Convolutional Neural Network and Convex Optimization

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Abstract

Latent Dirichlet allocation(LDA) is a generative topic model to find latent topics in a text corpus. It can be trained via collapsed Gibbs sampling. In this project, we train LDA models on two datasets, Classic400 and BBCSport dataset. We discuss possible ways to evaluate goodness-of-fit and to detect overfitting problem of LDA model, and we use these criteria to choose proper hyperparameters, observe convergence, and evaluate the models, the criteria we use include perplexity, VI-distance, visualization of clustering results, and highest-probability words.

1 Introduction

Deep learning

Convex optimization

SVM-loss

2 Sub-model Convolutional Network

2.1 Theoretical basis: Convolutional neural network

Convolutional neural networks(CNN) are a special kind of deep neural networks. It exploits local correlation by enforcing a local connectivity pattern between neurons of adjacent layers. For a certain hidden layer m, the hidden units in it are connected to a local subset of units in the $(m-1)$th layer. Additionally, each sparse filter h_i is replicated across the entire visual field. The replicated units share the same parametrization, i.e. the same weight vector and same bias. The layer is called feature map.

Mathematically, a feature map h^k is obtained by convolving the input with a linear filter, adding a bias term and then applying a non-linear function, it can be shown as follow:

$$h^k_{ij} = \mathrm{f}((W^k * x)_{ij} + b_k) \tag{1}$$

where W^k and b_k are weight and bias of kth feature map, and $\mathrm{f}(\cdot)$ is the nolinearity. In our experiments, Rectified Linear Units(ReLU) nonlinearity is used, which has been shown to be more efficient than conventional function $\tanh(\cdot)$.[1] ReLU nonlinearity is as follow:

$$f(x) = \max(0, x) \tag{2}$$

Another important type of layers is pooling. It is a form of non-linear down-sampling. There are several types of pooling, two common types of which are max-pooling and average-pooling. They partition the input image into a set of non-overlapping or overlapping rectangles and outputs the

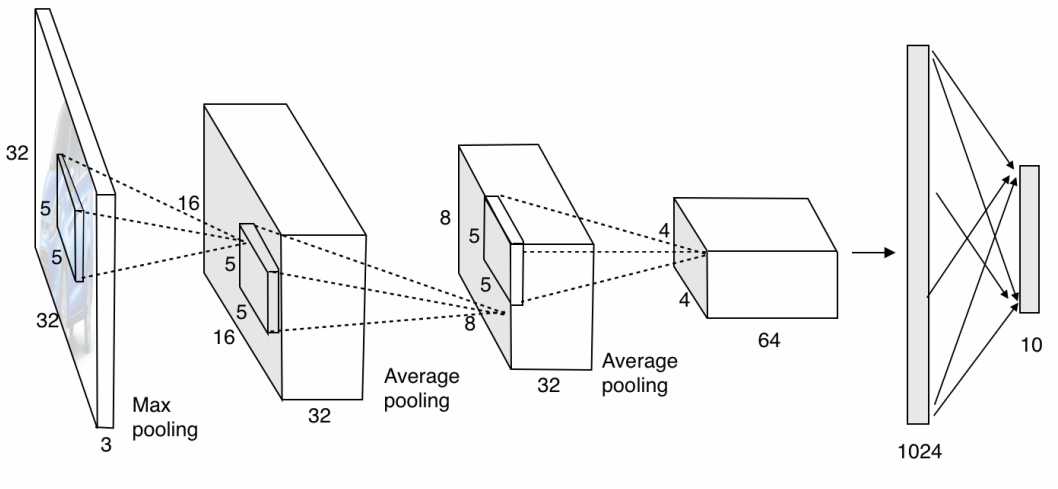


Figure 1: The architecture of our CNN.

maximum/average value for each such sub-region. By pooling, the model can reduce the computational complexity for upper layers, and can provide a form of translation invariance.

Typically, the last layer of a CNN is a logistic regression layer. Each unit of the output reflects a class membership probability:

$$P(Y = i|x, W, b) = softmax_i(Wx + b) = \frac{e^{W_i x + b_i}}{\sum_j e^{W_j x + b_j}} \tag{3}$$

The parameters of the network are trained using back propagation[2]. The loss function used for training is the negative-log likelihood of the training dataset D under the model:

$$L = \sum_{i=0}^{|D|} \log(P(Y = y^{(i)}|x^{(i)}, W, b)) \tag{4}$$

Finally, the prediction of the model is done by taking the argmax of the vector of $P(Y = i|x, W, b)$:

$$y_{pred} = \text{argmax}_i P(Y = i|x, W, b) \tag{5}$$

2.2 Overall architecture

The overall architecture of our CNN is shown in Figure 1. There are three convolutional layers and pooling layers alternatively. Overlapping pooling is performed. Each pooling layer consists of a grid of pooling units spaced $s = 2$ pixels apart, each summarizing a neighborhood of size 3×3 centered at the location of the pooling unit. The output of the network is a vector of class membership probability with 10 units, corresponding to 10 classes in our CIFAR-10 dataset[1].

2.3 Dropout and sub-model combination

Dropout is a recently-introduced technique to reduce overfitting [1]. It consists of setting to zero the output of each hidden neuron with probability of 0.5 in training procedure. So every time a training example is presented, the neural network samples a different architecture, which we denote here as a sub-model m_k. All these sub-models share weights. At test time, we use all neurons but multiply their outputs by 0.5, which is an approximation to taking the geometric mean of the predictive

[1] http://www.cs.toronto.edu/ kriz/cifar.html

distributions $P_{m_k} = [P_{m_k}(Y = 1), P_{m_k}(Y = 2), ..., P_{m_k}(Y = d)]^t$ produced by the sub-models (where d is the number of classes):

$$\begin{aligned}(P_{m_1}(Y = i) \cdot P_{m_2}(Y = i) \cdot \cdots \cdot P_{m_n}(Y = i))^{\frac{1}{n}} &= \frac{e^{(b_i + W_i \frac{1}{n} \sum_{k=1}^{n} h_{m_k})}}{(\sum_{j=1}^{d} e^{(nb_j + W_j \sum_{k=1}^{n} h_{m_k})})^{\frac{1}{n}}} \\ &= \frac{e^{(b_i + W_i \cdot h_{comb})}}{(\sum_{j=1}^{d} e^{(nb_j + W_j \sum_{k=1}^{n} h_{m_k})})^{\frac{1}{n}}}\end{aligned} \tag{6}$$

$$P_{comb}(Y = i) = \frac{e^{b_i + W_i \cdot h_{comb}}}{\sum_{j=1}^{d} e^{b_j + W_j \cdot h_{comb}}} \tag{7}$$

where h_{m_k} is the neurons of the penultimate layer of sub-model m_k, and h_{comb} is the that of the combined model by using all the neurons but multiply them by 0.5. $P_{comb}(\cdot)$ is the class membership probabilities of the combined model.

Apparently, the predictive distribution of the combined model is only a biased approximation of taking the mean of the predictive distribution of all sub-models.

In our experiments, the architecture is shown in Figure 1, dropout is performed in the output of penultimate layer, and $d = 10$ is the number of classes of our dataset.

Here, we want to explore a better option of combining the sub-models. Rather than giving an approximation, we want to actually taking the linear combination of the predictive distribution of n sub-models:

$$P_{l.comb}(Y = i) = \sum_{k=1}^{n} l_k \times P_{m_k}(Y = i) \tag{8}$$

where l_k is the weight of the distribution of kth model. The best weight $l = [l_1, l_2, ..., l_n]^t$ can be obtained solving following optimization problem:

minimize $\sum_{i=1}^{N} \|P_i \cdot l - y_i\|_2^2$,

subject to $l \geq 0$.

with the variable l, where N is the number of all the training examples, y_i is the 10×1 binary column vector indicating the true label of ith data point, and $P_i = [P_{m_1}, P_{m_2}, ..., P_{m_n}]$ is a $10 \times n$ matrix. By minimizing the sum of squared l2 norm of difference between predicted distribution and true label, we find the non-negative weight vector l.

The objective function can be simplified as following:

$$\begin{aligned}\sum_{i=1}^{N} \|P_i \cdot l - y_i\|_2^2 &= \sum_{i=1}^{N} (P_i \cdot l - y_i)^t (P_i \cdot l - y_i) \\ &= (P \cdot l - y)^t (P \cdot l - y) \\ &= l^t P^t P l - 2 y^t P l + y^t y\end{aligned} \tag{9}$$

where $y = \left[y_1^t, y_2^t, ...y_N^t\right]^t$ is the concatenation of label indicator vectors of all data points, which is a $10N \times 1$ vector. $P = \left[P_1^t, P_2^t, ..., P_n^t\right]^t$ is the concatenation of probability distributions of all data points, which is a $10N \times n$ matrix. Then the optimization problem can be written as follow:

minimize $l^t P^t P l - 2 y^t P l + y^t y$,

subject to $l \geq 0$.

with the variable l. This is a Quadratic Optimization Problem (QP), apparently a convex optimization problem, and is easy to solve.

2.4 Sub-model combination in non-dropout CNN

Now let's move back to CNN without dropout training. The same idea of sub-model combination can also be utilized to improve the performance of CNN when the network is trained without dropout.

The sub-models can be obtained by similar fashion with the dropout sub-models: given the already trained CNN model without dropout, randomly set penultimate units to zero with probability of 50%, and multiply the remaining units by 2:

$$\Pr(h^j_{m_i} = 2h^j_{orig}) = \Pr(h^j_{m_i} = 0) = \frac{1}{2}. \tag{10}$$

where h_{m_i} is the 1024 penultimate-layer unit vector of the sub-model m_i, h_{orig} is the 1024-unit vector of the trained CNN model, and $h^j_{(\cdot)}$ is the jth element of the vector.

Then, we can obtain the predictive distribution of each sub-model P_{m_k}, and the new model takes linear combination of the predictive distribution of n sub-models, which is the same as the dropout condition:

$$P_{l.comb}(Y = i) = \sum_{k=1}^{n} l_k \times P_{m_k}(Y = i) \tag{11}$$

Therefore, the optimization problem is very similar with dropout condition, and the only difference is the multiplication by 2 when obtaining the penultimate layer of sub-models.

3 Convex Loss functions

Deep neural network is well-known for its highly non-convexity. But we can still borrow some ideas from the convex optimization literature, where people have found many useful convex loss functions for classification tasks. In this section, we will talk about three different convex loss functions, and discuss how to use them in multiclass classification problem within the deep learning architecture.

3.1 Cross-entropy

Cross-entropy is the most standard loss function for neural networks, which is defined by:

$$H(p, q) = -\sum_x p(x) log q(x), \tag{12}$$

where p and q are ground-truth posterior probability and estimated posterior probability respectively. Cross-entropy can be directly used for multiclass classfication. This has been discussed in Section 2.1.

3.2 Hinge Loss

Hinge loss is widely used in Support Vector Machines (SVMs). Given training data and its corresponding labels (x_n, y_n), $n = 1, ..., N$, $x_n \in R^D$, $t_n \in -1, +1$, for a binary classification problem, SVMs learning includes the following convex optimization:

$$\begin{array}{lll} \min\limits_{w,\psi} & \frac{1}{2}w^T w + C\sum_{n=1}^{N}\psi_n & \\ \text{s.t.} & w^T x_n t_n \quad \geq & 1 - \psi_n \forall n \\ & \psi_n \quad \geq 0 & \forall n \end{array} \tag{13}$$

Hinge loss, while doesn't have a clear probability interpretation as CE, can be regarded as a maximum margin object function. And it can be directly used in the deep learning architecture by deriving the corresponding unconstraint optimization problem:

$$\min_w \quad \frac{1}{2}w^T w + C\sum_{n=1}^{N} max(1 - w^T x_n t_n, 0) \tag{14}$$

The second term of the object function is the Hinge loss. For the first term, there is a specific term called Weight Decay in the deep learning literature(which can also be seen as L2 regularization). The derivative w.r.t x is:

$$\frac{\partial l(x)}{\partial x_n} = -Ct_n(\mathbb{I}(1 > w^T x_n t_n)), \tag{15}$$

which is fast to compute.

Another similar loss function is the squared hinge loss:

$$\sum_{n=1}^{N} max(1 - w^T x_n t_n, 0)^2, \tag{16}$$

which is also differentiable and easy to compute. It imposes a bigger loss for points which violate the margin.

To predict the class label, for a binary classification problem, it's simply:

$$\begin{cases} +1, if \quad w^T x > 0 \\ -1, \quad otherwise \end{cases} \tag{17}$$

3.3 Multiclass Deep Neural Network with Hinge Loss

Many methods have been proposed to generaliza SVM to deal with multiclass problem. Here we talk about two most popular ways: One-Versus-All method and One-Versus-One method.

3.3.1 One-Versus-All

This is the earliest method for SVM multiclass classification. The basic idea is to train K SVM models where K is the number of classes. The ith SVM uses the data with label i as the positive samples and the data with other labels as the negative samples. Interestingly, this idea can be easily implemented in deep learning architecture. We can have K output units on top of the penultimate layer with the hinge loss. Then each output unit corresponds to one of these One-Versus-All SVMs. We can also regard this as replacing the softmax and cross-entropy layer with the hinge loss layer. This kind of method works well for problem with a small number of classes. When the class number grows larger, the imbalance between positive and negative samples for each SVM becomes intolerable.

3.3.2 One-Versus-One

The One-Versus-One method is to construct $K(K-1)/2$ classifiers. Each is responsible for one of the $K(K-1)/2$ class pairs. While testing, we simply let all the binary classifiers vote for the most probable one, which is also called the "Max Wins" strategy.To incorporate this method to deep learning architecture, we can have $K(K-1)/2$ output units, each of which corresponds to one classifier. All of the units use hinge loss. For each training data, only $K-1$ of these units are activated. The other units are temperorily cut off. This is illustrated in Fig. 2

The good property here is that for each SVM, the positive and negative training samples are balanced, no matter how many classes there are. However, The number of SVMs needed are quadratic in K, which makes it not scalable.

3.4 Ranking Loss

Another way to directly model the classification problem is the pairwise-ranking loss. Since we just want to pick the one with the highest linear output at test time. This lead to the following minimization problem:

$$Loss = \sum_{n=1}^{N} \sum_{i \in C_n^*} max(0, 1 - f_j(x_n + f_i(x_n))), \tag{18}$$

where j is the label of the nth data and C_n^* indicates the set of all the other labels. This loss can be directly generalized to multilabel predition problem and is widely used in many recommandation systems.

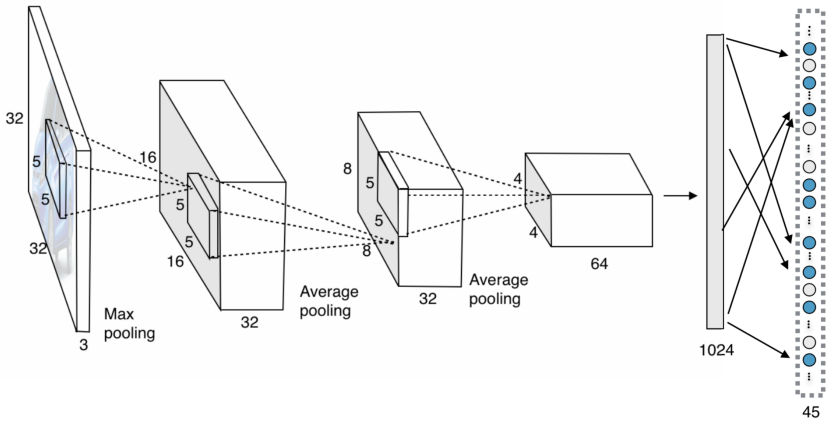


Figure 2: Deep Neural Network with One-Versus-One Hinge Loss

4 Experiments

4.1 Sub-model convolutional network

We use Theano[3] to train and test the CNN model, and cvx toolbox[2] in matlab to solve the convex optimization problem finding best weights. The training and test data are CIFAR-10 dataset.

We separately train the model with and without dropout, and the the result on the test set is shown in Table 1. Accuracy of dropout network is about 2% higher than nondropout network, which shows the advantage of dropout method.

Then, we randomly extract 4800 sub-models from dropout/non-dropout network respectively, find the optimal weight l by solving the convex optimization problem using different number of sub-models. The plot of the accuracy on test set versus number of sub-models is shown in Figure 3. The dotted line in both figures are the accuracy of the original model, which is the approximation of geometric mean of all possible sub-models.

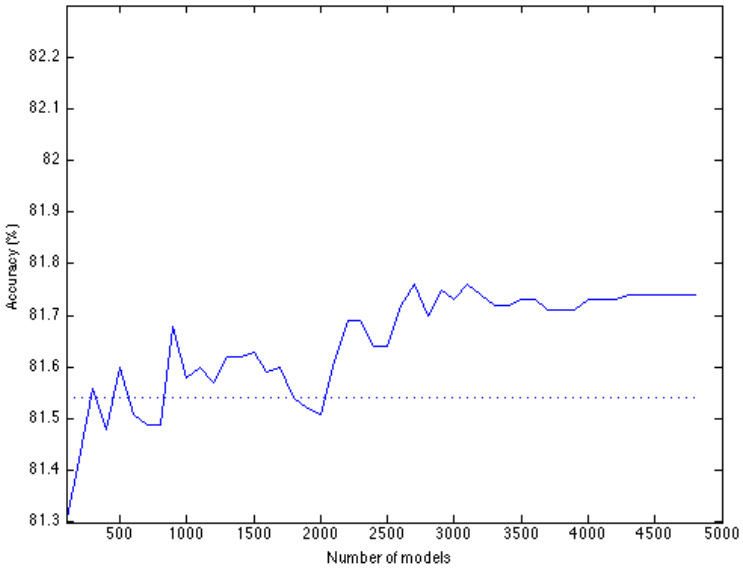
Clearly, the accuracy tend to increase with the number of sub-models used. This is intuitive: the sub-models are chosen randomly, the more sub-models we use, the more probable we have useful sub-models and better combinations. As is shown in Figure 3(a), for the model trained by dropout, the improvement is limited: approximately 0.2% improvement is achieved. However, for network trained without dropout, the improvement by weighted combination of sub-models is much more significant: the accuracy of original model is 79.52%, and the weighed combination of sub-models is always better than the original model, even when there are only 100 sub-models. The improvement is up to ???? when the number of sub-models reaches to ???.

4.2 The role of dropout

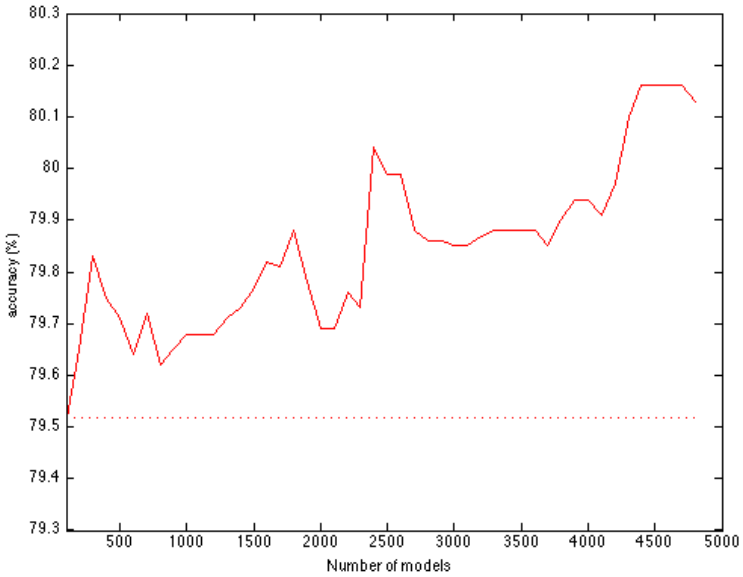
The reason of the lower improvement for dropout network is explained in this section. Dropout trains different sub-model at a time, but the weights are shared by all the sub-models. This procedure forces the network to learn more robust features that are useful for many different random sub-models, and after training, the sub-models in the dropout network can give similar results for all the data. This is the eventual goal of the dropout training. In other words, the sub-models in the dropout network are similar to each other, therefore whatever combination of them would not achieve much improvement. On the other hand, the network trained without dropout doesn't have the invariant property, thus the sub-models are quite different to each other, leading to greater improvement by combining them.

Figure 4 illustrates this effect of dropout training more clearly. accuracies achieved by 4800 sub-models for nondropout/ dropout network are shown in the two histograms. Clearly, the sub-models

[2]http://cvxr.com

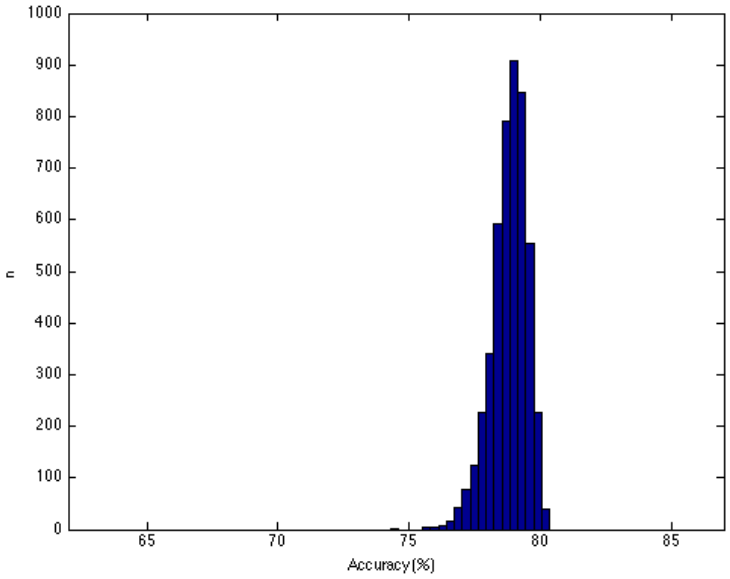


(a) Accuracy-number of sub-models for dropout network

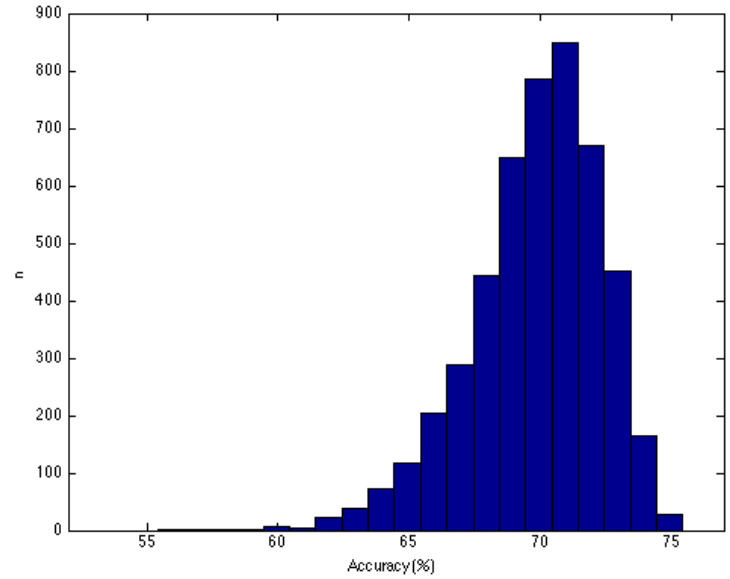


(b) Accuracy-number of sub-models for nondropout network

Figure 3: Accuracy-number of sub-models.



(a) Histogram of accuracies of sub-models of dropout network



(b) Histogram of accuracies of sub-models of nondropout network

Figure 4: Histograms of sub-models.

of dropout network are much more concentrated than those of the nondropout network. This shows the larger variance of the sub-models in nondropout network.

4.3 Convolutional network with different convex loss functions.

For this part, we use Caffe to do the experiments. Caffe is the most popular and fastest deep convolutional network implementation for the time being. It provides the cross-entropy loss. For the other loss functions, we implemented by ourself. We are going to compare cross-entropy(CE), One-

Network	Accuracy on test set (%)
Dropout	81.540
Non-dropout	79.517

Table 1: Accuracy of networks

Loss	Accuracy on test set (%)	WeightDecay
CE	77.85	750
1vsALL-L1	80.25	10
1vsALL-L2	80.18	100
1vs1-L1	77.80	10
RANK	77.60	100

Table 2: Accuracy of networks

Versus-All hinge loss(1vsAll-L1), One-Versus-All square hinge loss(1vsALL-L2), One-Versus-One hinge loss(1vs1-L1), rank loss(RANK).

4.3.1 Classification results

Table 2 shows the results for different loss functions and the corresponding relative weight decay used for the best results. For all of them, we use a similar strategy to train the network. The learning rate is initialized to 0.001. Before reaching the final point, we decrease the learning rate twice(for each time we reduce it by a factor of 10). The results clearly shows that One-Versus-All hinge loss and square hinge loss outperform other methods by a large margin. Due to time limit, all the results shown above is the best from the parameters that we have tried.

4.3.2 Convergence comparison

We also plot the accuracy rate on the validation set for the first 50000 iterations while training(see Fig. 5). We can find that under the same learning rate(0.001), the One-Versus-All hinge loss and square hinge loss converge the fastest. Cross-entropy gives the smoothest curve.

Please note that even though in this dataset One-Versus-All hinge loss seems to outperform cross-entropy by a large margin, it doesn't mean that we can use them as the standard loss in the future. By some preliminary experiments, the One-Versus-All hinge loss doesn't work on CIFAR100, which is a 100 class extention of CIFAR10. Cross-entropy is standard because of its stability. Also, for One-Versus-One hinge loss and rank loss, we can not say for sure that they perform worse than the others since the sets of parameters we have tried on them are too limited. This is why many people don't like neural networks. Tuning the parameters is a nightmare. However, we do find that by borrowing ideas from the convex optimization literature, we do see some improvements on some certain tasks.

5 Conclusion

References

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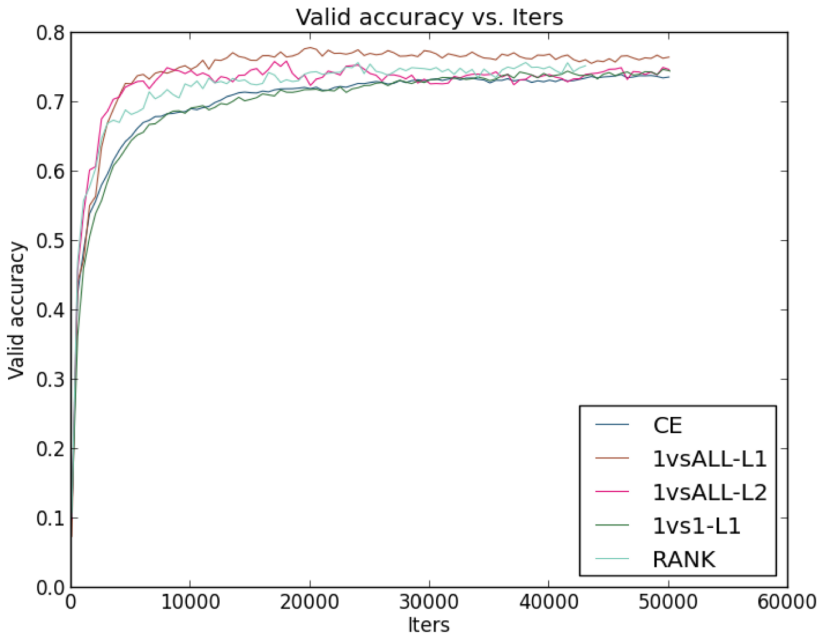

Figure 5: Comparison for different loss functions while training