Semi-supervised Experiment Problem Collection

Deep Learning via Embedding Model

Describe Dataset in JSON

It's very annoying to adapt the model for new dataset when code lines like filename and `tf.placeholder` shape have to be modified every time. So writing `json` configuration file would be a better idea than changing the code mannually in source code or command line input.

Blind To Classifications

Try normalization anyway:

```
from sklearn import preprocessing
fn = '/home/yangminz/Semi-supervised_Embedding/dataset/PaviaU.mat'
dset = sio.loadmat(fn)
x = dset['paviaU'].reshape(shape_[0]*shape_[1], shape_[2])
x = preprocessing.scale(x)
x = x.reshape(shape_)
```

Taxing Coumputation

A profusion of computation lies in *finding neighbors*, or $\mathbf{W_{ij}}$. It's not cheap at all because it involves distance computation and ording:

$$\sqrt{(\mathbf{x_1}-\mathbf{x_2})^T(\mathbf{x_1}-\mathbf{x_2})}$$

$\mathbf{W_{ij}}$ is crucial to manifold or graph method since it indicates the internel structure or *space distribution* of the dataset.

The paper Deep Learning via Semi-supervised Embedding provides the solution or substitution for such arduous computation in section *3.1 Labeling Unlabeled Data as Neighbors(Building the Graph)*:

> However, there are also many other ways of collecting neighboring unlabeled data that do not involve computing k-nn. For example, if one has access to unlabeled sequence data the following tricks can be used.

The trick is to take advantage of the physical properties of data itself. Here for `paviaU` dataset, we pick the actual neighbor of a 'pixel' as its neighbor. Without distance computation and ordering, the computation is much faster.

According to the paper, the tricks can be subsumed into the following conditions by their datasets:

- image
- text
- speech

Difficult to Perform Batch Computation for Loss

To impletement loss with unlabeled samples, it's import to combine supervised loss with embedding loss. One can consult this stackoverflow post to figure out how to impletement embedding loss with unlabeled samples. There are some tricks for $\mathbf{W_{ij}}$.

Notice that it is difficult to impletement this embedding loss within a batch. Because a batch of data in `tf.placeholder` cannot get $\mathbf{W_{ij}}$ with each other. If we have a batch in size 3 like `[x[0], x[1], x[2]]`, then we must do something like:

```
for i in [0, 1, 2]:
for j in [0, 1, 2]:
W[i][j] = get_weight(x, i, j)
```

But as far as I know, it seems that this is impossible to impletement with `Tensorflow` because it requires indexing within `tf.placeholder`.

Fortunately the algoritm in the paper actually did not impletement batch form like:

$$\sum_{i=1} l(f(x_i), y_i) + \lambda \sum_{i,j=1}^{M+U} L(f(x_i), f(x_j), W_{ij})$$

Instead, it picks a pair of labeled, random neighbor, random unlabeled at every epoch. This makes it much more easier to impletement. It sounds like not fast. But with the new design of neighboring, the computation is not slow at all.

And remember to make the loss to scalar by `tf.reduce_sum` or `tf.reduce_mean`.

Weight Reusing

Originally, the code was designed like:

```
def forward(x):
    y = Dense(128, activation='tanh')(x)
    y = Dense(1, activation='sigmoid')(y)
    return y

y1 = forward(x1)
y2 = forward(x2)
```

However, weights would not be reused in this way because everytime the script calls `forward`, a new layer would be allocated when building up the graph. As a result, we get 2 seperate networks.

Layer initialization should be put outside the function:

```
layers = [
    Dense(128, activation='tanh'),
    Dense(1, activation='sigmoid')]

def forward(x):
y = x
for layer in layers:
y = layer(y)

y1 = forward(x1)
y2 = forward(x2)
```

It's much more convinent since the structure of the network can easily be adjusted and extended in `list` like:

```
layer_3 = layer_1[:5] + layer_2[4:]
```

Such implemention is possible by `Keras`.

Distance and `nan` Problem

In EmbedNN experiment with `g50c` dataset, the model sometimes converges to `nan` when use different distance in unlabeled embedding. For *Laplacian Eigenmaps*,

$$\sum_{ij} L(f_i, f_j, W_{ij}) = \sum_{ij} W_{ij} ||f_i - f_j||^2$$

can work while Euclidean distance:

$$\sum_{ij} L(f_i, f_j, W_{ij}) = \sum_{ij} W_{ij} ||f_i - f_j||$$

would give `nan`. There seems some delicate math backend.

And *Siamese Networks* embedding function:

$$L(f_i, f_j, W_{ij}) = \max(0, m||f_i f_j||_2)^2, \text{ if } W_{ij} = 0$$

can work when $||f_i f_j||_2 = (f_i - f_j)^T (f_i - f_j)$ while simple Euclidean distance would not give meaningful results.

S3VM loss

Standard optimization for *S3VM* is:

$$\sum_{\text{labeled}} \max(0, 1 - y_i f(x_i)) + \lambda_1 + ||h||^2_{\mathcal{HK}} + \lambda_2 \sum_{\text{unlabeled}} \max(0, 1 - |f(x_i)|)$$

Here we use the final unlabeled term in the combined loss which contains neighbor embedding loss based on manifold(graph) and this *S3VM* loss:

$$L_{\text{supervised}} + \alpha L_{\text{manifold}} + \beta L_{\text{cluster}}$$

Note that here $\beta + \alpha = 1$ and f is not the *SVM* kernel in original model but deep neural network embedding here.

A little experiment here can detect the model preference between $ L_{\text{neighbor}}$ and L_{s3vm}. Iterate `100000` labeled data with absolute hinge loss and *Siamese Networks* embedding:

Alpha	0.0	1.0	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1
Beta	0.0	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Accuracy	66.08%	39.16%	36.64%	45.52%	14.35%	48.74%	41.80%	41.46%	51.82%	56.18%	63.75%

Correct Distinguishing, Error Labeling

The classifier can distinguish classes from each other. However, the corresponding labels are misclassified. For example, `[2, 2, 4, 3, 3]` would be classified as `[1, 1, 6, 2, 2]`. They are correctly distinguished but wrongly classified.

The test data is the one to blame. One should be extremly careful when prepare "one-hot" labeling otherwise such weird error would occur.

For example, the following function

```
def OneHot(data, width):
    tmp = np.zeros((data.size, width))
    tmp[np.arange(data.size), data] = 1
    return tmp
```

returns one at their indices, `[0, 1, 0, 0]` for `data=1` and `width=4`. Sometimes similar function would give one-hot at their counting position, `[1, 0, 0, 0]`. Here `data=1` means *the first digit* rather than index `1`.

Improve the Accuracy

Tested with `paviaU`.

- Change Embedding Algorithm
  Lapalacian Eigenmaps seems to work better than *Siamese Networks*:

nb_labeled	supervised	manifold	Alpha	cluster	Beta	Radius	Accuracy
100000	'abs_hinge'	'SN'	0.5	'S3VM'	0.5	1	41.80%
100000	'abs_hinge'	'LE'	0.5	'S3VM'	0.5	1	65.52%

- Absolute Quadratic Loss
  Use absolute quadratic loss may be better for labeled data:

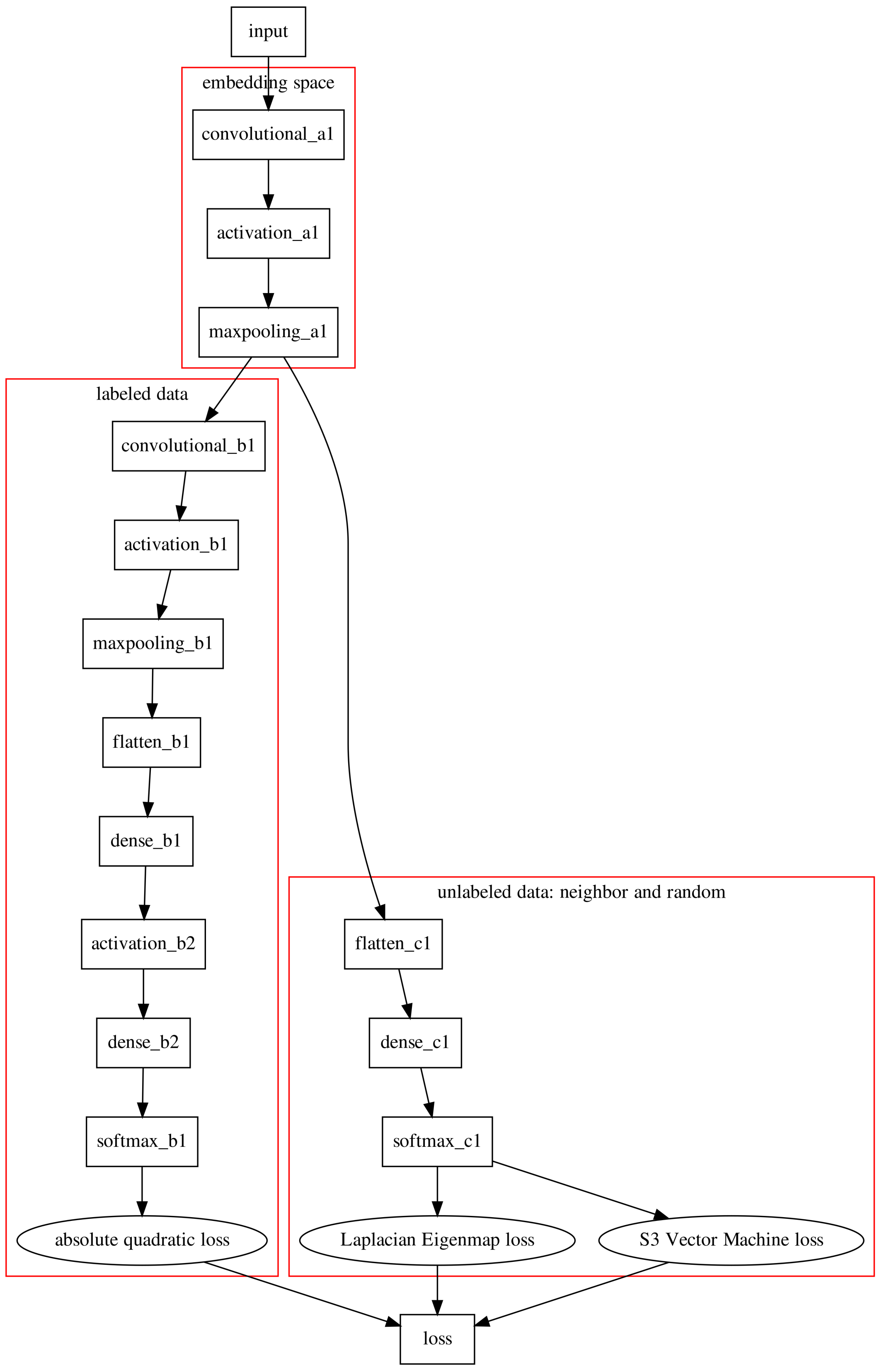
$$\mathcal{L}(y, y_t) = \max(0, 1 - |y_t \cdot y|)^2$$

nb_labeled	supervised	manifold	Alpha	cluster	Beta	Radius	Accuracy
100000	'abs_hinge'	'LE'	0.5	'S3VM'	0.5	1	65.52%
100000	'abs_quadratic'	'LE'	0.5	'S3VM'	0.5	1	69.93%

- Neighbor Radius
  For manifold(graph) loss, appropriate neighbor radius may help the accuracy(to avoid overfitting).
  But in fact this does not help:

nb_labeled	supervised	manifold	Alpha	cluster	Beta	Radius	Accuracy
100000	'abs_quadratic'	'LE'	0.5	'S3VM'	0.5	1	69.93%
100000	'abs_quadratic'	'LE'	0.5	'S3VM'	0.5	2	67.34%
100000	'abs_quadratic'	'LE'	0.5	'S3VM'	0.5	3	62.05%

- Other Model Structure
  Try *Auxiliary EmbedCNN*:


input
embedding space
convolutional_a1
activation_a1
maxpooling_a1
labeled data
convolutional_b1
activation_b1
maxpooling_b1
flatten_b1
dense_b1
activation_b2
dense_b2
softmax_b1
absolute quadratic loss
unlabeled data: neighbor and random
flatten_c1
dense_c1
softmax_c1
Laplacian Eigenmap loss
S3 Vector Machine loss
loss

This model gives a relatively high accuracy with `100000` labeled data, `'abs_quadratic'` supervised loss and `'S3VM'` unsupervised loss:

Alpha	0.0	1.0	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1
Beta	0.0	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Accuracy	68.10%	58.66%	62.87%	63.00%	62.16%	69.43%	69.58%	70.43%	71.62%	74.18%	77.37%

But it does not mean the more intricate the architecture is, the higher the accuracy will be. If the auxiliary net for unsupervised data is another stack of convolutional and maxpooling layers, the accuracy can decrease.

Other Models

Semi-supervised Support Vector Machine: Memory Error

SVM would take a lot of memory, e.g. $O(n^2)$ for kernel. Thus to run *S3VM*, the size of dataset should not be large. *SVM* is especially useful when the number of data is not so big, otherwise other brute algorithm would also work well, which makes *SVM* algorithm less competitive. So try less data to fit *S3VM* unless you have very large memory.

It's better to be noticed that currently it is not easy at all to find a repository for *multi-classification semi-supervised SVM*. The most common code is *multi-classification SVM* or *binary S3VM*.

Discriminative Restricted Boltzmann Machine

Semi-supervised DRBM algorithm is proposed in paper Classification using Discriminative Restricted Boltzmann Machines:

$$\mathcal{L}_{\text{semi-sup}}(\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{unlab}}) = \mathcal{L}_{\text{TYPE}}(\mathcal{D}_{\text{train}}) + \beta \mathcal{L}_{\text{unsup}}(\mathcal{D}_{\text{unlab}})$$

$$= -\sum_{i=1}^{|\mathcal{D}_{\text{train}}|} \log p(y_i|\mathbf{x_i}) - \beta \sum_{i=1}^{|\mathcal{D}_{\text{unlab}}|} \log p(\mathbf{x_i})$$

or

$$= -\sum_{i=1}^{|\mathcal{D}_{\text{train}}|} \log p(y_i|\mathbf{x_i}) - \alpha \sum_{i=1}^{|\mathcal{D}_{\text{train}}|} \log p(y_i, \mathbf{x_i}) - \beta \sum_{i=1}^{|\mathcal{D}_{\text{unlab}}|} \log p(\mathbf{x_i})$$

The implementation of *semi-supervised DRBM* consulted other people's code. The most common repository is *RBM*. I only found two repositories implemented by `Tensorflow` or `Theano`, both of them are supervised only.

The extension to semi-supervised is not difficult, as long as one pay attention to the *contrastive divergence algorithm*. The following code would illustrate:

```
def _calc_unsupervised_grads(self, x):
    x0, h0, x1, h1 = self._gibbs_un_sampling_step(x)

    h0 = tf.reshape(h0, [-1, self.num_hidden, 1])
    x0 = tf.reshape(x0, [-1, self.num_visible, 1])
    h1 = tf.reshape(h1, [-1, self.num_hidden, 1])
    x1 = tf.reshape(x1, [-1, self.num_visible, 1])

    # no gradient for U, but use zero to take place here
    d_U_unsup = tf.constant(0.0)
    d_W_unsup = tf.reduce_mean(tf.matmul(h0, x0, transpose_b=True) - tf.matmul(h1, x1, transpose_b

    d_b_unsup = tf.reduce_sum(x0 - x1, 0)
    d_c_unsup = tf.reduce_sum(h0 - h1, 0)
    d_d_unsup = tf.constant(0.0)
    return d_U_unsup, d_W_unsup, d_b_unsup, d_c_unsup, d_d_unsup
```

We know that the difference between supervised and semi-supervised is one-hot label `y`. Thus make the gradients related to `y` be `tf.constant(0.0)` would make them contribute nothing to the loss. Meanwhile `Tensorflow` can work even we have no method to figure out the shape of the `tf.placeholder` batch.

All-0 Prediction

Sometimes the model would predict the same label(`0` for dataset of `[0, 1, 2, 3, 4]` for example) in `EmbedCNN` and `Ladder Network(LN)`.

For EmbedCNN

The problem for EmbedCNN can usually be solved by:

- Try different initializers. Replace the default initializer with `lecun_uniform` for example.
- Clip gradient. Limit the gradient so they won't go to infinite. Code is usually like:

```
opt = tf.train.AdagradOptimizer(lr)
gvs = opt.compute_gradients(loss_)
clipped_gvs = [(tf.clip_by_value(grad, -1.0, 1.0), var) for grad, var in gvs]
train_step = opt.apply_gradients(clipped_gvs)
```

- Use different activations. For example, use `tanh` and `sigmoid` instead of using `relu` only.
- Sometimes directly use a 2-layer `dense` network would give a good result.
- Add `Dropout` layer to the network.

For LN

The major problem is `houston` dataset. It's weird because the LN with the same architecture works well on `paviaU` and `indian`. But for `houston`, the prediction will be `[0, 0, 0, ..., 0]`. A little debug tip here:

- Run the model in very short time(10 epoches for example) first and print all predicted labels. In this way, one can save a lot of time to verify if his model works before entering the time-costing training.
- Make sure that training dataset is reasonable. The split of labeled and unlabeled training data should reasonable: each class should at least have a certain and balanced number of data.
- Transform dataset. Shuffle, crop or PCA the true dataset and then train it to see if model can make multi-label prediction. If the model still make prediction like `[0, ..., 0]`, there must be something wrong with the dataset instead of the model.
- Remove the predicted class. If the model always predict `2` for dataset with `[0, 1, 2, 3, 4]`, try remove the `2` data and train with `[0, 1, 3, 4]` to see if the model still only predict `2`.
- Check the weights and layer output. Check weights after training to see if it is the weights that cause the problem. Especially the weight of the last layer.

Then we can finally locate the problem is weight and loss become `nan` in training. This problem is most probably caused by infinite gradient or loss. Thus clip it would make the situation much better.

However, one may find that Tensorflow's `clip_by_value` would give errors. This is mainly because the gradient itself is `nan` and loss is `inf`. Here in `houston` dataset, when the labeled loss is around 2.5, the unlabeled loss is 3000, 5000, inf.

This problem can be traced back to the selection of unlabeled data instead of the architecture of the network, if one break at the batch input code line to check. There are so many duplicated unlabeled data. This will not affect EmbedCNN since it picks only one unlabeled sample at a time, but will greatly influence LN.

Now can check if it is the unlabeled data unshuffled. Because if not shuffled, the data in batch would be very similar or even the same arccording to the physical properties of dataset. The problem can be solved by shuffling.

Improve Ladder Networks, Houston

The original loss in the paper Semi-Supervised Learning with Ladder Network is:

$$C = C_{\text{supervised cost}} + C_{\text{unsupervised denosing cost}}$$

Give the unsupervised part a coefficient `alpha < 1.0` so that the unstructured unlabeled part would not strongly affect the labeled one:

$$C = C_{\text{supervised cost}} + \alpha C_{\text{unsupervised denosing cost}}$$