Graph Convolutional Networks for Classification with a Structured Label Space

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Abstract

It is a usual practice to ignore any structural information underlying classes in multi-class classification. In this paper, we propose a graph convolutional network (GCN) augmented neural network classifier to exploit a known, underlying graph structure of labels. The proposed approach resembles an (approximate) inference procedure in, for instance, a conditional random field (CRF), however without losing any modelling flexibility. The proposed method can easily scale up to thousands of labels. We evaluate the proposed approach on the problems of document classification and object recognition and report both accuracies and graph-theoretic metrics that correspond to the consistency of the model’s prediction. The experiment results reveal that the proposed model outperforms a baseline method which ignores the graph structures of a label space.

Introduction

Multi-class classification is one of the most common problems in machine learning. A multi-class classifier predicts one label out of a set of mutually exclusive labels based on the known assignments in a training data.

However, such an approach does not take into account the complex dependencies among output variables and potentially leads to two problems. First, a multi-class classification model usually assumes mutually independent labels. The assumption holds on some computer vision tasks such as object recognition on ILSVRC (Russakovsky et al., 2015), in which classes are mutually exclusive leaf nodes of WordNet (Miller, 1995) (e.g., an object is not supposed to be both of a dog and of a cat). However, such an assumption does not apply to many other tasks, for example, a document can be labeled by multiple topics, which are statistically related. Second, the quality of top-k predictions is poorly evaluated. A naive multi-class classification framework evaluates top-k accuracy, which only measures the model’s ability to exactly match the true label. It ignores the relevance of other top predictions. This is critical especially in a dataset with highly correlated classes. For example, an image labeled with ‘husky’ is classified as ‘dog’ or ‘mammal’. Though neither matches the ground truth exactly, ‘dog’ is clearly a better prediction than ‘mammal’. Ideally, in a graph that encodes the relations among these three classes, the semantic distance from ‘dog’ to ‘husky’ is shorter than from ‘mammal’ to ‘husky’.

A known label relation can be exploited as a guide for a model to produce a cluster of predictions that are close to the ground truth in a structured label space. As a result, both classification accuracy and the relevancies of top predictions can be improved. Graphs have been shown to encode a complex geometry and can be used with strong mathematical tools such as spectral graph theory (Chung, 1997). Information propagation on such a graph that encodes label relations can be used to guide a classifier better incorporate relevance structures underlying the labels.

There have been work on incorporating the label structure in multi-class classification. They however come with two major shortcomings. First, classification with label relations is often confined to a certain type of graph (Deng et al., 2014). However, underlying label relations of a certain task may exist in various ways such as co-occurrence statistic or conceptual similarity. Second, most of the recent work approximates the pairwise relation with graphical models such as conditional random fields (CRF) and Markov random fields (MRFs) (Schwing and Urtasun, 2015). These often require complicated inference steps during training and prediction.

In this paper, we explore a novel way to perform multi-class classification combining deep neural networks (DNNs) with graph convolutional networks (GCNs) (Bruna et al., 2013) that allows flexible encoding of label structure. The GCNs improve classification accuracy and top prediction relevancy by exploiting the rich structure underlying the output variables. In particular, we propose a model structure that approaches a classification problem from the perspective of context-dependent graph representation learning. The proposed model stacks graph convolution layers on the concatenation of input and class latent variables to extract label-wise features, which are then decoded by a tied-weight decoder. The entire network is then trained as a deterministic deep neural network, bypassing any need for iterative inference steps. This significantly simplifies both training and prediction, and enables efficient learning on large datasets. We also propose several graph-theoretic metrics to evaluate the relevancy of top predictions.

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Related Work

Graph as Output

Structured Prediction with Label Relations Structured prediction approaches have been introduced in (Taskar, Guestrin, and Koller, 2004), (Tsotschantaridis et al., 2005), (Lampert, 2011), (Bi and Kwok, 2012), (Bi and Kwok, 2011), (Zhang, Shah, and Kakadiariis, 2017), in which a set of class labels are predicted jointly under a fixed loss function.

The goal of our work is clearly distinguished from the aforementioned works which are based on structured prediction. Structured prediction can be viewed as a variation of multi-label classification in that it takes input data with multiple assignments during training and jointly predicts a set of class labels for new observations during testing. In our work, the proposed models are trained on single-labeled data, and we demonstrate that incorporating label relation with multi-class classifier can not only improve accuracy but also produce top-n predictions that are closely related to the ground truth.

Multi-Class Classification with Label Relations Deng et al. (2014) incorporated WordNet (Miller, 1995) in image object recognition and demonstrated that exploiting label relations not only improves multi-class classification accuracy but also multi-label classification performance by setting hard constraints on the exclusive and inclusive relation between labels. This model was further extended for soft label relations using the Ising model in (Ding et al., 2015).

There are three major differences between this approach and the proposed approach. First, we do not impose any constraints on the graph structure other than requiring the availability of pairwise relations among nodes. Deng et al. (2014) on the other hand proposed to use a special kind of representation (the HEX graph) to express and enforce exclusion, inclusion, and overlap relations. Second, the proposed model is trained strictly with a single-labeled data, while Deng et al. (2014) and Ding et al. (2015) are equivalent to add multiple labels during training by using hard constraints. For example, if ‘husky’ is noted as a true label, the hard constraint forces the ‘dog’ label to turn on, indicating that this instance is an example of both the husky class and the dog class. Third, we train and use the entire model as a deterministic network, while Deng et al. (2014) and Ding et al. (2015) require a complicated inference step to model a conditional probability in the test time, potentially leading to mismatch between training and test.

Graph as Input

DNNs combined with graphical models have been found powerful on capturing statistical dependencies between the variables of interest in recent years. Some paper on this topic worked on generalizing neural networks for arbitrarily structured graphs, e.g., (Duvenaud et al., 2015; Li et al., 2015; Jain et al., 2015), while others have utilized graph convolution based on spectral graph theory (Bruna et al., 2013) to define parameterized filters that are used in a multi-layer neural network model. These work aim at modeling structured input data.

Graph Convolutional Networks GCNs are a type of neural network model that takes a graph as an input and output, for instance, labels. Previous works focused on exploiting different GCN structures. For instance, Defferrard, Bresson, and Vandergheynst (2016) approximated smooth filters in the spectral domain using Chebyshev polynomials with free parameters that are learned in a neural network-like model. Kipf and Welling (2016) started from the framework of spectral graph convolutions, and introduced simplifications that enable both significantly faster training times and higher predictive accuracy.

The main difference between the proposed method and the previously mentioned works is in the input data structure. The method proposed in this paper applies GCN as a layer in DNN to model data with structured output instead of structured input. In particular, the proposed model projects structured labels into a high-dimensional space and forward label hidden states conditioned on input data to GCN layers for feature extraction and classification.

Classification with External Knowledge

External knowledge of label relations (e.g., a taxonomy) is beneficial to guide the traditional classification systems. Recent works have begun to investigate new ways to integrate richer knowledge in a variety of tasks. For example, Grauman, Sha, and Hwang (2011), Hwang, Grauman, and Sha (2012) and Deng et al. (2014) took the WordNet category taxonomy to improve image object recognition. McAuley and Leskovec (2012) and Johnson, Ballan, and Fei-Fei (2015) used metadata from a social network to improve image classification. Ordonez et al. (2013) leveraged associated image captions to estimate entry-level labels of visual objects. Hu et al. (2016) used label relation graphs and concept layers for layered predictions.

The proposed method is a novel approach to incorporating external knowledge about label relations and is not task-specific. The label structure can be extracted in arbitrary ways according to a practitioner’s preference.

Model

Given an input variable \( x \in \mathcal{X} \) and output variables \( y = (y_1, y_2, ..., y_N) \) where \( y_i \in \{1, ..., |\mathcal{Y}_i|\} \), the score function \( F \) parametrized by \( \omega \in \mathbb{R}^w \) is modeled by the mapping \( F : \mathcal{X} \times \mathcal{Y} \times \mathbb{R}^w \rightarrow \mathbb{R} \).

The prediction procedure amounts to finding the configuration \( y^* \) that maximizes score function:

\[
y^* = \arg \max_{\hat{y} \in \mathcal{Y}} \max_{\omega} F(x, \hat{y}; \omega).
\]

The best configuration \( y^* \) is equivalently maximizing probability distribution

\[
p(\hat{y}|x, \omega) \propto \exp(F(x, \hat{y}; \omega)),
\]

since the exponential function is a monotonically increasing function and the normalization constant is independent of the configuration \( \hat{y} \).
Learning procedure finds a parameter vector $\omega^*$ that maximizes the log likelihood given a training set $\mathcal{D} = \{(x_1, y_1), \ldots, (x_N, y_N)\}$:

$$\omega^* = \arg \max_{\omega \in \mathbb{R}^{e'}} \log \prod_{(x,y) \in \mathcal{D}} p(x, y; \omega). \quad (3)$$

Consider a CRF defined over random variables $\mathcal{Y}$ given an observation $\mathcal{X}$ with a unary potential function $\psi_1(y_i, x; \omega_1)$ parametrized by $\omega_1$ and a pairwise potential function $\psi_2(y_i, y_j, x; \omega_2)$ parametrized by $\omega_2$. For simplicity, we omit parameters $\omega, \omega_1$, and $\omega_2$ whenever we can from here on.

In a flat classification model, label random variables are independent. Therefore, score function of output $y_i$ consists of only unitary terms:

$$F(x, y_i) = \psi_1(y_i, x). \quad (4)$$

In a scenario where pairwise relations among label random variables are taken into account, the score function consists of both unary and pairwise potentials:

$$F(x, y_i) = \psi_1(y_i, x) + \sum_{j=1, j \neq i}^N \psi_2(y_i, y_j, x). \quad (5)$$

By allowing the score function to depend not only on unary potentials but also pairwise potentials, the model explicitly encodes the graphical structure of the label space.

The proposed approach approximates the score function $F(x, y; \omega)$ with a neural network that has GCN layers to incorporate label relations represented by a graph $G = (\mathcal{V}, \mathcal{A})$, where $\mathcal{V}$ consists of all vertices and $\mathcal{A} \in \mathbb{R}^{N \times N}$ is an adjacency matrix, which is a representative description of the graph structure. In order to model the score function $F(x, y; \omega)$, based on input and pairwise label relations, the following steps are taken in the proposed approach: i) input representation (Fig. 1-(a-1)), ii) context-dependent label representation (Fig. 1-(a-2)), (b); iii) graph convolutional network (Fig. 1-(c)); iv) tied-weight decoder (Fig. 1-(d)).

**Input Representation** Let $x \in \mathbb{R}^D$ be the input data and $E : \mathbb{R}^D \rightarrow \mathbb{R}^{d_e}$ be an embedding function that maps $x$ to a continuous space. For example, in the task of document classification, $E(\cdot)$ can be a continuous bag-of-words (CBOW) lookup table (Mikolov et al., 2013); in the case of object recognition, it can be a convolutional neural network (CNN, (LeCun et al., 1990)). After the input encoding $E(x)$, the latent input representation $z \in \mathbb{R}^{d_z}$ is extracted by an affine transformation followed by a non-linear activation function:

$$z = \sigma(E(x)W + b),$$

where $W \in \mathbb{R}^{d_z \times d_e}$ and $b \in \mathbb{R}^{d_z}$ are trainable parameters and biases, and $\sigma(\cdot)$ is a non-linear activation, such as tanh.

**Context-Dependent Label Representation** After the input latent representation $z$ is extracted, each label $y_i$ is embedded in a $d_l$-dimensional vector $v_i \in \mathbb{R}^{d_l}$ which is jointly learned during training. Context-dependent label vector $v_i$ for label $y_i$ is initialized by concatenating the latent input representation $z$ and label vector $v_i$:

$$v_i = [z; v_i]. \quad (7)$$

A graph feature matrix $V \in \mathbb{R}^{N \times (d_l + d_z)}$ is constructed so that the $i$-th row of $V$ is $v_i$, i.e., $V = [v_1, v_2, \ldots, v_1, \ldots, v_N]^{\top}$. $V$ is in other words a feature matrix that simultaneously encodes labels and input.

**Graph Convolutional Network** The context-dependent feature matrix $V$ is fed the first GCN layer: $U^{(0)} = V$.

At the $t$-th layer, a graph convolutional network (GCN) takes an input feature matrix $U^{(t)} \in \mathbb{R}^{N \times d_t}$ and an adjacency matrix $\mathcal{A} \in \mathbb{R}^{N \times N}$, and produces an output $U^{(t+1)} \in \mathbb{R}^{N \times d_{t+1}}$, where $d_{t+1}$ is the number of output features per node. Kipf and Welling (2016) introduced a simplified graph convolution iteration step defined as:

$$U^{(t+1)} = \sigma(\mathcal{A}U^{(t)}W^{(t)}),$$

where $W^{(t)}$ is a learnable weight matrix and $\sigma$ is a non-linear activation function.
We use features extracted by 
Input Representation 
tracted from the WordNet canine subgraph. WordNet depicts 
channel feature maps size of 8x8 from the final convolutional layer. We do not fine-tune the network.

Tied-Weight Decoder  
After K iterations of graph convolution, the graph feature \( U^{(K+1)} \) is extracted. A fully connected decoder maps \( U^{(K+1)} \) to the number of labels as follows:

\[
F = U^{(K+1)} \omega,
\]

where \( \omega \in \mathbb{R}^{d_{K+1}} \).

Instead of using fully-connected decoder, the graph feature vector \( u_i \) of label \( y_i \) is decoded by tying output weight with input latent representation \( z \) and label representation \( v_i \). The label score \( F_i \) is obtained as follows:

\[
F_i = u_i z + u_i v_i
\]

where \( u_i \) is the \( i \)-th row of \( U^{(K+1)} \). Note that because of the decoding procedure, \( z \) and \( v_i \) need to have the same dimension.

Experiments Overview

In this section, we describe the details of the experiment settings including data collection and preprocessing. The proposed model is assessed in two experiments: a document classification task on an in-house dataset and a visual object recognition task on a canine image dataset. Dataset statistics are summarized in Table 1.

| Dataset          | Task                | Nodes (Labels) | Edges | Data Size |
|------------------|---------------------|----------------|-------|-----------|
| Canine image dataset | Object recognition | 170            | 170   | 23,800    |
| Document         | Document classification | 251          | 15,498| 28,916    |

Object Recognition on Canine Image Dataset

Image data collection  
We collect a new dataset consisting of images of canines using an approach inspired by Evtimova et al. (2017). We crawl the nodes in the subtree of the ‘canine’ synset in WordNet. For each node, we collect the word and query the word in Flickr to retrieve up to 140 images. We filter out the nodes with less than 140 images. The dataset is split into 100/20/20 images for training/validation/testing sets respectively.

Label graph construction  
The adjacency matrix is extracted from the WordNet canine subgraph. WordNet depicts hierarchical relations among a set of synsets.

Input Representation  
We use features extracted by ResNet-34 (He et al., 2016) that is trained on ImageNet for visual object recognition. The 512-dimensional feature vector is extracted after applying average pooling to the 512-channel feature maps size of 8x8 from the final convolutional layer. We do not fine-tune the network.

Proposed Model: GCNTD  
There are two evaluation scenarios in this task: the trained model is evaluated on a testing set consists of all nodes (all), or only leaf-nodes (leaf). We evaluate baseline and proposed models on both scenarios. We denote the proposed model on image object recognition task by GCNTD.

Baselines  
We compare the GCNTD with the following baselines.

• MLP  
The baseline model uses multi-layer perceptron (MLP) instead of the proposed GCN layers to map the contextual hidden state \( z \) to the classes. We denote this model as MLP.

• MLP-CRF  
Inspired by Ding et al. (2015), this baseline adds an Ising model as a layer on top of MLP. The Ising model is an undirected graphical model which defines the joint distribution of configurations of \( n \) binary random variables \( y \) in graph \( G = (V, E) \) by a Boltzmann distribution,

\[
p_\beta(y) = \frac{1}{Z_\beta} \exp(-\beta E(y)),
\]

where \( Z_\beta \) is the normalization constant, and \( \beta \) is a temperature variable that will be omitted later by fixing it to 1. \( E(y) \) is the energy function of the configuration \( y \), which takes into account local energy potentials \( h_i y_i \) as well as pairwise energy potential \( J_{ij} y_i y_j \).

\[
E(y) = \sum_{(i,j) \in G} J_{ij} y_i y_j + \sum_{i=1}^n h_i y_i.
\]

To formulate this model, assume we have a set of \( n \) possible labels, represented as the bit vector \( y = \{y_1, y_2, ..., y_n\} \), where \( y_i \in \{1, -1\} \). Also, assume we have an input feature vector \( x = \{x_1, x_2, ..., x_d\} \), and a discriminative model which maps this to the score vector \( z = [z_1, z_2, ..., z_n] \). In this model an MLP is used for the mapping. We define the conditional probability as follow:

\[
p(y|z) = \frac{1}{Z(x)} \prod_{i=1}^n \psi(y_i, z_i) \prod_{(i,j) \in E} \phi(y_i, y_j),
\]

where \( \psi(y_i, z_i) = \exp(-y_i z_i) \), and \( \phi(y_i, y_j) \) is the edge-specific potential function.

We confi gure the pairwise energy function \( E(y_i, y_j) \) between a pair \( (i, j) \) of an Ising model as follows:

\[
E(y_i, y_j; u) = -u_{ij} y_i y_j
\]

\[
= \begin{cases} 
  u_{ij} & y_i \neq y_j \\
  -u_{ij} & y_i = y_j 
\end{cases}
\]

where \( u_{ij} \) is the interaction parameter defined as follow:

\[
u_{ij} = \begin{cases} 
  u & (i, j) \in E \\
  0 & else
\end{cases}
\]

We set \( \phi(y_i, y_j) \propto \exp(-E(y_i, y_j; u)) \). The product of the pairwise factor function \( \phi(y_i, y_j) \) can be written in the
terms of sum of pairwise every functions $E(y_i, y_j; u_{ij})$:

$$
\prod_{(i,j) \in \mathcal{G}} \phi(y_i, y_j) \propto \exp\left(- \sum_{(i,j) \in \mathcal{G}} J_{ij} y_i y_j - \sum_{i=1}^{n} h_i y_i \right),
$$

(16)

where

$$J_{ij} = -u_{ij}
$$

(17)

$$h_i = 0
$$

(18)

To incorporate local evidence, we can rewrite Eq. 13 as follows:

$$p(y \mid z) \propto \exp\left(- \sum_{(i,j) \in \mathcal{G}} E(y_i, y_j; u_{ij}) + \sum_{i=1}^{n} \log \psi(y_i, z_i) \right)
$$

$$= \exp\left( \sum_{(i,j) \in \mathcal{G}} u_{ij} y_i y_j - \sum_{i=1}^{n} z_i y_i \right).
$$

(19)

We apply mean-field inference (MF) in our experiment. We fine-tune MLP parameters and $u$ on validation set using top-1 accuracy.

- **GCNTD-fc/id** Another baseline is to set the adjacency matrix in GCNTD as fully-connected (fc) or identity matrix (id).

We evaluate the graph-theoretic metrics of baseline models on WordNet canine graph.

**Document Classification**

**Data collection and preprocessing** For this task, we use an in-house dataset that is composed of various types of web page content including whitepapers, news articles, and blog posts. Each document has one human-added label that summarizes the primary information of the content. The labels are topics covering company names, business, finance, accounting, marketing, human resource, technology, lifestyle, and etc. The dataset is split by 60%/20%/20% for training/validation/testing sets respectively. The documents are lowercased and tokenized. The vocabulary set contains the most frequent 100,000 tokens including uni-grams and bi-grams.

**Label graph construction** The label graph is built by measuring pairwise similarities based on the label definitions. The label definition is queried from Wikipedia. If the label name does not have an exact match, the top-three suggested by Wikipedia are selected, and their Wikipedia definitions are concatenated as an alternative. The definitions are further tokenized into words and vectorized. We experiment with definition vectors that are created by TF-IDF weighted average of pre-trained word vectors. We construct the adjacency matrix by computing pairwise cosine similarity of definition vectors. The $[i,j]$ entry of an adjacency matrix $A \in \mathbb{R}^{|\mathcal{G}| \times |\mathcal{G}|}$ is

$$A_{i,j, i \neq j} = \frac{\mu_i \cdot \mu_j}{\|\mu_i\|_2 \|\mu_j\|_2},
$$

(20)

in which $\mu_i$ and $\mu_j$ are the $i$-th and $j$-th label’s definition vector respectively. We build a discrete adjacency matrix $\bar{A}$ by setting a threshold $\epsilon$ on the continuous adjacency matrix:

$$\bar{A}_{i,j} = \begin{cases} 1 & \text{if } A_{i,j} \geq \epsilon \\ 0 & \text{otherwise.} \end{cases}
$$

(21)

In the experiment, we set $\epsilon$ as the 75% percentile of all entries in $A$. As a result the discrete adjacency matrix $\bar{A}$ has on average 29.74 edges per node.

**Input Representation** After preprocessing, the document vectors are embedded in a CBOW manner (Mikolov et al., 2013). In detail, let $C \in \mathbb{R}^{v \times d_e}$ be a trainable embedding matrix, where $v$ is the vocabulary size and $d_e$ the embedding dimension, and $c_i$ be the of $i$-th row of $C$, the embedding function $E(\cdot)$ for document with tokens indices $D = \{d_1, d_2, \ldots, d_N\}$ is:

$$E(x) = \frac{1}{N} \sum_{i=1}^{N} c_{d_i}.
$$

(22)

**Models** We denote the structure of proposed model, GCN with tied-weight decoder, as GCNTD.

**Baselines**

- **MLP** Similarly, we denote baseline models as MLPn. In this experiment we test $n=1, 2, 4$. Note that this baseline model for document classification is equivalent to (Joulin et al., 2016) with word bi-gram. Such a model is shown to achieve near SoTA performances on several benchmarks of document classification (Joulin et al., 2016).

- **MLP-CRF**

- **GCNTD-fc/id**

We evaluate the graph-theoretic performance of these baseline models on definition based graph of GCNTD.

**Training Configurations**

All models are trained by minimizing negative log-likelihood (NLL) using back-propagation using Adam (Kingma and Ba, 2014) optimizer with an initial learning rate of 0.001. Additionally, a learning rate annealing is applied after each time the validation error does not decrease.

For GCNTD models, the number of GCN iterations is set to be two. For both GCNTDs and MLPs, trainings are early-stopped based on top-1 accuracy on validation set. We grid search embedding size $d_e$, learning rate, and minibatch size on validation set. Metrics are reported on testing set using the best model according to validation set.

**Evaluation**

Apart from the top-1 and top-10 accuracies, we suggest several graph-theoretic metrics to understand the performance of the proposed GCNTD model. We refer to ‘predictions’ as the 10 labels that are predicted with the highest confidence, if not otherwise specified. The following are our evaluation metrics:
• **Top-1/top-10 accuracy** The percentage of test cases when the true label is predicted in top-1/top-10 predictions.

• **One-hop precision@k** The fraction of top-k predictions that overlaps with the true label and its one-hop neighbors. By default $k = 10$.

• **One-hop recall@k** The fraction of the true label and its one-hop neighbors that overlaps with top-k predictions. By default $k = 10$.

• **Top-1/top-10 distance** Distance refers to the shortest path between a certain prediction and the true label on the graph, if they are connected at all. Top-1 distance is the distance between top-1 prediction and true label, and top-10 distance is the average distance between top-10 predictions and true label.

• **Diameter** The diameter of a graph is the maximum eccentricity of any vertex in the graph. In other words, it is the greatest distance between any pair of vertices. Here the diameter refers to the diameter of the subgraph that the predictions form.

The one-hop precision and recall are similar to those in multi-label classification framework. For simplicity, we refer to them as precision and recall. In these metrics, it is assumed that the true label’s one-hop neighbors on the graph are also potential true labels. Let true label and its one-hop neighbors be $T$ and predictions be $P$, the precision and recall are: $\text{precision} = \frac{|T \cap P|}{|P|}, \text{recall} = \frac{|T \cap P|}{|T|}$. In addition to the ability of model to exactly match the ground truth, these two metrics also measure the ability of the model to find a small cluster around ground truth. Higher values on top-1/top-10 accuracy, precision, and recall indicate stronger predictive power.

Top-1/top-10 distances and diameter, on the other hand, measure the coherence of predictions from a graphical perspective. Since the graph captures label relations, the labels that are closer to each other on the graph are more related. In the case of the definition-based label graph in document classification task, the graph captures semantic similarities. These metrics hence measure how centralized the predictions are with respect to the true label or themselves from a semantic perspective. Lower values indicate semantically more related labels.

**Results and Discussions**

We examine various aspects of the proposed GCNTD model. We compare the performance between GCNTD and MLP on the aforementioned metrics in document classification and object recognition. In addition, on document classification, we i) analyze ensemble model performance on top-1/top-10 accuracy; ii) analyze the contribution of model architecture component; iii) conduct a degree analysis to understand the prediction behavior from a graph perspective.

**Object Recognition on Canine Image Dataset**

The results are shown in Table 2-(A). The models are trained on all nodes and evaluated on both all nodes (all) and leaf nodes (leaf) of WordNet hierarchy.

![Image](320x506 to 558x583)

**Figure 2:** Precision and recall on top-k predictions. GCNTD refers to average precision/recall of 10 GCNTD in Table 2-(A), and MLP refers to that of MLP. GCNTD significantly outperforms MLP, and the improvement grows as k increases.

![Image](329x654 to 497x664)

**Figure 3:** The impact of ensemble method on top-1/top-10 accuracy in document classification. The single model result refer to the average accuracy of ten single models with identical hyperparameter settings. Ensemble refers to the accuracy of an ensemble of such 10 models. Ensemble has a stronger boosting effect on GCNTD than MLPs on both top-1 and top-10 accuracies.

In both cases, the models that consider underlying label structure (i.e. GCNTF and MLP-CRF) achieve higher performances on graph-theoretic metrics while the MLP outperforms on accuracy. In particular, MLP-CRF achieves the highest precision and recall on all nodes and leaf nodes respectively. Such result indicates that the explicitly defined energy functions in graphical model are beneficial for predicting labels closer to the ground truth than the MLP and the GCNTD on WordNet hierarchy.

To further explore the performance of GCNTD on a dataset with more complex pairwise relations, we experiment on document classification with labels highly correlated to each other.

**Document Classification**

Results are shown in Table 2-(B). In general, the GCNTD outperforms the MLP on all metrics, and outperforms MLP-CRF on accuracies, precision, and recall. GCNTD-fc achieves the highest accuracies, indicating the benefit of message passing under the extreme case where labels are fully-connected.

Figure 2 shows a comparison on top-k precision and recall between GCNTD and MLP. This demonstrates that the GCNTD tends to find a smaller cluster of predictions that are closer to ground truth. Since the label graph, in this case, is constructed by measuring definition similarities, the GCNTD can be thought of as making predictions that are semantically closer and more related to the ground truth: a
Table 2: Classification accuracy and graph-theoretic metrics on document classification and object recognition. Note that higher scores mean better performance for the first three columns, while lower scores mean better performance for the others. The best result on each evaluation metric is highlighted.

Panel A: Object recognition on ImageNet canine subset with GCNTD and MLP evaluated on the testing set with all nodes (all) or with only leaf nodes (leaf). GCNTD has better performance on graph-theoretic metrics such as top-10 distance and diameter, while MLP achieves higher accuracy. The better result on each metric in each testing scenario is highlighted.

| Test data | Top-1 (top-10) accuracy | Precision | Recall | Top-1 (top-10) distance | Diameter |
|-----------|-------------------------|-----------|--------|------------------------|----------|
| GCNTD     | .8235 (.9476)           | .6116     | .1794  | .2358 (.13520)         | 2.4008   |
| MLP       | .8060 (.9447)           | .5045     | .1460  | .2790 (.14840)         | 2.8142   |
| MLP-CRF   | .8446 (.9557)           | .5028     | .1465  | .2248 (.14823)         | 2.8238   |
| GCNTD-id  | .8141 (.9497)           | .5992     | .1635  | .2547 (1.3438)         | 2.4253   |
| GCNTD-fc  | .7487 (.9067)           | .4608     | .1329  | .3719 (.15386)         | 2.9368   |

Panel B: Document classification results of GCNTD and MLP. The GCNTD significantly improves the MLP-CRF and the MLP on accuracies, precision, and recall. GCNTD-fc achieves the highest accuracies among all models.

| Top-1 (top-10) accuracy | Precision | Recall | Top-1 (top-10) distance | Diameter |
|--------------------------|-----------|--------|------------------------|----------|
| GCNTD-id                 | .7387     | .1468  | .5954                  | 2.0671   | .33706 |
| MLP                      | .4396 (.7513) | .1424 | .5703                  | 2.0232   | .52373 |
| MLP-CRF                  | .4157 (.7458) | .1622 | .6472                  | 1.9732   | .32879 |
| GCNTD-id                 | .4038 (.7034) | .1302 | .5186                  | 2.1674   | .36433 |
| GCNTD-fc                 | .4208 (.7372) | .1402 | .5588                  | 2.1091   | .37511 |

smaller diameter indicates semantically closer predictions, and a smaller distance indicates that the predictions are semantically closer to the ground truth.

Architecture Component Analysis As shown in table 2-(B), the GCNTD outperforms the MLP on almost all metrics. Our hypotheses are i) GCN layer improves top predic-
tions relevancy and coherence by enabling information propagation across the structured label space and ii) a tied-weight decoder can effectively boost the top-1/top-10 accuracy.

To measure their contributions independently, different components in the proposed model are sequentially added and evaluated on document dataset.

The results are presented in Table 3. The MLP can be viewed as our implementation of Joulin et al. (2016) with bi-gram and zero MLP layer. Their implementation is denoted as fastText and evaluated as a reference for our MLP implementation.

As shown in the results of ‘GCN+fully-connected layer’ in Table 3, applying GCN layers significantly improves the performance on all graph-theoretic metrics. For example, diameter decreases by 26.7% and precision increases by 31.0%. This validates our first hypothesis that GCN layer improves classification performance by enabling information propagation across the structured label space. However, the top-1/top-10 accuracy also decreases dramatically. A possible explanation is that the undirected information propagation limits the model’s ability to produce the highest score for the correct label during training.

The ‘GCN+tied-weight decoder’ component of Table 3 shows the performance of replacing a fully-connected layer with tied-weight decoder on the previous model (‘GCN+fully-connected layer’), hence enforces information inflow of true label.

Degree Analysis The purpose of degree analysis is to understand the prediction behavior of GCNTD from a graph perspective. The degree of a graph node (or vertex) v in a graph G is the number of graph edges which touch v. The node degree is a common feature for tasks such as node similarity and classification (Lorrain and White, 1971). Degree analysis is helpful to understand the prediction preference of models.

The result is shown in Figure 4, displaying the average node degree of the k-th prediction (confidence from high to low, up to the 10th prediction) of a model. We observe a clear downward trend on the average node degrees of GCNTD top predictions, while the top-1 prediction from MLP has a much lower degree than the follow-up predictions. This re-
tions relevancy and coherence by enabling information propagation across the structured label space and ii) a tied-weight decoder can effectively boost the top-1/top-10 accuracy.

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Figure 4: Average node degree of k-th prediction in GCNTD and MLP. GCNTD refers to a group of six GCNTDs, and MLP refers to a group of ten MLP1-s. The average node degree values refer to that of k-th prediction (confidence high to low) on testing set produced by a certain group of models. Average node degree on graph is provided as a reference. In general, predictions of MLP have higher node degrees than those of GCNTD. Top-1 prediction of MLP has a lower degree than the rest, while that of GCNTD is the contrary.

Table: Average node degree for different prediction indexes.

| Prediction index | GCNTD | MLP |
|------------------|-------|-----|
| 1                | 67.5  | 62.6|
| 2                | 67.0  | 62.2|
| 3                | 66.8  | 62.1|
| 4                | 66.6  | 61.9|
| 5                | 66.4  | 61.7|
| 6                | 66.2  | 61.5|
| 7                | 66.0  | 61.3|
| 8                | 65.8  | 61.1|
| 9                | 65.6  | 60.9|
| 10               | 65.4  | 60.7|

Acknowledgements

Meihao Chen and Zhuoru Lin thank Nicholas Halecky, Jeffery Payne, Oleg Khavronin, Patrick Kelley, and Lindsay Reynolds for discussion and support on this work. Kyunghyun Cho thanks support by Tencent, eBay, Facebook, Google and NVIDIA, and was partly supported by Samsung Advanced Institute of Technology (Next Generation Deep Learning: from pattern recognition to AI). This work is completed during Zhuoru Lin’s internship with Bombora Inc.

Appendix

In this section we provide details for inference of the baseline MLP-CRF model.

Probability base for mean-field inference

In this section we calculate the conditional probability $p(y_k = 1|y_{i\neq k}, z)$, where $z$ is the local evidence $z = MLP(x)$. By Bayes rule we must have:

$$p(y_k = 1|y_{i\neq k}, z) = \frac{p(y_k = 1, y_{i\neq k} | z)}{\sum_{m \in \{-1, 1\}} p(y_k, y_{i\neq k} | z)}.$$  \hspace{1cm} (23)

The conditional probability $p(y_k = 1, y_{i\neq k} | z)$ is calculated by:

$$p(y_k = 1, y_{i\neq k} | z) = \frac{1}{Z} \exp(z_k + \sum_{i>k} u_{ik} y_i + \sum_{i>j, i\neq k} u_{ij} y_j - \sum_{i\neq k} y_i z_i).$$ \hspace{1cm} (24)

Assuming $y_{i\neq k}$ to be constant, we can rewrite Eq. 24 as:

$$p(y_k = 1, y_{i\neq k} | z) = \frac{1}{Z} \exp(z_k),$$ \hspace{1cm} (25)

where $\alpha = z_k + \sum_{i>k} u_{ik}$, and $c = \exp(\sum_{i>j, i\neq k} u_{ij} y_j - \sum_{i\neq k} y_i z_i)$.

Similarly:

$$p(y_k = -1, y_{i\neq k} | z) = \frac{1}{Z} \exp(-\alpha).$$ \hspace{1cm} (26)

Now we can use Eq. 25 and Eq. 26 to calculate Eq. 23:

$$p(y_k = 1|y_{i\neq k}, z) = \frac{\exp(\alpha)}{\exp(\alpha) + \exp(-\alpha)}.$$ \hspace{1cm} (27)

$$= \frac{1}{1 + \exp(-2\alpha)}.$$ \hspace{1cm} (28)

Algorithm

Based on the probability derived in previous section, the following algorithm is used to get $p(y | z)$.

\begin{algorithm}
\begin{algorithmic}
\STATE Input: Local evidence $z$
\STATE Result: Posterior belief $p(y | z)$
\STATE initialization: $\mu_k = \text{sigmoid}(2z_k)$
\WHILE{not converged}
\FOR{$\mu_k$ in $\mu$}
\STATE $\mu_k = \text{sigmoid}(2(z_k + \sum_{i \neq k} u_{ik} \mu_i))$
\ENDFOR
\ENDWHILE
\end{algorithmic}
\end{algorithm}

References

Bi, W., and Kwok, J. T. 2011. Multi-label classification on tree-and-dag-structured hierarchies. In Proceedings of the 28th International Conference on Machine Learning (ICML-11), 17–24.
Bi, W., and Kwok, J. T. 2012. Mandatory leaf node prediction in hierarchical multilabel classification. In Pereira, F.; Burges, C. J. C.; Bottou, L.; and Weinberger, K. Q., eds., Advances in Neural Information Processing Systems 25. Curran Associates, Inc., 153–161.

Bruna, J.; Zaremba, W.; Szlam, A.; and LeCun, Y. 2013. Spectral networks and locally connected networks on graphs. CoRR abs/1312.6203.

Chung, F. R. 1997. Spectral graph theory. Number 92. American Mathematical Soc.

Defferrard, M.; Bresson, X.; and Vandergheynst, P. 2016. Convolutional neural networks on graphs with fast localized spectral filtering. CoRR abs/1606.09375.

Deng, J.; Ding, N.; Jia, Y.; Frome, A.; Murphy, K.; Bengio, S.; Li, Y.; Neven, H.; and Adam, H. 2014. Large-scale object classification using label relation graphs. In European Conference on Computer Vision, 48–64. Springer.

Ding, N.; Deng, J.; Murphy, K.; and Neven, H. 2015. Probabilistic label relation graphs with ising models. CoRR abs/1503.04428.

Duvenaud, D. K.; Maclaurin, D.; Iparraguirre, J.; Bombarell, R.; Hirzel, T.; Aspuru-Guzik, A.; and Adams, R. P. 2015. Convolutional networks on graphs for learning molecular fingerprints. In Cortes, C.; Lawrence, N. D.; Lee, D. D.; Sugiyama, M.; and Garnett, R., eds., Advances in Neural Information Processing Systems 28. Curran Associates, Inc., 2224–2232.

Evitimova, K.; Drozdov, A.; Kiela, D.; and Cho, K. 2017. Emergent language in a multi-modal, multi-step referential game. arXiv preprint arXiv:1705.01428.

Grauman, K.; Sha, F.; and Hwang, S. J. 2011. Learning a tree of metrics with disjoint visual features. In Advances in neural information processing systems, 621–629.

He, K.; Zhang, X.; Ren, S.; and Sun, J. 2016. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition, 770–778.

Hu, H.; Zhou, G.-T.; Deng, Z.; Liao, Z.; and Mori, G. 2016. Learning structured inference neural networks with label relations. In The IEEE Conference on Computer Vision and Pattern Recognition (CVPR).

Hwang, S. J.; Grauman, K.; and Sha, F. 2012. Semantic kernel forests from multiple taxonomies. In Advances in neural information processing systems, 1718–1726.

Jain, A.; Zamir, A. R.; Savarese, S.; and Saxena, A. 2015. Structural-rnn: Deep learning on spatio-temporal graphs. CoRR abs/1511.05493.

Johnson, J.; Ballan, L.; and Fei-Fei, L. 2015. Love thy neighbors: Image annotation by exploiting image metadata. In Proceedings of the IEEE international conference on computer vision, 4624–4632.

Joulin, A.; Grave, E.; Bojanowski, P.; and Mikolov, T. 2016. Bag of tricks for efficient text classification. CoRR abs/1607.01759.

Kingma, D., and Ba, J. 2014. Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980.

Kipf, T. N., and Welling, M. 2016. Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907.

Lampert, C. H. 2011. Maximum margin multi-label structured prediction. In Advances in Neural Information Processing Systems, 289–297.

LeCun, Y.; Boser, B. E.; Denker, J. S.; Henderson, D.; Howard, R. E.; Hubbard, W. E.; and Jackel, L. D. 1990. Handwritten digit recognition with a back-propagation network. In Advances in neural information processing systems, 396–404.

Li, Y.; Tarlow, D.; Brockschmidt, M.; and Zemel, R. S. 2015. Gated graph sequence neural networks. CoRR abs/1511.05493.

Lorrain, F., and White, H. C. 1971. Structural equivalence of individuals in social networks. The Journal of mathematical sociology 1(1):49–80.

McAuley, J., and Leskovec, J. 2012. Image labeling on a network: using social-network metadata for image classification. Computer Vision–ECCV 2012 828–841.

Mikolov, T.; Chen, K.; Corrado, G.; and Dean, J. 2013. Efficient estimation of word representations in vector space. arXiv preprint arXiv:1301.3781.

Miller, G. A. 1995. Wordnet: a lexical database for english. Communications of the ACM 38(11):39–41.

Ordonez, V.; Deng, J.; Choi, Y.; Berg, A. C.; and Berg, T. L. 2013. From large scale image categorization to entry-level categories. In Proceedings of the IEEE International Conference on Computer Vision, 2768–2775.

Russakovsky, O.; Deng, J.; Su, H.; Krause, J.; Satheesh, S.; Ma, S.; Huang, Z.; Karpathy, A.; Khosla, A.; Bernstein, M.; et al. 2015. Imagenet large scale visual recognition challenge. International Journal of Computer Vision 115(3):211–252.

Schwing, A. G., and Urtasun, R. 2015. Fully connected deep structured networks. CoRR abs/1503.02351.

Taskar, B.; Guestrin, C.; and Koller, D. 2004. Max-margin markov networks. In Advances in neural information processing systems, 25–32.

Tschantzaris, I.; Joachims, T.; Hofmann, T.; and Altun, Y. 2005. Large margin methods for structured and interdependent output variables. Journal of machine learning research 6(Sep):1453–1484.

Zhang, L.; Shah, S.; and Kakadiaris, I. 2017. Hierarchical multi-label classification using fully associative ensemble learning. Pattern Recognition 70:89–103.