Lab 4

- Tuan Nguyen
- Deep learning Spring 2017
- Dr. Martin Hagan

Debugging one_layer_theano.py

```
In [1]: import numpy as np
import theano
import theano.tensor as T

In [2]: rng = np.random

In [3]: input = np.array([[1],[2],[3],[4]])
target = np.array([[3],[5],[7],[9]])
```

--> Input and Target values (very small dataset with 4 data points)

```
In [4]: p = T.dmatrix("p")
t = T.dmatrix("t")
```

--> Just like placeholders in TensorFlow, p and t are symbolic matrixes (that will be fed values later)

```
In [5]: # initialize the weight
w = theano.shared(rng.randn(1), name="w")
# initialize the bias
b = theano.shared(0., name="b")
```

--> W and b are weight and bias, just like Variable in TensorFlow

```
In [6]: a = w^*p + b
```

--> a linear layer (perceptron) with single neuron

```
In [7]: e = t - a
    e2 = T.sqr(e)
    perf = T.sum(e2)
```

--> compute performance, which is sum square error between a (actual output) and t (target)

```
In [8]: gw, gb = T.grad(perf, [w, b])
```

--> compute gradient of the performance, respect to weight and bias

--> declare a train function then run train function for 1000 times

The network tried to approximate linear equation y = 2 * x + 1. And the weight (1.99) and bias (1.00) are very close to the correct ones.

Theano for Problem 3 HW1

```
In [31]: import numpy as np
import theano
import theano.tensor as T
%matplotlib inline
import matplotlib.pyplot as plt

In [32]: input = np.array([[-1],[0],[1]])
target = np.array([[-1.5],[0.5],[2.5]])
```

--> changed the input and target

-->changed initial value for w from random to zero

```
In [37]: iterations = 1000
a = w*p + b

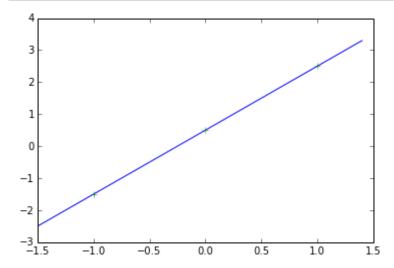
In [38]: e = t - a
e2 = T.sqr(e)
perf = T.sum(e2)
In [39]: gw, gb = T.grad(perf, [w, b])
```

--> change learning rate from 0.01 to 0.1 as required

Plotting network response

```
x = np.array([np.arange(-1.5, 1.5, 0.1)])
In [42]:
Out[42]: array([[ -1.50000000e+00,
                                    -1.40000000e+00,
                                                      -1.3000000e+00,
                  -1.2000000e+00,
                                    -1.10000000e+00,
                                                      -1.00000000e+00,
                  -9.0000000e-01,
                                    -8.00000000e-01,
                                                      -7.00000000e-01,
                  -6.00000000e-01,
                                    -5.00000000e-01,
                                                      -4.00000000e-01,
                  -3.0000000e-01,
                                    -2.00000000e-01,
                                                      -1.00000000e-01,
                   1.33226763e-15,
                                     1.00000000e-01,
                                                       2.00000000e-01,
                   3.00000000e-01,
                                     4.00000000e-01,
                                                       5.0000000e-01,
                   6.0000000e-01,
                                     7.00000000e-01,
                                                       8.0000000e-01,
                   9.0000000e-01,
                                     1.00000000e+00,
                                                       1.10000000e+00,
                   1.20000000e+00,
                                     1.3000000e+00,
                                                       1.4000000e+0011)
In [43]: y = predict(x)
         У
Out[43]: array([[-2.5, -2.3, -2.1, -1.9, -1.7, -1.5, -1.3, -1.1, -0.9, -0.7, -
         0.5,
                 -0.3, -0.1, 0.1, 0.3, 0.5, 0.7, 0.9, 1.1, 1.3, 1.5,
          1.7,
                  1.9, 2.1, 2.3, 2.5, 2.7, 2.9, 3.1, 3.3]
```

```
In [44]: plt.plot(x[0], y[0])
  plt.plot(input, target,'+')
  plt.show()
```



Boltzmann machine

In [3]: """This tutorial introduces restricted boltzmann machines (RBM) using Th Boltzmann Machines (BMs) are a particular form of energy-based model whi contain hidden variables. Restricted Boltzmann Machines further restrict to those without visible-visible and hidden-hidden connections. from future import print function import timeit try: import PIL.Image as Image except ImportError: import Image import numpy import theano import theano.tensor as T import os from theano.sandbox.rng mrg import MRG RandomStreams as RandomStreams from utils import tile_raster_images from logistic sgd import load data

NOTE: have to download utils.py and logistic_sgd.py from http://deeplearning.net/tutorial/code (http://deeplearning.net/tutorial/code)

```
In [4]:
        # start-snippet-1
        class RBM(object):
            """Restricted Boltzmann Machine (RBM)
            def init (
                self,
                input=None,
                n visible=784,
                n hidden=500,
                W=None,
                hbias=None,
                vbias=None,
                numpy rng=None,
                theano rng=None
            ):
                RBM constructor. Defines the parameters of the model along with
                basic operations for inferring hidden from visible (and vice-ver
                as well as for performing CD updates.
                :param input: None for standalone RBMs or symbolic variable if R
                part of a larger graph.
                :param n visible: number of visible units
                :param n hidden: number of hidden units
                :param W: None for standalone RBMs or symbolic variable pointing
                shared weight matrix in case RBM is part of a DBN network; in a
                the weights are shared between RBMs and layers of a MLP
                :param hbias: None for standalone RBMs or symbolic variable poin
                to a shared hidden units bias vector in case RBM is part of a
                different network
                :param vbias: None for standalone RBMs or a symbolic variable
                pointing to a shared visible units bias
                self.n visible = n visible
                self.n_hidden = n_hidden
                if numpy rng is None:
                    # create a number generator
                    numpy rng = numpy.random.RandomState(1234)
                if theano rng is None:
                    theano rng = RandomStreams(numpy rng.randint(2 ** 30))
                if W is None:
                    # W is initialized with `initial W` which is uniformely
                    # sampled from -4*sqrt(6./(n visible+n hidden)) and
                    # 4*sqrt(6./(n hidden+n visible)) the output of uniform if
                    # converted using asarray to dtype theano.config.floatX so
                    # that the code is runable on GPU
                    initial W = numpy.asarray(
```

```
numpy rng.uniform(
                low=-4 * numpy.sqrt(6. / (n_hidden + n_visible)),
                high=4 * numpy.sqrt(6. / (n_hidden + n_visible)),
                size=(n visible, n hidden)
            dtype=theano.config.floatX
        )
        # theano shared variables for weights and biases
        W = theano.shared(value=initial W, name='W', borrow=True)
    if hbias is None:
        # create shared variable for hidden units bias
        hbias = theano.shared(
            value=numpy.zeros(
                n hidden,
                dtype=theano.config.floatX
            ),
            name='hbias',
            borrow=True
        )
    if vbias is None:
        # create shared variable for visible units bias
        vbias = theano.shared(
            value=numpy.zeros(
                n visible,
                dtype=theano.config.floatX
            ),
            name='vbias',
            borrow=True
        )
    # initialize input layer for standalone RBM or layer0 of DBN
    self.input = input
    if not input:
        self.input = T.matrix('input')
    self.W = W
    self.hbias = hbias
    self.vbias = vbias
    self.theano rng = theano rng
    # **** WARNING: It is not a good idea to put things in this list
    # other than shared variables created in this function.
    self.params = [self.W, self.hbias, self.vbias]
    # end-snippet-1
def free energy(self, v sample):
    ''' Function to compute the free energy '''
    wx b = T.dot(v sample, self.W) + self.hbias
    vbias term = T.dot(v sample, self.vbias)
    hidden term = T.sum(T.log(1 + T.exp(wx b)), axis=1)
    return -hidden_term - vbias_term
def propup(self, vis):
    '''This function propagates the visible units activation upwards
    the hidden units
```

Note that we return also the pre-sigmoid activation of the layer. As it will turn out later, due to how Theano deals with optimizations, this symbolic variable will be needed to write down a more stable computational graph (see details in the reconstruction cost function) 1 1 1 pre sigmoid activation = T.dot(vis, self.W) + self.hbias return [pre sigmoid activation, T.nnet.sigmoid(pre sigmoid activ def sample h given v(self, v0 sample): ''' This function infers state of hidden units given visible uni # compute the activation of the hidden units given a sample of # the visibles pre sigmoid h1, h1 mean = self.propup(v0 sample) # get a sample of the hiddens given their activation # Note that theano rng.binomial returns a symbolic sample of dty # int64 by default. If we want to keep our computations in float # for the GPU we need to specify to return the dtype floatX h1 sample = self.theano rng.binomial(size=h1 mean.shape, n=1, p=h1 mean, dtype=theano.config.floatX) return [pre sigmoid h1, h1 mean, h1 sample] def propdown(self, hid): '''This function propagates the hidden units activation downward the visible units Note that we return also the pre sigmoid activation of the layer. As it will turn out later, due to how Theano deals with optimizations, this symbolic variable will be needed to write down a more stable computational graph (see details in the reconstruction cost function) . . . pre sigmoid activation = T.dot(hid, self.W.T) + self.vbias return [pre sigmoid activation, T.nnet.sigmoid(pre sigmoid activ def sample v given h(self, h0 sample): ''' This function infers state of visible units given hidden uni # compute the activation of the visible given the hidden sample pre sigmoid v1, v1 mean = self.propdown(h0 sample) # get a sample of the visible given their activation # Note that theano rng.binomial returns a symbolic sample of dty # int64 by default. If we want to keep our computations in float # for the GPU we need to specify to return the dtype floatX v1 sample = self.theano rng.binomial(size=v1 mean.shape, n=1, p=v1 mean, dtype=theano.config.floatX) return [pre sigmoid v1, v1 mean, v1 sample] def gibbs hvh(self, h0 sample): ''' This function implements one step of Gibbs sampling, starting from the hidden state''' pre sigmoid v1, v1 mean, v1 sample = self.sample v given h(h0 salpre sigmoid h1, h1 mean, h1 sample = self.sample h given v(v1 sa return [pre sigmoid v1, v1 mean, v1 sample,

```
pre sigmoid h1, h1 mean, h1 sample]
def gibbs vhv(self, v0 sample):
    ''' This function implements one step of Gibbs sampling,
        starting from the visible state'''
    pre sigmoid h1, h1 mean, h1 sample = self.sample h given v(v0 sa
    pre_sigmoid_v1, v1_mean, v1_sample = self.sample v given h(h1 sa
    return [pre sigmoid h1, h1 mean, h1 sample,
            pre sigmoid v1, v1 mean, v1 sample]
# start-snippet-2
def get cost updates(self, lr=0.1, persistent=None, k=1):
    """This functions implements one step of CD-k or PCD-k
    :param lr: learning rate used to train the RBM
    :param persistent: None for CD. For PCD, shared variable
        containing old state of Gibbs chain. This must be a shared
        variable of size (batch size, number of hidden units).
    :param k: number of Gibbs steps to do in CD-k/PCD-k
    Returns a proxy for the cost and the updates dictionary. The
    dictionary contains the update rules for weights and biases but
    also an update of the shared variable used to store the persiste
    chain, if one is used.
    .....
    # compute positive phase
    pre sigmoid ph, ph mean, ph sample = self.sample h given v(self.
    # decide how to initialize persistent chain:
    # for CD, we use the newly generate hidden sample
    # for PCD, we initialize from the old state of the chain
    if persistent is None:
        chain_start = ph_sample
    else:
        chain_start = persistent
    # end-snippet-2
    # perform actual negative phase
    # in order to implement CD-k/PCD-k we need to scan over the
    # function that implements one gibbs step k times.
    # Read Theano tutorial on scan for more information :
    # http://deeplearning.net/software/theano/library/scan.html
    # the scan will return the entire Gibbs chain
        [
            pre sigmoid nvs,
            nv means,
            nv samples,
            pre sigmoid nhs,
            nh means,
            nh samples
        ],
        updates
    ) = theano.scan(
```

```
self.gibbs hvh,
        # the None are place holders, saying that
        # chain start is the initial state corresponding to the
        # 6th output
        outputs info=[None, None, None, None, chain start],
        n steps=k,
        name="gibbs hvh"
    # start-snippet-3
    # determine gradients on RBM parameters
    # note that we only need the sample at the end of the chain
    chain end = nv samples[-1]
    cost = T.mean(self.free energy(self.input)) - T.mean(
        self.free energy(chain end))
    # We must not compute the gradient through the gibbs sampling
    gparams = T.grad(cost, self.params, consider constant=[chain end
    # end-snippet-3 start-snippet-4
    # constructs the update dictionary
    for gparam, param in zip(gparams, self.params):
        # make sure that the learning rate is of the right dtype
        updates[param] = param - qparam * T.cast(
            dtype=theano.config.floatX
        )
    if persistent:
        # Note that this works only if persistent is a shared variab
        updates[persistent] = nh samples[-1]
        # pseudo-likelihood is a better proxy for PCD
        monitoring cost = self.get pseudo likelihood cost(updates)
    else:
        # reconstruction cross-entropy is a better proxy for CD
        monitoring_cost = self.get_reconstruction_cost(updates,
                                                        pre sigmoid n
    return monitoring cost, updates
    # end-snippet-4
def get pseudo likelihood cost(self, updates):
    """Stochastic approximation to the pseudo-likelihood"""
    # index of bit i in expression p(x i \mid x \{ \setminus i \})
    bit_i_idx = theano.shared(value=0, name='bit_i_idx')
    # binarize the input image by rounding to nearest integer
    xi = T.round(self.input)
    # calculate free energy for the given bit configuration
    fe xi = self.free energy(xi)
    # flip bit x i of matrix xi and preserve all other bits x {\i}
    # Equivalent to xi[:,bit_i_idx] = 1-xi[:, bit_i_idx], but assign
    # the result to xi flip, instead of working in place on xi.
    xi flip = T.set subtensor(xi[:, bit i idx], 1 - xi[:, bit i idx]
    # calculate free energy with bit flipped
    fe xi flip = self.free energy(xi flip)
```

def get_reconstruction_cost(self, updates, pre_sigmoid_nv):
 """Approximation to the reconstruction error

return cost

0.00

Note that this function requires the pre-sigmoid activation as input. To understand why this is so you need to understand a bit about how Theano works. Whenever you compile a Theano function, the computational graph that you pass as input gets optimized for speed and stability. This is done by changing several parts of the subgraphs with others. One such optimization expresses terms of the form log(sigmoid(x)) in terms of softplus. We need this optimization for the cross-entropy since sigmoid of numbers larger than 30. (or even less then that) turn to 1. and numbers smaller than -30. turn to 0 which in terms will force theano to compute log(0) and therefore we will get either -inf or NaN as cost. If the value is expressed in terms of softplus we do not get this undesirable behaviour. This optimization usually works fine, but here we have a special case. The sigmoid is applied inside the scan op, while the log is outside. Therefore Theano will only see log(scan(..)) instead of log(sigmoid(..)) and will not apply the wanted optimization. We can not go and replace the sigmoid in scan with something else also, because this only needs to be done on the last step. Therefore the easiest and more efficient way is to get also the pre-sigmoid activation as an output of scan, and apply both the log and sigmoid outside scan such that Theano can catch and optimize the expression.

```
cross_entropy = T.mean(
    T.sum(
        self.input * T.log(T.nnet.sigmoid(pre_sigmoid_nv)) +
        (1 - self.input) * T.log(1 - T.nnet.sigmoid(pre_sigmoid_axis=1))
)
return cross entropy
```

```
In [5]: def test rbm(learning rate=0.1, training epochs=15,
                    dataset='mnist.pkl.gz', batch_size=20,
                    n chains=20, n samples=10, output folder='rbm plots',
                    n hidden=500):
            .....
           Demonstrate how to train and afterwards sample from it using Theano.
           This is demonstrated on MNIST.
            :param learning rate: learning rate used for training the RBM
            :param training epochs: number of epochs used for training
            :param dataset: path the the pickled dataset
            :param batch size: size of a batch used to train the RBM
            :param n chains: number of parallel Gibbs chains to be used for samp
            :param n samples: number of samples to plot for each chain
           datasets = load data(dataset)
           train_set_x, train_set_y = datasets[0]
           test set x, test set y = datasets[2]
           # compute number of minibatches for training, validation and testing
           n train batches = train set x.get value(borrow=True).shape[0] // bat
           # allocate symbolic variables for the data
           index = T.lscalar() # index to a [mini]batch
           x = T.matrix('x') # the data is presented as rasterized images
           rng = numpy.random.RandomState(123)
           theano rng = RandomStreams(rng.randint(2 ** 30))
           # initialize storage for the persistent chain (state = hidden
           # layer of chain)
           persistent chain = theano.shared(numpy.zeros((batch size, n hidden),
                                                       dtype=theano.config.flo
                                            borrow=True)
           # construct the RBM class
            rbm = RBM(input=x, n visible=28 * 28,
                     n hidden=n hidden, numpy rng=rng, theano rng=theano rng)
           # get the cost and the gradient corresponding to one step of CD-15
           cost, updates = rbm.get cost updates(lr=learning rate,
                                               persistent=persistent chain, k=
           Training the RBM
           if not os.path.isdir(output folder):
               os.makedirs(output folder)
```

```
os.chdir(output folder)
# start-snippet-5
# it is ok for a theano function to have no output
# the purpose of train rbm is solely to update the RBM parameters
train rbm = theano.function(
    [index],
    cost,
    updates=updates,
    givens={
        x: train_set_x[index * batch_size: (index + 1) * batch size]
    },
    name='train rbm'
)
plotting time = 0.
start time = timeit.default timer()
# go through training epochs
for epoch in range(training epochs):
    # go through the training set
   mean cost = []
    for batch index in range(n train batches):
        mean cost += [train rbm(batch index)]
    print('Training epoch %d, cost is ' % epoch, numpy.mean(mean cos
    # Plot filters after each training epoch
    plotting start = timeit.default timer()
    # Construct image from the weight matrix
    image = Image.fromarray(
        tile raster images(
           X=rbm.W.get value(borrow=True).T,
            img shape=(28, 28),
           tile shape=(10, 10),
           tile spacing=(1, 1)
        )
    )
    image.save('filters_at_epoch_%i.png' % epoch)
    plotting stop = timeit.default timer()
    plotting time += (plotting stop - plotting start)
end time = timeit.default timer()
pretraining_time = (end_time - start_time) - plotting_time
print ('Training took %f minutes' % (pretraining time / 60.))
# end-snippet-5 start-snippet-6
Sampling from the RBM
######################################
# find out the number of test samples
number_of_test_samples = test_set_x.get_value(borrow=True).shape[0]
# pick random test examples, with which to initialize the persistent
test idx = rng.randint(number of test samples - n chains)
```

```
persistent vis chain = theano.shared(
    numpy.asarray(
        test set x.get value(borrow=True)[test idx:test idx + n chai
        dtype=theano.config.floatX
    )
# end-snippet-6 start-snippet-7
plot every = 1000
# define one step of Gibbs sampling (mf = mean-field) define a
# function that does `plot every` steps before returning the
# sample for plotting
(
    [
        presig hids,
        hid mfs,
        hid samples,
        presig vis,
        vis mfs,
        vis samples
    ],
    updates
) = theano.scan(
    rbm.gibbs vhv,
    outputs info=[None, None, None, None, persistent vis chain
    n steps=plot every,
    name="gibbs vhv"
)
# add to updates the shared variable that takes care of our persiste
# chain :.
updates.update({persistent vis chain: vis samples[-1]})
# construct the function that implements our persistent chain.
# we generate the "mean field" activations for plotting and the actu
# samples for reinitializing the state of our persistent chain
sample fn = theano.function(
    [],
    [
        vis mfs[-1],
        vis_samples[-1]
    ],
    updates=updates,
    name='sample fn'
)
# create a space to store the image for plotting ( we need to leave
# room for the tile spacing as well)
image data = numpy.zeros(
    (29 * n samples + 1, 29 * n chains - 1),
    dtype='uint8'
for idx in range(n samples):
    # generate `plot_every` intermediate samples that we discard,
    # because successive samples in the chain are too correlated
    vis mf, vis sample = sample fn()
    print(' ... plotting sample %d' % idx)
    image data[29 * idx:29 * idx + 28, :] = tile raster images(
        X=vis mf,
```

```
img_shape=(28, 28),
    tile_shape=(1, n_chains),
    tile_spacing=(1, 1)
)

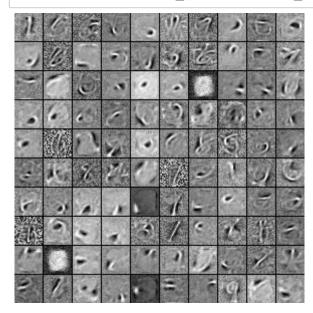
# construct image
image = Image.fromarray(image_data)
image.save('samples.png')
# end-snippet-7
os.chdir('../')
```

```
In [7]: | if name == ' main ':
            test rbm()
        ... loading data
        Training epoch 0, cost is
                                   -90.8270998815
        Training epoch 1, cost is
                                   -80.5750399886
        Training epoch 2, cost is
                                   -74.5885131451
        Training epoch 3, cost is
                                   -72.1490817319
        Training epoch 4, cost is
                                   -68.5374212061
        Training epoch 5, cost is
                                   -63.5795446906
        Training epoch 6, cost is
                                   -65.7429554572
        Training epoch 7, cost is
                                   -68.1725534948
        Training epoch 8, cost is
                                   -68.3253752854
        Training epoch 9, cost is
                                   -64.4359574712
        Training epoch 10, cost is
                                    -61.0471123121
        Training epoch 11, cost is
                                    -61.5234953063
        Training epoch 12, cost is
                                   -64.6232410604
        Training epoch 13, cost is
                                    -62.710471344
        Training epoch 14, cost is
                                    -62.4188898712
        Training took 27.488739 minutes
         ... plotting sample 0
         ... plotting sample 1
         ... plotting sample 2
         ... plotting sample 3
         ... plotting sample 4
         ... plotting sample 5
         ... plotting sample 6
         ... plotting sample 7
         ... plotting sample 8
         ... plotting sample 9
```

In [1]: from IPython.display import Image
Image(filename='rbm_plots/samples.png')

In [3]: Image(filename='rbm_plots/filters_at_epoch_14.png')

Out[3]:



Questions

1. What are the arguments to the Theano function command.

```
theano.function(inputs=[x,y], # list of input variables
outputs=..., # what values to be returned
updates=..., # "state" values to be modified
givens=..., # substitutions to the graph
```

2. How do you set a default value for a function argument?

```
f = function([x, In(y, value=1)], z)
```

In this statement, In(y, value=1) will set 1 as the default value for argument y.

3. What are shared variables used for?

Variable with Storage that is shared between functions that it appears in. It is normally used for weight and bias

4. Does the Theano grad function return numpy arrays, or symbolic Theano variables?

It returns symbolic Theano variables.

5. Is it possible to enforce the shape of a Theano variable when building a graph?

I do not totally understand this question. My best guess is No, because when building a graph, normally we already knew the shape (size) of all factors. So it makes sense to avoid the changing

6. What does "broadcasting" mean in Theano?

Numpy does broadcasting of arrays of different shapes during arithmetic operations. What this means in general is that the smaller array (or scalar) is broadcasted across the larger array so that they have compatible shapes. Here is an example:

```
>>> a = numpy.asarray([1.0, 2.0, 3.0])
>>> b = 2.0
>>> a * b
array([ 2., 4., 6.])
```