)). Since our data points are coming from a compact space, there exists a finite sub-cover to any union of open sets. Hence, the finite query property is a straightforward result of compactness.

In summary, we show that CNNs have Lipschitz continuous loss functions, making them generalize to unseen images. In addition, when the underlying data distribution has Lipschitz continuous regression functions, we further show, under reasonable assumptions, it is enough to label a small subset of the dataset as long as it covers the space efficiently. Since the difference between the empirical loss over unseen images and the optimal loss is bounded by \(\delta(\lambda^L + 2\lambda^\mu)\), direct minimization of \(\delta\) is a theoretically sound approach to this problem, validating our space-covering heuristic.

![Figure 4: Results on Active Learning for Weakly-Supervised Model (error bars are 3-std-dev)](image1)

![Figure 5: Results on Active Learning for Fully-Supervised Model (error bars are 3-std-dev)](image2)

### 6 Experimental Results

We tested our algorithm on the problem of classification using three different datasets. We performed experiments on CIFAR[18] and Caltech-256[12] datasets for image classification and on SVHN[24] dataset for digit classification. CIFAR[18] dataset has two tasks; one coarse-grained and one fine-grained. There are 100 fine-grained categories and 10 coarse-grained categories defined as strict supersets of some of these fine-grained categories. We performed experiments on both.

We also conducted experiments on active learning for fully-supervised models as well as active learning for weakly-supervised models. In our experiments, we start with small set of the images sampled uniformly at random from the dataset as an initial pool. The weakly-supervised model
has access to labeled examples as well as unlabelled examples. The fully-supervised model only has access to the labeled data points. We run all experiments with five random initializations of the initial pool of labeled points and use the average classification accuracy as a metric. We plot the accuracy vs the number of labeled points. We also plot error bars as three standard deviations. We run the query algorithm iteratively; in other words, we solve the discrete optimization problem

\[
\min_{k+1} \|s_{k+1}\|_b \mathbb{E}_{x,y \sim p_Z} [l(x, y; A_{s_0, \ldots, s_k})]
\]

for each point on the accuracy vs number of labelled examples graph. We present the results in Figures 4 and 5.

We compare our algorithm with uniformly at random sampling as well as the uncertainty oracle explained in Section 4.1. We also compared our algorithm with CEAL [35] which is to the best-of-our-knowledge, the only active learning algorithm presented for CNNs. Since it is a weakly-supervised approach utilizing unlabeled data points, we only include it in the weakly-supervised analysis.

Figures 4 and 5 suggests that our algorithm outperforms all other baselines in all experiments; for the case of weakly-supervised models, by a large margin. We believe the effectiveness of our approach in the weakly-supervised case is due to the better feature learning. Weakly-supervised models provide better feature spaces resulting in accurate geometries. Since our method is geometric, it performs significantly better with better feature spaces. We also observed that our algorithm is less effective in CIFAR-100 and Caltech-256 when compared with CIFAR-10 and SVHN. This can easily be explained using our theoretical analysis. Our generalization bound scales with the number of classes, hence it is better to have fewer classes.

**Optimality of the k-Center Solution:** Our proposed method uses the greedy 2-OPT solution for the k-Center problem as an initialization and checks the feasibility of a mixed integer program (MIP). Internally, we use LP-relaxation of the defined MIP and use branch-and-bound to obtain integer solutions. The utility obtained by solving this expensive MIP should be investigated. We compare the average run-time of MIP\(^1\) with the run-time of 2-OPT solution in Table 1. We also compare the accuracy obtained with optimal k-Center solution and the 2-OPT solution in Figure 6 on CIFAR-100 dataset.

| Distance Matrix | Greedy (2-OPT) | MIP (per iteration) | MIP (total) | Total |
|-----------------|---------------|---------------------|-------------|-------|
| 104.2           | 2             | 7.5                 | 244.03      | 360.23|

As shown in the Table 1 although the run-time of MIP is not polynomial in worst-case, in practice it converges in a tractable amount of time for a dataset of 50k images. Hence, our algorithm can easily be applied in practice. Figure 6 suggests a small but significant drop in the accuracy when the 2-OPT solution is used. Hence, we conclude that unless the scale of the dataset is too restrictive, using our proposed optimal solver is desired. Even with the accuracy drop, our active learning strategy using 2-OPT solution still outperforms the other baselines. Hence, we can conclude that our algorithm can scale to any dataset size with small accuracy drop even if solving MIP is not feasible.

In addition to the active learning, our algorithm can also be used for unsupervised subset selection. We further performed experiments on this setting and discuss them in the supplementary materials.

### 7 Conclusion

We described an active learning algorithm for CNNs. Our empirical analysis showed that classical uncertainty based methods have limited applicability to the CNNs. We design a simple but effective active learning algorithm for CNNs using geometric intuitions. We further validated our algorithm using both theoretical analysis and an empirical study. Empirical results on three datasets showed state-of-the-art performance by a large margin.

\(^1\) On Intel Core i7-5930K@3.50GHz and 64GB memory
References

[1] M. Abadi, A. Agarwal, P. Barham, E. Brevdo, Z. Chen, C. Citro, G. S. Corrado, A. Davis, J. Dean, M. Devin, et al. Tensorflow: Large-scale machine learning on heterogeneous distributed systems. [arXiv:1603.04467], 2016.

[2] C. Berlind and R. Urner. Active nearest neighbors in changing environments. In ICML, 2015.

[3] K. Brinker. Incorporating diversity in active learning with support vector machines. In ICML, volume 3, pages 59–66, 2003.

[4] W. J. Cook, W. H. Cunningham, W. R. Pulleyblank, and A. Schrijver. Combinatorial optimization, volume 605. Springer, 1998.

[5] S. Dasgupta. Analysis of a greedy active learning strategy. In NIPS, 2004.

[6] J. Donahue, P. Krähenbühl, and T. Darrell. Adversarial feature learning. [arXiv:1605.09782] 2016.

[7] V. Dumoulin, I. Belghazi, B. Poole, A. Lamb, M. Arjovsky, O. Mastropietro, and A. Courville. Adversarially learned inference. [arXiv:1606.00704], 2016.

[8] E. Elhamifar, G. Sapiro, A. Yang, and S. Shankar Sastry. A convex optimization framework for active learning. In ICCV, 2013.

[9] Y. Freund, H. S. Seung, E. Shamir, and N. Tishby. Selective sampling using the query by committee algorithm. Machine learning, 28(2-3), 1997.

[10] D. Golovin and A. Krause. Adaptive submodularity: Theory and applications in active learning and stochastic optimization. Journal of Artificial Intelligence Research, 42:427–486, 2011.

[11] I. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, and Y. Bengio. Generative adversarial nets. In NIPS, 2014.

[12] G. Griffin, A. Holub, and P. Perona. Caltech-256 object category dataset. Technical Report 7694, California Institute of Technology, 2007.

[13] A. Guillory and J. Bilmes. Interactive submodular set cover. [arXiv:1002.3345] 2010.

[14] I. Gurobi Optimization. Gurobi optimizer reference manual, 2016.

[15] S. Har-Peled and A. Kushal. Smaller coresets for k-median and k-means clustering. In Annual Symposium on Computational geometry. ACM, 2005.

[16] A. J. Joshi, F. Porikli, and N. Papanikolopoulos. Multi-class active learning for image classification. In CVPR, 2009.

[17] A. Kapoor, K. Grauman, R. Urtasun, and T. Darrell. Active learning with gaussian processes for object categorization. In ICCV, 2007.

[18] A. Krizhevsky and G. Hinton. Learning multiple layers of features from tiny images. Technical report, University of Toronto, 2009.

[19] D. D. Lewis. A sequential algorithm for training text classifiers: Corrigendum and additional data. SIGIR Forum, 29(2):13–26, 1995.

[20] X. Li and Y. Guo. Adaptive active learning for image classification. In CVPR, 2013.

[21] L. v. d. Maaten and G. Hinton. Visualizing data using t-sne. Journal of Machine Learning Research, 9(Nov):2579–2605, 2008.

[22] A. Krizhevsky and G. Hinton. Learning multiple layers of features from tiny images. Technical report, University of Toronto, 2009.

[23] D. D. Lewis. A sequential algorithm for training text classifiers: Corrigendum and additional data. SIGIR Forum, 29(2):13–19, Sept. 1995.

[24] X. Li and Y. Guo. Adaptive active learning for image classification. In CVPR, 2013.

[25] L. v. d. Maaten and G. Hinton. Visualizing data using t-sne. Journal of Machine Learning Research, 9(Nov):2579–2605, 2008.

[26] A. Krizhevsky and G. Hinton. Learning multiple layers of features from tiny images. Technical report, University of Toronto, 2009.

[27] D. D. Lewis. A sequential algorithm for training text classifiers: Corrigendum and additional data. SIGIR Forum, 29(2):13–19, Sept. 1995.

[28] X. Li and Y. Guo. Adaptive active learning for image classification. In CVPR, 2013.

[29] L. v. d. Maaten and G. Hinton. Visualizing data using t-sne. Journal of Machine Learning Research, 9(Nov):2579–2605, 2008.

[30] A. K. McCallumzy and K. Nigamy. Employing em and pool-based active learning for text classification. In ICML, 1998.

[31] Y. Netzer, T. Wang, A. Coates, A. Bissacco, B. Wu, and A. Y. Ng. Reading digits in natural images with unsupervised feature learning. In NIPS workshop on deep learning and unsupervised feature learning, 2011.

[32] A. Radford, L. Metz, and S. Chintala. Unsupervised representation learning with deep convolutional generative adversarial networks. [arXiv:1511.06434] 2015.

[33] A. Rasmus, M. Berglund, M. Honkala, H. Valpola, and T. Raiko. Semi-supervised learning with ladder networks. In NIPS, 2015.
A Proofs of the Theorems and Lemmas Provided in the Main Paper

A.1 Proof for Lemma 1

**Proof.** We will start with showing that softmax function defined over $C$ class is $\sqrt{\frac{C-1}{C}}$-Lipschitz continuous. It is easy to show that for any differentiable function $f : \mathbb{R}^n \to \mathbb{R}^m$, 

$$
\|f(x) - f(y)\|_2 \leq \|J\|_F \|x - y\|_2 \forall x, y \in \mathbb{R}^n
$$

where $\|J\|_F = \max_x \|J\|_F$ and $J$ is the Jacobian matrix of $f$.

Softmax function is defined as 

$$
f(x)_i = \frac{\exp(x_i)}{\sum_{j=1}^{C} \exp(x_j)}, i = 1, 2, \ldots C
$$

For brevity, we will denote $f_i(x)$ as $f_i$. The Jacobian matrix will be, 

$$
J = \begin{bmatrix}
    f_1(1-f_1) & -f_1f_2 & \ldots & -f_1f_C \\
    -f_2f_1 & f_2(1-f_2) & \ldots & -f_2f_C \\
    \ldots & \ldots & \ldots & \ldots \\
    -f Cf_1 & -f Cf_2 & \ldots & f_C(1-f_C)
\end{bmatrix}
$$

Now, Frobenius norm of above matrix will be,

$$
\|J\|_F = \sqrt{\sum_{i=1}^{C} \sum_{j=1}^{C} f_i^2 f_j^2 + \sum_{i=1}^{C} f_i^2(1-f_i)^2}
$$
It is straightforward to show that \( f_\epsilon = \frac{1}{\epsilon} \) is the optimal solution for \( \|J\|_F^* = \max_x \|J\|_F \). Hence, putting \( f_\epsilon = \frac{1}{\epsilon} \) in above equation, we get \( \|J\|_F^* = \sqrt{\frac{C - 1}{C}} \).

Now, consider two inputs \( x \) and \( \tilde{x} \), such that their representation at layer \( d \) is \( x^d \) and \( \tilde{x}^d \). Let’s consider any convolution or fully-connected layer as \( x_j^d = \sum_i w_{i,j} x_i^{d-1} \). If we assume, \( \sum_i |w_{i,j}| \leq \alpha \ \forall i, j, d \), for any convolutional or fully-connected layer, we can state:

\[
\|x^d - \tilde{x}^d\|_2 \leq \alpha \|x^{d-1} - \tilde{x}^{d-1}\|_2
\]

On the other hand, using \( |a - b| \leq |\max(0, a) - \max(0, b)| \) and the fact that max pool layer can be written as a convolutional layer such that only one weight is 1 and others are 0, we can state for ReLU and max-pool layers,

\[
\|x^d - \tilde{x}^d\|_2 \leq \|x^{d-1} - \tilde{x}^{d-1}\|_2
\]

Combining with the Lipschitz constant of soft-max layer,

\[
\|\text{CNN}(x; w) - \text{CNN}(\tilde{x}; w)\|_2 \leq \frac{\sqrt{C - 1}}{C} \alpha^{n_e + n_j} \|x - \tilde{x}\|_2
\]

### A.2 Proof for Proposition 1

In order to prove the Proposition 1, we use the robustness bound from [39].

**Proof.** We will start with

\[
\left| E_{x,y \sim p_Z} [l(x, y, A_s)] - \frac{1}{n} \sum_{i \in [n]} l(x_i, y_i, A_s) \right|
\]

\[
\overset{(a)}{\leq} \left| \sum_{j \in [K]} E[l(x, y)| (x, y) \in C_j] \mu_j - \sum_{j \in [K]} E[l(x, y)| (x, y) \in C_j] \frac{|n_j|}{n} \right|
\]

\[
+ \left| \sum_{j \in [K]} E[l(x, y)| (x, y) \in C_j] \frac{|n_j|}{n} - \frac{1}{n} \sum_{i \in [n]} l(x_i, y_i) \right|
\]

\[
\overset{(b)}{\leq} \left| \sum_{j \in [K]} E[l(x, y)| (x, y) \in C_j] \mu_j - \frac{|n_j|}{n} \right| + \frac{1}{n} \left| \sum_{j \in [K]} \sum_{i \in n_j} E[l(x, y)| (x, y) \in C_j] - l(x_i, y_i) \right|
\]

\[
\overset{(c)}{\leq} \sum_{j \in [K]} E[l(x, y)| z \in C_j] \mu_j - \frac{|n_j|}{n} + \frac{\lambda}{\epsilon}
\]

Here, with brevity we denoted \( l(x, y, A_s) \) as \( l(x, y) \). In (a), we used the fact that the space has an \( \epsilon \) cover; and denote the cover as \( \{C_j\}_{j \in [K]} \) such that each \( C_j \) has diameter at most \( \epsilon \). We further defined an auxiliary variable \( \mu_j = \mathbb{P}(x, y) \in C_j \) and \( n_j = \sum_i 1[ (x_i, y_i) \in C_j ] \) and used triangle inequality. In (b), we used \( i \in n_j \) to represent \( (x_i, y_i) \in C_j \). Finally, in (c) we used the fact that each ball has diameter at most \( \epsilon \) and the loss function is \( \lambda\)-Lipschitz.

We can bound \( E[l(x, y)| z \in C_j] \) with maximum loss \( L \) and use Breteganolle-Huber-Carol inequality (cf Proposition A6.6 of [34]) in order to bound \( \sum_j \mu_j - \frac{|n_j|}{n} \).

Combining all; with probability at least \( 1 - \gamma \),

\[
\left| E_{x, y \sim p_Z} [l(x, y, A_s)] - \frac{1}{n} \sum_{i \in [n]} l(x_i, y_i, A_s) \right| \leq \lambda \epsilon + L \sqrt{\frac{2K \log 2 + 2 \log(1/\gamma)}{n}}
\]

\( \square \)
A.3 Proof for Theorem 1

Before starting our proof, we state the Claim 1 from [2]. Fix some \( p, p' \in [0, 1] \) and \( y' \in \{0, 1\} \). Then,

\[
p_{y \sim p}(y \neq y') \leq p_{y \sim p'}(y \neq y') + |p - p'|
\]

**Proof.** We will start our proof with bounding \( E[l(x_i, y_i)] \). We have a condition which states that there exists and \( x_j \) in \( \delta \) ball around \( x_i \) such that \( x_j \) has 0 loss.

\[
E[l(x_i, y_i)] = \sum_{k \in [C]} p_{y_i \sim \eta_k(x_i)}(y_i = k)l(x_i, k) \leq \sum_{k \in [C]} p_{y_i \sim \eta_k(x_j)}(y_i = k)l(x_i, k) + \sum_{k \in [C]} |\eta_k(x_i) - \eta_k(x_j)|l(x_i, k)
\]

With abuse of notation, we represent \( \{y_i = k\} \sim \eta_k(x_i) \) with \( y_i \sim \eta_k(x_j) \). We use Claim 1 in \((d)\), and Lipschitz property of regression function and bound of loss in \((d)\). Then, we can further bound the remaining term as;

\[
\sum_{k \in [C]} p_{y_i \sim \eta_k(x_j)}(y_i = k)l(x_i, k) = \sum_{k \in [C]} p_{y_i \sim \eta_k(x_j)}(y_i = k)[l(x_i, k) - l(x_j, k)] + \sum_{k \in [C]} p_{y_i \sim \eta_k(x_j)}(y_i = k)l(x_j, k) \leq \delta \lambda^l
\]

where last step is coming from the fact that the trained classifier assumed to have 0 loss over training points. If we combine them,

\[
E[l(x_i, y_i)] \leq \delta (\lambda^l + \lambda^l LC)
\]

We further use the Hoefding’s Bound and conclude that with probability at least \( 1 - \gamma \),

\[
\frac{1}{n} \sum_{i \in [n]} l(x_i, y_i) \leq \delta (\lambda^l + \lambda^l LC) + \sqrt{\frac{L^2 \log(1/\gamma)}{2n}}
\]

\(\square\)