Deep Learning Tutorial

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CHAPTER

ONE

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CHAPTER

TWO

DEEP LEARNING TUTORIALS

Deep Learning is a new area of Machine Learning research, which has been introduced with the objective of moving Machine Learning closer to one of its original goals: Artificial Intelligence. See these course notes for a brief introduction to Machine Learning for AI and an introduction to Deep Learning algorithms.

Deep Learning is about learning multiple levels of representation and abstraction that help to make sense of data such as images, sound, and text. For more about deep learning algorithms, see for example:

- The monograph or review paper Learning Deep Architectures for AI (Foundations & Trends in Machine Learning, 2009).
- The ICML 2009 Workshop on Learning Feature Hierarchies webpage has a list of references.
- The LISA public wiki has a reading list and a bibliography.
- Geoff Hinton has readings from last year's NIPS tutorial.

The tutorials presented here will introduce you to some of the most important deep learning algorithms and will also show you how to run them using Theano. Theano is a python library that makes writing deep learning models easy, and gives the option of training them on a GPU.

The algorithm tutorials have some prerequisites. You should know some python, and be familiar with numpy. Since this tutorial is about using Theano, you should read over the Theano basic tutorial first. Once you've done that, read through our *Getting Started* chapter – it introduces the notation, and [downloadable] datasets used in the algorithm tutorials, and the way we do optimization by stochastic gradient descent.

The purely supervised learning algorithms are meant to be read in order:

1. *Logistic Regression* - using Theano for something simple
2. *Multilayer perceptron* - introduction to layers
3. *Deep Convolutional Network* - a simplified version of LeNet5

The unsupervised and semi-supervised learning algorithms can be read in any order (the auto-encoders can be read independently of the RBM/DBN thread):

- *Auto Encoders, Denoising Autoencoders* - description of autoencoders
- *Stacked Denoising Auto-Encoders* - easy steps into unsupervised pre-training for deep nets
- *Restricted Boltzmann Machines* - single layer generative RBM model
- *Deep Belief Networks* - unsupervised generative pre-training of stacked RBMs followed by supervised fine-tuning

Building towards including the mcRBM model, we have a new tutorial on sampling from energy models:

- *HMC Sampling* - hybrid (aka Hamiltonian) Monte-Carlo sampling with scan()

Building towards including the Contractive auto-encoders tutorial, we have the code for now:

- Contractive auto-encoders code - There is some basic doc in the code.

Energy-based recurrent neural network (RNN-RBM):

- *Modeling and generating sequences of polyphonic music*

CHAPTER

THREE

GETTING STARTED

These tutorials do not attempt to make up for a graduate or undergraduate course in machine learning, but we do make a rapid overview of some important concepts (and notation) to make sure that we're on the same page. You'll also need to download the datasets mentioned in this chapter in order to run the example code of the up-coming tutorials.

3.1 Download

On each learning algorithm page, you will be able to download the corresponding files. If you want to download all of them at the same time, you can clone the git repository of the tutorial:

```
git clone git://github.com/lisa-lab/DeepLearningTutorials.git
```

3.2 Datasets

3.2.1 MNIST Dataset

(mnist.pkl.gz)

The MNIST dataset consists of handwritten digit images and it is divided in 60,000 examples for the training set and 10,000 examples for testing. In many papers as well as in this tutorial, the official training set of 60,000 is divided into an actual training set of 50,000 examples and 10,000 validation examples (for selecting hyper-parameters like learning rate and size of the model). All digit images have been size-normalized and centered in a fixed size image of 28 x 28 pixels. In the original dataset each pixel of the image is represented by a value between 0 and 255, where 0 is black, 255 is white and anything in between is a different shade of grey.

Here are some examples of MNIST digits:

For convenience we pickled the dataset to make it easier to use in python. It is available for download here. The pickled file represents a tuple of 3 lists : the training set, the validation set and the testing set. Each of the three lists is a pair formed from a list of images and a list of class labels for each of the images. An image is represented as numpy 1-dimensional array

of 784 (28 x 28) float values between 0 and 1 (0 stands for black, 1 for white). The labels are numbers between 0 and 9 indicating which digit the image represents. The code block below shows how to load the dataset.

```
import cPickle, gzip, numpy

# Load the dataset
f = gzip.open('mnist.pkl.gz', 'rb')
train_set, valid_set, test_set = cPickle.load(f)
f.close()
```

When using the dataset, we usually divide it in minibatches (see *Stochastic Gradient Descent*). We encourage you to store the dataset into shared variables and access it based on the minibatch index, given a fixed and known batch size. The reason behind shared variables is related to using the GPU. There is a large overhead when copying data into the GPU memory. If you would copy data on request (each minibatch individually when needed) as the code will do if you do not use shared variables, due to this overhead, the GPU code will not be much faster then the CPU code (maybe even slower). If you have your data in Theano shared variables though, you give Theano the possibility to copy the entire data on the GPU in a single call when the shared variables are constructed. Afterwards the GPU can access any minibatch by taking a slice from this shared variables, without needing to copy any information from the CPU memory and therefore bypassing the overhead. Because the datapoints and their labels are usually of different nature (labels are usually integers while datapoints are real numbers) we suggest to use different variables for labes and data. Also we recomand using different variables for the training set, validation set and testing set to make the code more readable (resulting in 6 different shared variables).

Since now the data is in one variable, and a minibatch is defined as a slice of that variable, it comes more natural to define a minibatch by indicating its index and its size. In our setup the batch size stays constant through out the execution of the code, therefore a function will actually require only the index to identify on which datapoints to work. The code below shows how to store your data and how to access a minibatch:

```
def shared_dataset(data_xy):
    """ Function that loads the dataset into shared variables

    The reason we store our dataset in shared variables is to allow
    Theano to copy it into the GPU memory (when code is run on GPU).
    Since copying data into the GPU is slow, copying a minibatch everytime
    is needed (the default behaviour if the data is not in a shared
    variable) would lead to a large decrease in performance.
    """
    data_x, data_y = data_xy
    shared_x = theano.shared(numpy.asarray(data_x, dtype=theano.config.floatX))
    shared_y = theano.shared(numpy.asarray(data_y, dtype=theano.config.floatX))
    # When storing data on the GPU it has to be stored as floats
    # therefore we will store the labels as ''floatX'' as well
    # (''shared_y'' does exactly that). But during our computations
    # we need them as ints (we use labels as index, and if they are
    # floats it doesn't make sense) therefore instead of returning
    # ''shared_y'' we will have to cast it to int. This little hack
    # lets us get around this issue
```

```
        return shared_x, T.cast(shared_y, 'int32')

    test_set_x, test_set_y = shared_dataset(test_set)
    valid_set_x, valid_set_y = shared_dataset(valid_set)
    train_set_x, train_set_y = shared_dataset(train_set)

    batch_size = 500    # size of the minibatch

    # accessing the third minibatch of the training set

    data  = train_set_x[2 * 500: 3 * 500]
    label = train_set_y[2 * 500: 3 * 500]
```

The data has to be stored as floats on the GPU (the right `dtype` for storing on the GPU is given by `theano.config.floatX`). To get around this shortcomming for the labels, we store them as float, and then cast it to int.

Note: If you are running your code on the GPU and the dataset you are using is too large to fit in memory the code will crash. In such a case you should store the data in a shared variable. You can however store a sufficiently small chunk of your data (several minibatches) in a shared variable and use that during training. Once you got through the chunk, update the values it stores. This way you minimize the number of data transfers between CPU memory and GPU memory.

3.3 Notation

3.3.1 Dataset notation

We label data sets as $\mathcal{D}$. When the distinction is important, we indicate train, validation, and test sets as: $\mathcal{D}_{train}$, $\mathcal{D}_{valid}$ and $\mathcal{D}_{test}$. The validation set is used to perform model selection and hyper-parameter selection, whereas the test set is used to evaluate the final generalization error and compare different algorithms in an unbiased way.

The tutorials mostly deal with classification problems, where each data set $\mathcal{D}$ is an indexed set of pairs $(x^{(i)}, y^{(i)})$. We use superscripts to distinguish training set examples: $x^{(i)} \in \mathcal{R}^D$ is thus the i-th training example of dimensionality D. Similarly, $y^{(i)} \in \{0, ..., L\}$ is the i-th label assigned to input $x^{(i)}$. It is straightforward to extend these examples to ones where $y^{(i)}$ has other types (e.g. Gaussian for regression, or groups of multinomials for predicting multiple symbols).

3.3.2 Math Conventions

- W: upper-case symbols refer to a matrix unless specified otherwise
- W_{ij}: element at i-th row and j-th column of matrix W
- $W_{i\cdot}, W_i$: vector, i-th row of matrix W
- $W_{\cdot j}$: vector, j-th column of matrix W

- b: lower-case symbols refer to a vector unless specified otherwise
- b_i: i-th element of vector b

3.3.3 List of Symbols and acronyms

- D: number of input dimensions.
- $D_h^{(i)}$: number of hidden units in the i-th layer.
- $f_\theta(x)$, $f(x)$: classification function associated with a model $P(Y|x,\theta)$, defined as $\text{argmax}_k P(Y = k|x,\theta)$. Note that we will often drop the θ subscript.
- L: number of labels.
- $\mathcal{L}(\theta, \mathcal{D})$: log-likelihood $\mathcal{D}$ of the model defined by parameters θ.
- $\ell(\theta, \mathcal{D})$ empirical loss of the prediction function f parameterized by θ on data set $\mathcal{D}$.
- NLL: negative log-likelihood
- θ: set of all parameters for a given model

3.3.4 Python Namespaces

Tutorial code often uses the following namespaces:

```
import theano
import theano.tensor as T
import numpy
```

3.4 A Primer on Supervised Optimization for Deep Learning

What's exciting about Deep Learning is largely the use of unsupervised learning of deep networks. But supervised learning also plays an important role. The utility of unsupervised *pre-training* is often evaluated on the basis of what performance can be achieved after supervised *fine-tuning*. This chapter reviews the basics of supervised learning for classification models, and covers the minibatch stochastic gradient descent algorithm that is used to fine-tune many of the models in the Deep Learning Tutorials. Have a look at these introductory course notes on gradient-based learning for more basics on the notion of optimizing a training criterion using the gradient.

3.4.1 Learning a Classifier

Zero-One Loss

The models presented in these deep learning tutorials are mostly used for classification. The objective in training a classifier is to minimize the number of errors (zero-one loss) on unseen examples. If $f : R^D \rightarrow$

$\{0, ..., L\}$ is the prediction function, then this loss can be written as:

$$\ell_{0,1} = \sum_{i=0}^{|\mathcal{D}|} I_{f(x^{(i)}) \neq y^{(i)}}$$

where either $\mathcal{D}$ is the training set (during training) or $\mathcal{D} \cap \mathcal{D}_{train} = \emptyset$ (to avoid biasing the evaluation of validation or test error). I is the indicator function defined as:

$$I_x = \begin{cases} 1 & \text{if } x \text{ is True} \\ 0 & \text{otherwise} \end{cases}$$

In this tutorial, f is defined as:

$$f(x) = \text{argmax}_k P(Y = k|x, \theta)$$

In python, using Theano this can be written as :

```
# zero_one_loss is a Theano variable representing a symbolic
# expression of the zero one loss ; to get the actual value this
# symbolic expression has to be compiled into a Theano function (see
# the Theano tutorial for more details)
zero_one_loss = T.sum(T.neq(T.argmax(p_y_given_x), y))
```

Negative Log-Likelihood Loss

Since the zero-one loss is not differentiable, optimizing it for large models (thousands or millions of parameters) is prohibitively expensive (computationally). We thus maximize the log-likelihood of our classifier given all the labels in a training set.

$$\mathcal{L}(\theta, \mathcal{D}) = \sum_{i=0}^{|\mathcal{D}|} \log P(Y = y^{(i)}|x^{(i)}, \theta)$$

The likelihood of the correct class is not the same as the number of right predictions, but from the point of view of a randomly initialized classifier they are pretty similar. Remember that likelihood and zero-one loss are different objectives; you should see that they are corralated on the validation set but sometimes one will rise while the other falls, or vice-versa.

Since we usually speak in terms of minimizing a loss function, learning will thus attempt to **minimize** the **negative** log-likelihood (NLL), defined as:

$$NLL(\theta, \mathcal{D}) = -\sum_{i=0}^{|\mathcal{D}|} \log P(Y = y^{(i)}|x^{(i)}, \theta)$$

The NLL of our classifier is a differentiable surrogate for the zero-one loss, and we use the gradient of this function over our training data as a supervised learning signal for deep learning of a classifier.

This can be computed using the following line of code :

```
# NLL is a symbolic variable ; to get the actual value of NLL, this symbolic
# expression has to be compiled into a Theano function (see the Theano
# tutorial for more details)
NLL = -T.sum(T.log(p_y_given_x)[T.arange(y.shape[0]), y])
# note on syntax: T.arange(y.shape[0]) is a vector of integers [0,1,2,...,len(y)].
# Indexing a matrix M by the two vectors [0,1,...,K], [a,b,...,k] returns the
# elements M[0,a], M[1,b], ..., M[K,k] as a vector.  Here, we use this
# syntax to retrieve the log-probability of the correct labels, y.
```

3.4.2 Stochastic Gradient Descent

What is ordinary gradient descent? it is a simple algorithm in which we repeatedly make small steps downward on an error surface defined by a loss function of some parameters. For the purpose of ordinary gradient descent we consider that the training data is rolled into the loss function. Then the pseudocode of this algorithm can be described as :

```
# GRADIENT DESCENT

while True:
    loss = f(params)
    d_loss_wrt_params = ... # compute gradient
    params -= learning_rate * d_loss_wrt_params
    if <stopping condition is met>:
        return params
```

Stochastic gradient descent (SGD) works according to the same principles as ordinary gradient descent, but proceeds more quickly by estimating the gradient from just a few examples at a time instead of the entire training set. In its purest form, we estimate the gradient from just a single example at a time.

```
# STOCHASTIC GRADIENT DESCENT
for (x_i,y_i) in training_set:
                            # imagine an infinite generator
                            # that may repeat examples (if there is only a finite training
    loss = f(params, x_i, y_i)
    d_loss_wrt_params = ... # compute gradient
    params -= learning_rate * d_loss_wrt_params
    if <stopping condition is met>:
        return params
```

The variant that we recommend for deep learning is a further twist on stochastic gradient descent using so-called "minibatches". Minibatch SGD works identically to SGD, except that we use more than one training example to make each estimate of the gradient. This technique reduces variance in the estimate of the gradient, and often makes better use of the hierarchical memory organization in modern computers.

```
for (x_batch,y_batch) in train_batches:
                            # imagine an infinite generator
                            # that may repeat examples
    loss = f(params, x_batch, y_batch)
    d_loss_wrt_params = ... # compute gradient using theano
    params -= learning_rate * d_loss_wrt_params
```

```
    if <stopping condition is met>:
        return params
```

There is a tradeoff in the choice of the minibatch size B. The reduction of variance and use of SIMD instructions helps most when increasing B from 1 to 2, but the marginal improvement fades rapidly to nothing. With large B, time is wasted in reducing the variance of the gradient estimator, that time would be better spent on additional gradient steps. An optimal B is model-, dataset-, and hardware-dependent, and can be anywhere from 1 to maybe several hundreds. In the tutorial we set it to 20, but this choice is almost arbitrary (though harmless).

Note: If you are training for a fixed number of epochs, the minibatch size becomes important because it controls the number of updates done to your parameters. Training the same model for 10 epochs using a batch size of 1 yields completely different results compared to training for the same 10 epochs but with a batchsize of 20. Keep this in mind when switching between batch sizes and be prepared to tweak all the other parameters acording to the batch size used.

All code-blocks above show pseudocode of how the algorithm looks like. Implementing such algorithm in Theano can be done as follows :

```
# Minibatch Stochastic Gradient Descent

# assume loss is a symbolic description of the loss function given
# the symbolic variables params (shared variable), x_batch, y_batch;

# compute gradient of loss with respect to params
d_loss_wrt_params = T.grad(loss, params)

# compile the MSGD step into a theano function
updates = [(params, params - learning_rate * d_loss_wrt_params)]
MSGD = theano.function([x_batch,y_batch], loss, updates=updates)

for (x_batch, y_batch) in train_batches:
    # here x_batch and y_batch are elements of train_batches and
    # therefore numpy arrays; function MSGD also updates the params
    print('Current loss is ', MSGD(x_batch, y_batch))
    if stopping_condition_is_met:
        return params
```

3.4.3 Regularization

There is more to machine learning than optimization. When we train our model from data we are trying to prepare it to do well on *new* examples, not the ones it has already seen. The training loop above for MSGD does not take this into account, and may overfit the training examples. A way to combat overfitting is through regularization. There are several techniques for regularization; the ones we will explain here are L1/L2 regularization and early-stopping.

L1 and L2 regularization

L1 and L2 regularization involve adding an extra term to the loss function, which penalizes certain parameter configurations. Formally, if our loss function is:

$$NLL(\theta, \mathcal{D}) = -\sum_{i=0}^{|\mathcal{D}|} \log P(Y = y^{(i)}|x^{(i)}, \theta)$$

then the regularized loss will be:

$$E(\theta, \mathcal{D}) = NLL(\theta, \mathcal{D}) + \lambda R(\theta)$$

or, in our case

$$E(\theta, \mathcal{D}) = NLL(\theta, \mathcal{D}) + \lambda ||\theta||_p^p$$

where

$$||\theta||_p = \left(\sum_{j=0}^{|\theta|} |\theta_j|^p \right)^{\frac{1}{p}}$$

which is the L_p norm of θ. λ is a hyper-parameter which controls the relative importance of the regularization parameter. Commonly used values for p are 1 and 2, hence the L1/L2 nomenclature. If p=2, then the regularizer is also called "weight decay".

In principle, adding a regularization term to the loss will encourage smooth network mappings in a neural network (by penalizing large values of the parameters, which decreases the amount of nonlinearity that the network models). More intuitively, the two terms (NLL and $R(\theta)$) correspond to modelling the data well (NLL) and having "simple" or "smooth" solutions ($R(\theta)$). Thus, minimizing the sum of both will, in theory, correspond to finding the right trade-off between the fit to the training data and the "generality" of the solution that is found. To follow Occam's razor principle, this minimization should find us the simplest solution (as measured by our simplicity criterion) that fits the training data.

Note that the fact that a solution is "simple" does not mean that it will generalize well. Empirically, it was found that performing such regularization in the context of neural networks helps with generalization, especially on small datasets. The code block below shows how to compute the loss in python when it contains both a L1 regularization term weighted by λ_1 and L2 regularization term weighted by λ_2

```
# symbolic Theano variable that represents the L1 regularization term
L1  = T.sum(abs(param))

# symbolic Theano variable that represents the squared L2 term
L2_sqr = T.sum(param ** 2)

# the loss
loss = NLL + lambda_1 * L1 + lambda_2 * L2
```

Early-Stopping

Early-stopping combats overfitting by monitoring the model's performance on a *validation set*. A validation set is a set of examples that we never use for gradient descent, but which is also not a part of the *test set*. The

validation examples are considered to be representative of future test examples. We can use them during training because they are not part of the test set. If the model's performance ceases to improve sufficiently on the validation set, or even degrades with further optimization, then the heuristic implemented here gives up on much further optimization.

The choice of when to stop is a judgement call and a few heuristics exist, but these tutorials will make use of a strategy based on a geometrically increasing amount of patience.

```
# early-stopping parameters
patience = 5000  # look as this many examples regardless
patience_increase = 2     # wait this much longer when a new best is
                          # found
improvement_threshold = 0.995  # a relative improvement of this much is
                               # considered significant
validation_frequency = min(n_train_batches, patience/2)
                              # go through this many
                              # minibatches before checking the network
                              # on the validation set; in this case we
                              # check every epoch

best_params = None
best_validation_loss = numpy.inf
test_score = 0.
start_time = time.clock()

done_looping = False
epoch = 0
while (epoch < n_epochs) and (not done_looping):
    # Report "1" for first epoch, "n_epochs" for last epoch
    epoch = epoch + 1
    for minibatch_index in xrange(n_train_batches):

        d_loss_wrt_params = ... # compute gradient
        params -= learning_rate * d_loss_wrt_params # gradient descent

        # iteration number. We want it to start at 0.
        iter = (epoch - 1) * n_train_batches + minibatch_index
        # note that if we do 'iter % validation_frequency' it will be
        # true for iter = 0 which we do not want. We want it true for
        # iter = validation_frequency - 1.
        if (iter + 1) % validation_frequency == 0:

            this_validation_loss = ... # compute zero-one loss on validation set

            if this_validation_loss < best_validation_loss:

                # improve patience if loss improvement is good enough
                if this_validation_loss < best_validation_loss * improvement_threshold:

                    patience = max(patience, iter * patience_increase)
                best_params = copy.deepcopy(params)
                best_validation_loss = this_validation_loss

        if patience <= iter:
```

```
            done_looping = True
            break

# POSTCONDITION:
# best_params refers to the best out-of-sample parameters observed during the optimization
```

If we run out of batches of training data before running out of patience, then we just go back to the beginning of the training set and repeat.

Note: The `validation_frequency` should always be smaller than the `patience`. The code should check at least two times how it performs before running out of patience. This is the reason we used the formulation `validation_frequency = min( value, patience/2.)`

Note: This algorithm could possibly be improved by using a test of statistical significance rather than the simple comparison, when deciding whether to increase the patience.

3.4.4 Testing

After the loop exits, the best_params variable refers to the best-performing model on the validation set. If we repeat this procedure for another model class, or even another random initialization, we should use the same train/valid/test split of the data, and get other best-performing models. If we have to choose what the best model class or the best initialization was, we compare the best_validation_loss for each model. When we have finally chosen the model we think is the best (on validation data), we report that model's test set performance. That is the performance we expect on unseen examples.

3.4.5 Recap

That's it for the optimization section. The technique of early-stopping requires us to partition the set of examples into three sets (training $\mathcal{D}_{train}$, validation $\mathcal{D}_{valid}$, test $\mathcal{D}_{test}$). The training set is used for minibatch stochastic gradient descent on the differentiable approximation of the objective function. As we perform this gradient descent, we periodically consult the validation set to see how our model is doing on the real objective function (or at least our empirical estimate of it). When we see a good model on the validation set, we save it. When it has been a long time since seeing a good model, we abandon our search and return the best parameters found, for evaluation on the test set.

3.5 Theano/Python Tips

3.5.1 Loading and Saving Models

When you're doing experiments, it can take hours (sometimes days!) for gradient-descent to find the best parameters. You will want to save those weights once you find them. You may also want to save your current-best estimates as the search progresses.

Pickle the numpy ndarrays from your shared variables

The best way to save/archive your model's parameters is to use pickle or deepcopy the ndarray objects. So for example, if your parameters are in shared variables `w, v, u`, then your save command should look something like:

```
>>> import cPickle
>>> save_file = open('path', 'wb')  # this will overwrite current contents
>>> cPickle.dump(w.get_value(borrow=True), save_file, -1)  # the -1 is for HIGHEST_PROTOCOL
>>> cPickle.dump(v.get_value(borrow=True), save_file, -1)  # .. and it triggers much more e
>>> cPickle.dump(u.get_value(borrow=True), save_file, -1)  # .. storage than numpy's defau
>>> save_file.close()
```

Then later, you can load your data back like this:

```
>>> save_file = open('path')
>>> w.set_value(cPickle.load(save_file), borrow=True)
>>> v.set_value(cPickle.load(save_file), borrow=True)
>>> u.set_value(cPickle.load(save_file), borrow=True)
```

This technique is a bit verbose, but it is tried and true. You will be able to load your data and render it in matplotlib without trouble, years after saving it.

Do not pickle your training or test functions for long-term storage

Theano functions are compatible with Python's deepcopy and pickle mechanisms, but you should not necessarily pickle a Theano function. If you update your Theano folder and one of the internal changes, then you may not be able to un-pickle your model. Theano is still in active development, and the internal APIs are subject to change. So to be on the safe side – do not pickle your entire training or testing functions for long-term storage. The pickle mechanism is aimed at for short-term storage, such as a temp file, or a copy to another machine in a distributed job.

Read more about serialization in Theano, or Python's pickling.

3.5.2 Plotting Intermediate Results

Visualizations can be very powerful tools for understanding what your model or training algorithm is doing. You might be tempted to insert `matplotlib` plotting commands, or `PIL` image-rendering commands into your model-training script. However, later you will observe something interesting in one of those pre-rendered images and want to investigate something that isn't clear from the pictures. You'll wished you had saved the original model.

If you have enough disk space, your training script should save intermediate models and a visualization script should process those saved models.

You already have a model-saving function right? Just use it again to save these intermediate models.

Libraries you'll want to know about: Python Image Library (PIL), matplotlib.

CHAPTER

FOUR

CLASSIFYING MNIST DIGITS USING LOGISTIC REGRESSION

Note: This sections assumes familiarity with the following Theano concepts: shared variables , basic arithmetic ops , T.grad , floatX. If you intend to run the code on GPU also read GPU.

Note: The code for this section is available for download here.

In this section, we show how Theano can be used to implement the most basic classifier: the logistic regression. We start off with a quick primer of the model, which serves both as a refresher but also to anchor the notation and show how mathematical expressions are mapped onto Theano graphs.

In the deepest of machine learning traditions, this tutorial will tackle the exciting problem of MNIST digit classification.

4.1 The Model

Logistic regression is a probabilistic, linear classifier. It is parametrized by a weight matrix W and a bias vector b. Classification is done by projecting data points onto a set of hyperplanes, the distance to which reflects a class membership probability.

Mathematically, this can be written as:

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

The output of the model or prediction is then done by taking the argmax of the vector whose i'th element is P(Y=i|x).

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

The code to do this in Theano is the following:

```
# generate symbolic variables for input (x and y represent a
# minibatch)
x = T.fmatrix('x')
y = T.lvector('y')

# allocate shared variables model params
b = theano.shared(numpy.zeros((10,)), name='b')
W = theano.shared(numpy.zeros((784, 10)), name='W')

# symbolic expression for computing the vector of
# class-membership probabilities
p_y_given_x = T.nnet.softmax(T.dot(x, W) + b)

# compiled Theano function that returns the vector of class-membership
# probabilities
get_p_y_given_x = theano.function(inputs=[x], outputs=p_y_given_x)

# print the probability of some example represented by x_value
# x_value is not a symbolic variable but a numpy array describing the
# datapoint
print 'Probability that x is of class %i is %f' % (i, get_p_y_given_x(x_value)[i])

# symbolic description of how to compute prediction as class whose probability
# is maximal
y_pred = T.argmax(p_y_given_x, axis=1)

# compiled theano function that returns this value
classify = theano.function(inputs=[x], outputs=y_pred)
```

We first start by allocating symbolic variables for the inputs x, y. Since the parameters of the model must maintain a persistent state throughout training, we allocate shared variables for W, b. This declares them both as being symbolic Theano variables, but also initializes their contents. The dot and softmax operators are then used to compute the vector $P(Y|x, W, b)$. The resulting variable p_y_given_x is a symbolic variable of vector-type.

Up to this point, we have only defined the graph of computations which Theano should perform. To get the actual numerical value of $P(Y|x, W, b)$, we must create a function `get_p_y_given_x`, which takes as input `x` and returns `p_y_given_x`. We can then index its return value with the index i to get the membership probability of the i th class.

Now let's finish building the Theano graph. To get the actual model prediction, we can use the `T.argmax` operator, which will return the index at which `p_y_given_x` is maximal (i.e. the class with maximum probability).

Again, to calculate the actual prediction for a given input, we construct a function `classify`. This function takes as argument a batch of inputs x (as a matrix), and outputs a vector containing the predicted class for each example (row) in x.

Now of course, the model we have defined so far does not do anything useful yet, since its parameters are still in their initial random state. The following section will thus cover how to learn the optimal parameters.

Note: For a complete list of Theano ops, see: list of ops

4.2 Defining a Loss Function

Learning optimal model parameters involves minimizing a loss function. In the case of multi-class logistic regression, it is very common to use the negative log-likelihood as the loss. This is equivalent to maximizing the likelihood of the data set $\mathcal{D}$ under the model parameterized by θ. Let us first start by defining the likelihood $\mathcal{L}$ and loss ℓ:

$$\mathcal{L}(\theta = \{W, b\}, \mathcal{D}) = \sum_{i=0}^{|\mathcal{D}|} \log(P(Y = y^{(i)}|x^{(i)}, W, b))$$
$$\ell(\theta = \{W, b\}, \mathcal{D}) = -\mathcal{L}(\theta = \{W, b\}, \mathcal{D})$$

While entire books are dedicated to the topic of minimization, gradient descent is by far the simplest method for minimizing arbitrary non-linear functions. This tutorial will use the method of stochastic gradient method with mini-batches (MSGD). See *Stochastic Gradient Descent* for more details.

The following Theano code defines the (symbolic) loss for a given minibatch:

```
loss = -T.mean(T.log(p_y_given_x)[T.arange(y.shape[0]), y])
# note on syntax: T.arange(y.shape[0]) is a vector of integers [0,1,2,...,len(y)].
# Indexing a matrix M by the two vectors [0,1,...,K], [a,b,...,k] returns the
# elements M[0,a], M[1,b], ..., M[K,k] as a vector.  Here, we use this
# syntax to retrieve the log-probability of the correct labels, y.
```

Note: Even though the loss is formally defined as the *sum*, over the data set, of individual error terms, in practice, we use the *mean* (`T.mean`) in the code. This allows for the learning rate choice to be less dependent of the minibatch size.

4.3 Creating a LogisticRegression class

We now have all the tools we need to define a `LogisticRegression` class, which encapsulates the basic behaviour of logistic regression. The code is very similar to what we have covered so far, and should be self explanatory.

```
class LogisticRegression(object):

    def __init__(self, input, n_in, n_out):
        """ Initialize the parameters of the logistic regression

        :type input: theano.tensor.TensorType
        :param input: symbolic variable that describes the input of the
                      architecture (e.g., one minibatch of input images)

        :type n_in: int
        :param n_in: number of input units, the dimension of the space in
                     which the datapoint lies

        :type n_out: int
        :param n_out: number of output units, the dimension of the space in
```

```
                    which the target lies
        """

        # initialize with 0 the weights W as a matrix of shape (n_in, n_out)
        self.W = theano.shared(value=numpy.zeros((n_in, n_out),
                                                 dtype=theano.config.floatX), name='W' )
        # initialize the baises b as a vector of n_out 0s
        self.b = theano.shared(value=numpy.zeros((n_out,),
                                                 dtype=theano.config.floatX), name='b' )

        # compute vector of class-membership probabilities in symbolic form
        self.p_y_given_x = T.nnet.softmax(T.dot(input, self.W) + self.b)

        # compute prediction as class whose probability is maximal in
        # symbolic form
        self.y_pred=T.argmax(self.p_y_given_x, axis=1)


    def negative_log_likelihood(self, y):
        """Return the mean of the negative log-likelihood of the prediction
        of this model under a given target distribution.

        .. math::

          \frac{1}{|\mathcal{D}|} \mathcal{L} (\theta=\{W,b\}, \mathcal{D}) =
          \frac{1}{|\mathcal{D}|} \sum_{i=0}^{|\mathcal{D}|} \log(P(Y=y^{(i)}|x^{(i)}, W,b
              \ell (\theta=\{W,b\}, \mathcal{D})


        :param y: corresponds to a vector that gives for each example the
                  correct label;

        Note: we use the mean instead of the sum so that
              the learning rate is less dependent on the batch size
        """
        return -T.mean(T.log(self.p_y_given_x)[T.arange(y.shape[0]), y])
```

We instantiate this class as follows:

```
# allocate symbolic variables for the data
x = T.fmatrix()  # the data is presented as rasterized images (each being a 1-D row vector
y = T.lvector()  # the labels are presented as 1D vector of [long int] labels

# construct the logistic regression class
classifier = LogisticRegression(
               input=x.reshape((batch_size, 28 * 28)), n_in=28 * 28, n_out=10)
```

Note that the inputs x and y are defined outside the scope of the `LogisticRegression` object. Since the class requires the input x to build its graph however, it is passed as a parameter of the `__init__` function. This is usefull in the case when you would want to concatenate such classes to form a deep network (case in which the input is not a new variable but the output of the layer below). While in this example we will not do that, the tutorials are designed such that the code is as similar as possible among them, making it easy to go from one tutorial to the other.

The last step involves defining a (symbolic) cost variable to minimize, using the instance method `classifier.negative_log_likelihood`.

```
cost = classifier.negative_log_likelihood(y)
```

Note how x is an implicit symbolic input to the symbolic definition of cost, here, because classifier.__init__ has defined its symbolic variables in terms of x.

4.4 Learning the Model

To implement MSGD in most programming languages (C/C++, Matlab, Python), one would start by manually deriving the expressions for the gradient of the loss with respect to the parameters: in this case $\partial \ell / \partial W$, and $\partial \ell / \partial b$, This can get pretty tricky for complex models, as expressions for $\partial \ell / \partial \theta$ can get fairly complex, especially when taking into account problems of numerical stability.

With Theano, this work is greatly simplified as it performs automatic differentiation and applies certain math transforms to improve numerical stability.

To get the gradients $\partial \ell / \partial W$ and $\partial \ell / \partial b$ in Theano, simply do the following:

```
# compute the gradient of cost with respect to theta = (W,b)
g_W = T.grad(cost, classifier.W)
g_b = T.grad(cost, classifier.b)
```

`g_W` and `g_b` are again symbolic variables, which can be used as part of a computation graph. Performing one-step of gradient descent can then be done as follows:

```
# compute the gradient of cost with respect to theta = (W,b)
g_W = T.grad(cost=cost, wrt=classifier.W)
g_b = T.grad(cost=cost, wrt=classifier.b)

# specify how to update the parameters of the model as a list of
# (variable, update expression) pairs
updates = [(classifier.W, classifier.W - learning_rate * g_W),
           (classifier.b, classifier.b - learning_rate * g_b)]

# compiling a Theano function `train_model` that returns the cost, but in
# the same time updates the parameter of the model based on the rules
# defined in `updates`
train_model = theano.function(inputs=[index],
        outputs=cost,
        updates=updates,
        givens={
            x: train_set_x[index * batch_size: (index + 1) * batch_size],
            y: train_set_y[index * batch_size]})
```

The `updates` list contains, for each parameter, the stochastic gradient update operation. The `givens` dictionary indicates with what to replace certain variables of the graph. The function `train_model` is then defined such that:

- the input is the mini-batch index `index` that together with the batch size(which is not an input since it is fixed) defines x with corresponding labels y

- the return value is the cost/loss associated with the x, y defined by the `index`
- on every function call, it will first replace `x` and `y` with the corresponding slices from the training set as defined by the `index` and afterwards it will evaluate the cost associated with that minibatch and apply the operations defined by the `updates` list.

Each time `train_model(index)` function is called, it will thus compute and return the appropriate cost, while also performing a step of MSGD. The entire learning algorithm thus consists in looping over all examples in the dataset, and repeatedly calling the `train_model` function.

4.5 Testing the model

As explained in *Learning a Classifier*, when testing the model we are interested in the number of misclassified examples (and not only in the likelihood). The `LogisticRegression` class therefore has an extra instance method, which builds the symbolic graph for retrieving the number of misclassified examples in each minibatch.

The code is as follows:

```
class LogisticRegression(object):

    ...

    def errors(self, y):
        """Return a float representing the number of errors in the minibatch
        over the total number of examples of the minibatch ; zero
        one loss over the size of the minibatch
        """
        return T.mean(T.neq(self.y_pred, y))
```

We then create a function `test_model` and a function `validate_model`, which we can call to retrieve this value. As you will see shortly, `validate_model` is key to our early-stopping implementation (see *Early-Stopping*). Both of these function will get as input a batch offset and will compute the number of missclassified examples for that mini-batch. The only difference between them is that one draws its batches from the testing set, while the other from the validation set.

```
# compiling a Theano function that computes the mistakes that are made by
# the model on a minibatch
test_model = theano.function(inputs=[index],
        outputs=classifier.errors(y),
        givens={
            x: test_set_x[index * batch_size: (index + 1) * batch_size],
            y: test_set_y[index * batch_size: (index + 1) * batch_size]})

validate_model = theano.function(inputs=[index],
        outputs=classifier.errors(y),
        givens={
            x: valid_set_x[index * batch_size: (index + 1) * batch_size],
            y: valid_set_y[index * batch_size: (index + 1) * batch_size]})
```

4.6 Putting it All Together

The finished product is as follows.

```
"""
This tutorial introduces logistic regression using Theano and stochastic
gradient descent.

Logistic regression is a probabilistic, linear classifier. It is parametrized
by a weight matrix :math:`W` and a bias vector :math:`b`. Classification is
done by projecting data points onto a set of hyperplanes, the distance to
which is used to determine a class membership probability.

Mathematically, this can be written as:

.. math::
  P(Y=i|x, W,b) &= softmax_i(W x + b) \\
                &= \frac {e^{W_i x + b_i}} {\sum_j e^{W_j x + b_j}}


The output of the model or prediction is then done by taking the argmax of
the vector whose i'th element is P(Y=i|x).

.. math::

  y_{pred} = argmax_i P(Y=i|x,W,b)


This tutorial presents a stochastic gradient descent optimization method
suitable for large datasets, and a conjugate gradient optimization method
that is suitable for smaller datasets.


References:

    - textbooks: "Pattern Recognition and Machine Learning" -
                 Christopher M. Bishop, section 4.3.2

"""
__docformat__ = 'restructedtext en'

import cPickle
import gzip
import os
import sys
import time

import numpy

import theano
import theano.tensor as T
```

```
class LogisticRegression(object):
    """Multi-class Logistic Regression Class

    The logistic regression is fully described by a weight matrix :math:`W`
    and bias vector :math:`b`. Classification is done by projecting data
    points onto a set of hyperplanes, the distance to which is used to
    determine a class membership probability.
    """

    def __init__(self, input, n_in, n_out):
        """ Initialize the parameters of the logistic regression

        :type input: theano.tensor.TensorType
        :param input: symbolic variable that describes the input of the
                      architecture (one minibatch)

        :type n_in: int
        :param n_in: number of input units, the dimension of the space in
                     which the datapoints lie

        :type n_out: int
        :param n_out: number of output units, the dimension of the space in
                      which the labels lie

        """

        # initialize with 0 the weights W as a matrix of shape (n_in, n_out)
        self.W = theano.shared(value=numpy.zeros((n_in, n_out),
                                                 dtype=theano.config.floatX),
                               name='W', borrow=True)
        # initialize the baises b as a vector of n_out 0s
        self.b = theano.shared(value=numpy.zeros((n_out,),
                                                 dtype=theano.config.floatX),
                               name='b', borrow=True)

        # compute vector of class-membership probabilities in symbolic form
        self.p_y_given_x = T.nnet.softmax(T.dot(input, self.W) + self.b)

        # compute prediction as class whose probability is maximal in
        # symbolic form
        self.y_pred = T.argmax(self.p_y_given_x, axis=1)

        # parameters of the model
        self.params = [self.W, self.b]

    def negative_log_likelihood(self, y):
        """Return the mean of the negative log-likelihood of the prediction
        of this model under a given target distribution.

        .. math::

            \frac{1}{|\mathcal{D}|} \mathcal{L} (\theta=\{W,b\}, \mathcal{D}) =
            \frac{1}{|\mathcal{D}|} \sum_{i=0}^{|\mathcal{D}|} \log(P(Y=y^{(i)}|x^{(i)}, W,
```

```
                \ell (\theta=\{W,b\}, \mathcal{D})

        :type y: theano.tensor.TensorType
        :param y: corresponds to a vector that gives for each example the
                  correct label

        Note: we use the mean instead of the sum so that
              the learning rate is less dependent on the batch size
        """
        # y.shape[0] is (symbolically) the number of rows in y, i.e.,
        # number of examples (call it n) in the minibatch
        # T.arange(y.shape[0]) is a symbolic vector which will contain
        # [0,1,2,... n-1] T.log(self.p_y_given_x) is a matrix of
        # Log-Probabilities (call it LP) with one row per example and
        # one column per class LP[T.arange(y.shape[0]),y] is a vector
        # v containing [LP[0,y[0]], LP[1,y[1]], LP[2,y[2]], ...,
        # LP[n-1,y[n-1]]] and T.mean(LP[T.arange(y.shape[0]),y]) is
        # the mean (across minibatch examples) of the elements in v,
        # i.e., the mean log-likelihood across the minibatch.
        return -T.mean(T.log(self.p_y_given_x)[T.arange(y.shape[0]), y])

    def errors(self, y):
        """Return a float representing the number of errors in the minibatch
        over the total number of examples of the minibatch ; zero one
        loss over the size of the minibatch

        :type y: theano.tensor.TensorType
        :param y: corresponds to a vector that gives for each example the
                  correct label
        """

        # check if y has same dimension of y_pred
        if y.ndim != self.y_pred.ndim:
            raise TypeError('y should have the same shape as self.y_pred',
                ('y', target.type, 'y_pred', self.y_pred.type))
        # check if y is of the correct datatype
        if y.dtype.startswith('int'):
            # the T.neq operator returns a vector of 0s and 1s, where 1
            # represents a mistake in prediction
            return T.mean(T.neq(self.y_pred, y))
        else:
            raise NotImplementedError()


def load_data(dataset):
    ''' Loads the dataset

    :type dataset: string
    :param dataset: the path to the dataset (here MNIST)
    '''

    #############
    # LOAD DATA #
```

```
    ############

    # Download the MNIST dataset if it is not present
    data_dir, data_file = os.path.split(dataset)
    if data_dir == "" and not os.path.isfile(dataset):
        # Check if dataset is in the data directory.
        new_path = os.path.join(os.path.split(__file__)[0], "..", "data", dataset)
        if os.path.isfile(new_path) or data_file == 'mnist.pkl.gz':
            dataset = new_path

    if (not os.path.isfile(dataset)) and data_file == 'mnist.pkl.gz':
        import urllib
        origin = 'http://www.iro.umontreal.ca/~lisa/deep/data/mnist/mnist.pkl.gz'
        print 'Downloading data from %s' % origin
        urllib.urlretrieve(origin, dataset)

    print '... loading data'

    # Load the dataset
    f = gzip.open(dataset, 'rb')
    train_set, valid_set, test_set = cPickle.load(f)
    f.close()
    #train_set, valid_set, test_set format: tuple(input, target)
    #input is an numpy.ndarray of 2 dimensions (a matrix)
    #witch row's correspond to an example. target is a
    #numpy.ndarray of 1 dimensions (vector)) that have the same length as
    #the number of rows in the input. It should give the target
    #target to the example with the same index in the input.

    def shared_dataset(data_xy, borrow=True):
        """ Function that loads the dataset into shared variables

        The reason we store our dataset in shared variables is to allow
        Theano to copy it into the GPU memory (when code is run on GPU).
        Since copying data into the GPU is slow, copying a minibatch everytime
        is needed (the default behaviour if the data is not in a shared
        variable) would lead to a large decrease in performance.
        """
        data_x, data_y = data_xy
        shared_x = theano.shared(numpy.asarray(data_x,
                                               dtype=theano.config.floatX),
                                 borrow=borrow)
        shared_y = theano.shared(numpy.asarray(data_y,
                                               dtype=theano.config.floatX),
                                 borrow=borrow)
        # When storing data on the GPU it has to be stored as floats
        # therefore we will store the labels as ``floatX'' as well
        # (``shared_y'' does exactly that). But during our computations
        # we need them as ints (we use labels as index, and if they are
        # floats it doesn't make sense) therefore instead of returning
        # ``shared_y'' we will have to cast it to int. This little hack
        # lets ous get around this issue
        return shared_x, T.cast(shared_y, 'int32')
```

```
    test_set_x, test_set_y = shared_dataset(test_set)
    valid_set_x, valid_set_y = shared_dataset(valid_set)
    train_set_x, train_set_y = shared_dataset(train_set)

    rval = [(train_set_x, train_set_y), (valid_set_x, valid_set_y),
            (test_set_x, test_set_y)]
    return rval


def sgd_optimization_mnist(learning_rate=0.13, n_epochs=1000,
                           dataset='mnist.pkl.gz',
                           batch_size=600):
    """
    Demonstrate stochastic gradient descent optimization of a log-linear
    model

    This is demonstrated on MNIST.

    :type learning_rate: float
    :param learning_rate: learning rate used (factor for the stochastic
                          gradient)

    :type n_epochs: int
    :param n_epochs: maximal number of epochs to run the optimizer

    :type dataset: string
    :param dataset: the path of the MNIST dataset file from
                 http://www.iro.umontreal.ca/~lisa/deep/data/mnist/mnist.pkl.gz

    """
    datasets = load_data(dataset)

    train_set_x, train_set_y = datasets[0]
    valid_set_x, valid_set_y = datasets[1]
    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] / batch_size
    n_valid_batches = valid_set_x.get_value(borrow=True).shape[0] / batch_size
    n_test_batches = test_set_x.get_value(borrow=True).shape[0] / batch_size

    ######################
    # BUILD ACTUAL MODEL #
    ######################
    print '... building the model'

    # 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
    y = T.ivector('y')  # the labels are presented as 1D vector of
                        # [int] labels

    # construct the logistic regression class
```

```
# Each MNIST image has size 28*28
classifier = LogisticRegression(input=x, n_in=28 * 28, n_out=10)

# the cost we minimize during training is the negative log likelihood of
# the model in symbolic format
cost = classifier.negative_log_likelihood(y)

# compiling a Theano function that computes the mistakes that are made by
# the model on a minibatch
test_model = theano.function(inputs=[index],
        outputs=classifier.errors(y),
        givens={
            x: test_set_x[index * batch_size: (index + 1) * batch_size],
            y: test_set_y[index * batch_size: (index + 1) * batch_size]})

validate_model = theano.function(inputs=[index],
        outputs=classifier.errors(y),
        givens={
            x: valid_set_x[index * batch_size:(index + 1) * batch_size],
            y: valid_set_y[index * batch_size:(index + 1) * batch_size]})

# compute the gradient of cost with respect to theta = (W,b)
g_W = T.grad(cost=cost, wrt=classifier.W)
g_b = T.grad(cost=cost, wrt=classifier.b)

# specify how to update the parameters of the model as a list of
# (variable, update expression) pairs.
updates = [(classifier.W, classifier.W - learning_rate * g_W),
           (classifier.b, classifier.b - learning_rate * g_b)]

# compiling a Theano function `train_model` that returns the cost, but in
# the same time updates the parameter of the model based on the rules
# defined in `updates`
train_model = theano.function(inputs=[index],
        outputs=cost,
        updates=updates,
        givens={
            x: train_set_x[index * batch_size:(index + 1) * batch_size],
            y: train_set_y[index * batch_size:(index + 1) * batch_size]})

###############
# TRAIN MODEL #
###############
print '... training the model'
# early-stopping parameters
patience = 5000  # look as this many examples regardless
patience_increase = 2  # wait this much longer when a new best is
                       # found
improvement_threshold = 0.995  # a relative improvement of this much is
                       # considered significant
validation_frequency = min(n_train_batches, patience / 2)
                       # go through this many
                       # minibatche before checking the network
```

```
                                # on the validation set; in this case we
                                # check every epoch

    best_params = None
    best_validation_loss = numpy.inf
    test_score = 0.
    start_time = time.clock()

    done_looping = False
    epoch = 0
    while (epoch < n_epochs) and (not done_looping):
        epoch = epoch + 1
        for minibatch_index in xrange(n_train_batches):

            minibatch_avg_cost = train_model(minibatch_index)
            # iteration number
            iter = (epoch - 1) * n_train_batches + minibatch_index

            if (iter + 1) % validation_frequency == 0:
                # compute zero-one loss on validation set
                validation_losses = [validate_model(i)
                                     for i in xrange(n_valid_batches)]
                this_validation_loss = numpy.mean(validation_losses)

                print('epoch %i, minibatch %i/%i, validation error %f %%' % \
                     (epoch, minibatch_index + 1, n_train_batches,
                     this_validation_loss * 100.))

                # if we got the best validation score until now
                if this_validation_loss < best_validation_loss:
                    #improve patience if loss improvement is good enough
                    if this_validation_loss < best_validation_loss *  \
                       improvement_threshold:
                        patience = max(patience, iter * patience_increase)

                    best_validation_loss = this_validation_loss
                    # test it on the test set

                    test_losses = [test_model(i)
                                   for i in xrange(n_test_batches)]
                    test_score = numpy.mean(test_losses)

                    print(('     epoch %i, minibatch %i/%i, test error of best'
                       ' model %f %%') %
                          (epoch, minibatch_index + 1, n_train_batches,
                           test_score * 100.))

            if patience <= iter:
                done_looping = True
                break

    end_time = time.clock()
    print(('Optimization complete with best validation score of %f %%,'
```

```
            'with test performance %f %%') %
                  (best_validation_loss * 100., test_score * 100.))
    print 'The code run for %d epochs, with %f epochs/sec' % (
        epoch, 1. * epoch / (end_time - start_time))
    print >> sys.stderr, ('The code for file ' +
                          os.path.split(__file__)[1] +
                          ' ran for %.1fs' % ((end_time - start_time)))

if __name__ == '__main__':
    sgd_optimization_mnist()
```

The user can learn to classify MNIST digits with SGD logistic regression, by typing, from within the DeepLearningTutorials folder:

```
python code/logistic_sgd.py
```

The output one should expect is of the form :

```
...
epoch 72, minibatch 83/83, validation error 7.510417 %
     epoch 72, minibatch 83/83, test error of best model 7.510417 %
epoch 73, minibatch 83/83, validation error 7.500000 %
     epoch 73, minibatch 83/83, test error of best model 7.489583 %
Optimization complete with best validation score of 7.500000 %,with test performance 7.489
The code run for 74 epochs, with 1.936983 epochs/sec
```

On an Intel(R) Core(TM)2 Duo CPU E8400 @ 3.00 Ghz the code runs with approximately 1.936 epochs/sec and it took 75 epochs to reach a test error of 7.489%. On the GPU the code does almost 10.0 epochs/sec. For this instance we used a batch size of 600.

CHAPTER

FIVE

MULTILAYER PERCEPTRON

Note: This section assumes the reader has already read through *Classifying MNIST digits using Logistic Regression*. Additionally, it uses the following new Theano functions and concepts: T.tanh, shared variables, basic arithmetic ops, T.grad, *L1 and L2 regularization*, floatX. If you intend to run the code on GPU also read GPU.

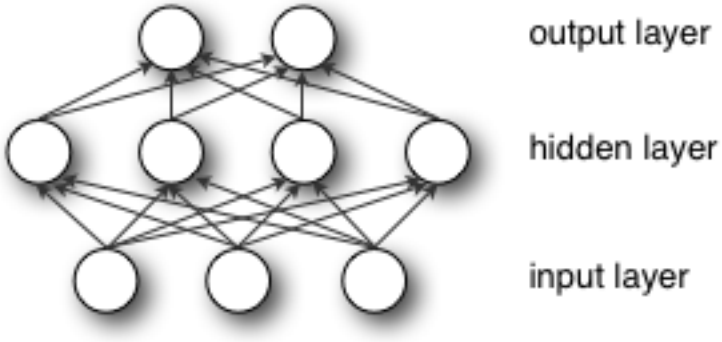
Note: The code for this section is available for download here.

The next architecture we are going to present using Theano is the single-hidden layer Multi-Layer Perceptron (MLP). An MLP can be viewed as a logistic regressor, where the input is first transformed using a learnt non-linear transformation Φ. The purpose of this transformation is to project the input data into a space where it becomes linearly separable. This intermediate layer is referred to as a **hidden layer**. A single hidden layer is sufficient to make MLPs a **universal approximator**. However we will see later on that there are substantial benefits to using many such hidden layers, i.e. the very premise of **deep learning**. See these course notes for an introduction to MLPs, the back-propagation algorithm, and how to train MLPs.

This tutorial will again tackle the problem of MNIST digit classification.

5.1 The Model

An MLP (or Artificial Neural Network - ANN) with a single hidden layer can be represented graphically as follows:



Formally, a one-hidden layer MLP constitutes a function $f : R^D \rightarrow R^L$, where D is the size of input vector

x and L is the size of the output vector $f(x)$, such that, in matrix notation:

$$f(x) = G(b^{(2)} + W^{(2)}(s(b^{(1)} + W^{(1)}x))),$$

with bias vectors $b^{(1)}$, $b^{(2)}$; weight matrices $W^{(1)}$, $W^{(2)}$ and activation functions G and s.

The vector $h(x) = \Phi(x) = s(b^{(1)} + W^{(1)}x)$ constitutes the hidden layer. $W^{(1)} \in R^{D \times D_h}$ is the weight matrix connecting the input vector to the hidden layer. Each column $W_{.i}^{(1)}$ represents the weights from the input units to the i-th hidden unit. Typical choices for s include $tanh$, with $tanh(a) = (e^a - e^{-a})/(e^a + e^{-a})$, or the logistic $sigmoid$ function, with $sigmoid(a) = 1/(1 + e^{-a})$. We will be using $tanh$ in this tutorial because it typically yields to faster training (and sometimes also to better local minima). Both the $tanh$ and $sigmoid$ are scalar-to-scalar functions but their natural extension to vectors and tensors consists in applying them element-wise (e.g. separately on each element of the vector, yielding a same-size vector).

The output vector is then obtained as: $o(x) = G(b^{(2)} + W^{(2)}h(x))$. The reader should recognize the form we already used for *Classifying MNIST digits using Logistic Regression*. As before, class-membership probabilities can be obtained by choosing G as the $softmax$ function (in the case of multi-class classification).

To train an MLP, we learn **all** parameters of the model, and here we use *Stochastic Gradient Descent* with minibatches. The set of parameters to learn is the set $\theta = \{W^{(2)}, b^{(2)}, W^{(1)}, b^{(1)}\}$. Obtaining the gradients $\partial \ell / \partial \theta$ can be achieved through the **backpropagation algorithm** (a special case of the chain-rule of derivation). Thankfully, since Theano performs automatic differentation, we will not need to cover this in the tutorial !

5.2 Going from logistic regression to MLP

This tutorial will focus on a single-layer MLP. We start off by implementing a class that will represent any given hidden layer. To construct the MLP we will then only need to throw a logistic regression layer on top.

```
class HiddenLayer(object):
    def __init__(self, rng, input, n_in, n_out, activation=T.tanh):
        """
        Typical hidden layer of a MLP: units are fully-connected and have
        sigmoidal activation function. Weight matrix W is of shape (n_in,n_out)
        and the bias vector b is of shape (n_out,).

        NOTE : The nonlinearity used here is tanh

        Hidden unit activation is given by: tanh(dot(input,W) + b)

        :type rng: numpy.random.RandomState
        :param rng: a random number generator used to initialize weights

        :type input: theano.tensor.dmatrix
        :param input: a symbolic tensor of shape (n_examples, n_in)

        :type n_in: int
        :param n_in: dimensionality of input

        :type n_out: int
        :param n_out: number of hidden units
```

```
        :type activation: theano.Op or function
        :param activation: Non linearity to be applied in the hidden
                           layer
        """
        self.input = input
```

The initial values for the weights of a hidden layer i should be uniformly sampled from a symmetric interval that depends on the activation function. For $tanh$ activation function results obtained in [Xavier10] show that the interval should be $[-\sqrt{\frac{6}{fan_{in}+fan_{out}}}, \sqrt{\frac{6}{fan_{in}+fan_{out}}}]$, where fan_{in} is the number of units in the $(i-1)$-th layer, and fan_{out} is the number of units in the i-th layer. For the sigmoid function the interval is $[-4\sqrt{\frac{6}{fan_{in}+fan_{out}}}, 4\sqrt{\frac{6}{fan_{in}+fan_{out}}}]$. This initialization ensures that, early in training, each neuron operates in a regime of its activation function where information can easily be propagated both upward (activations flowing from inputs to outputs) and backward (gradients flowing from outputs to inputs).

```
# `W` is initialized with `W_values` which is uniformely sampled
# from sqrt(-6./(n_in+n_hidden)) and sqrt(6./(n_in+n_hidden))
# for tanh activation function
# the output of uniform is converted using asarray to dtype
# theano.config.floatX so that the code is runable on GPU
# Note : optimal initialization of weights is dependent on the
#        activation function used (among other things).
#        For example, results presented in [Xavier10]_ suggest that you
#        should use 4 times larger initial weights for sigmoid
#        compared to tanh
#        We have no info for other function, so we use the same as tanh.
W_values = numpy.asarray(rng.uniform(
        low=-numpy.sqrt(6. / (n_in + n_out)),
        high=numpy.sqrt(6. / (n_in + n_out)),
        size=(n_in, n_out)), dtype=theano.config.floatX)
if activation == theano.tensor.nnet.sigmoid:
    W_values *= 4

self.W = theano.shared(value=W_values, name='W')

b_values = numpy.zeros((n_out,), dtype=theano.config.floatX)
self.b = theano.shared(value=b_values, name='b')
```

Note that we used a given non-linear function as the activation function of the hidden layer. By default this is `tanh`, but in many cases we might want to use something else.

```
self.output = activation(T.dot(input, self.W) + self.b)
# parameters of the model
self.params = [self.W, self.b]
```

If you look into theory this class implements the graph that computes the hidden layer value $h(x) = \Phi(x) = s(b^{(1)} + W^{(1)}x)$. If you give this as input to the `LogisticRegression` class, implemented in the previous tutorial *Classifying MNIST digits using Logistic Regression*, you get the output of the MLP. You can see this in the following short implementation of the `MLP` class :

```
class MLP(object):
  """Multi-Layer Perceptron Class
```

```
    A multilayer perceptron is a feedforward artificial neural network model
    that has one layer or more of hidden units and nonlinear activations.
    Intermediate layers usually have as activation function tanh or the
    sigmoid function (defined here by a ''HiddenLayer'' class)  while the
    top layer is a softamx layer (defined here by a ''LogisticRegression''
    class).
    """



    def __init__(self, rng, input, n_in, n_hidden, n_out):
        """Initialize the parameters for the multilayer perceptron

        :type rng: numpy.random.RandomState
        :param rng: a random number generator used to initialize weights

        :type input: theano.tensor.TensorType
        :param input: symbolic variable that describes the input of the
        architecture (one minibatch)

        :type n_in: int
        :param n_in: number of input units, the dimension of the space in
        which the datapoints lie

        :type n_hidden: int
        :param n_hidden: number of hidden units

        :type n_out: int
        :param n_out: number of output units, the dimension of the space in
        which the labels lie

        """

        # Since we are dealing with a one hidden layer MLP, this will
        # translate into a Hidden Layer connected to the LogisticRegression
        # layer
        self.hiddenLayer = HiddenLayer(rng = rng, input = input,
                                       n_in = n_in, n_out = n_hidden,
                                       activation = T.tanh)

        # The logistic regression layer gets as input the hidden units
        # of the hidden layer
        self.logRegressionLayer = LogisticRegression(
                                        input=self.hiddenLayer.output,
                                        n_in=n_hidden,
                                        n_out=n_out)
```

In this tutorial we will also use L1 and L2 regularization (see *L1 and L2 regularization*). For this, we need to compute the L1 norm and the squared L2 norm of the weights $W^{(1)}, W^{(2)}$.

```
# L1 norm ; one regularization option is to enforce L1 norm to
# be small
self.L1 = abs(self.hiddenLayer.W).sum() \
```

```
        + abs(self.logRegressionLayer.W).sum()

# square of L2 norm ; one regularization option is to enforce
# square of L2 norm to be small
self.L2_sqr = (self.hiddenLayer.W ** 2).sum() \
            + (self.logRegressionLayer.W ** 2).sum()

# negative log likelihood of the MLP is given by the negative
# log likelihood of the output of the model, computed in the
# logistic regression layer
self.negative_log_likelihood = self.logRegressionLayer.negative_log_likelihood
# same holds for the function computing the number of errors
self.errors = self.logRegressionLayer.errors

# the parameters of the model are the parameters of the two layer it is
# made out of
self.params = self.hiddenLayer.params + self.logRegressionLayer.params
```

As before, we train this model using stochastic gradient descent with mini-batches. The difference is that we modify the cost function to include the regularization term. `L1_reg` and `L2_reg` are the hyperparameters controlling the weight of these regularization terms in the total cost function. The code that computes the new cost is:

```
# the cost we minimize during training is the negative log likelihood of
# the model plus the regularization terms (L1 and L2); cost is expressed
# here symbolically
cost = classifier.negative_log_likelihood(y) \
     + L1_reg * classifier.L1 \
     + L2_reg * classifier.L2_sqr
```

We then update the parameters of the model using the gradient. This code is almost identical to the one for logistic regression. Only the number of parameters differ. To get around this (and write code that could work for any number of parameters) we will use the list of parameters that we created with the model `params` and parse it, computing a gradient at each step.

```
# compute the gradient of cost with respect to theta (stored in params)
# the resulting gradients will be stored in a list gparams
gparams = []
for param in classifier.params:
    gparam  = T.grad(cost, param)
    gparams.append(gparam)


# specify how to update the parameters of the model as a list of
# (variable, update expression) pairs
updates = []
# given two list the zip A = [a1, a2, a3, a4] and B = [b1, b2, b3, b4] of
# same length, zip generates a list C of same size, where each element
# is a pair formed from the two lists :
#    C = [(a1, b1), (a2, b2), (a3, b3) , (a4, b4)]
for param, gparam in zip(classifier.params, gparams):
    updates.append((param, param - learning_rate * gparam))
```

```
# compiling a Theano function `train_model` that returns the cost, butx
# in the same time updates the parameter of the model based on the rules
# defined in `updates`
train_model = theano.function(inputs=[index], outputs=cost,
        updates=updates,
        givens={
            x: train_set_x[index * batch_size:(index + 1) * batch_size],
            y: train_set_y[index * batch_size:(index + 1) * batch_size]})
```

5.3 Putting it All Together

Having covered the basic concepts, writing an MLP class becomes quite easy. The code below shows how this can be done, in a way which is analogous to our previous logistic regression implementation.

```
"""
This tutorial introduces the multilayer perceptron using Theano.

 A multilayer perceptron is a logistic regressor where
instead of feeding the input to the logistic regression you insert a
intermediate layer, called the hidden layer, that has a nonlinear
activation function (usually tanh or sigmoid) . One can use many such
hidden layers making the architecture deep. The tutorial will also tackle
the problem of MNIST digit classification.

.. math::

    f(x) = G( b^{(2)} + W^{(2)}( s( b^{(1)} + W^{(1)} x))),

References:

    - textbooks: "Pattern Recognition and Machine Learning" -
                 Christopher M. Bishop, section 5

"""
__docformat__ = 'restructedtext en'


import cPickle
import gzip
import os
import sys
import time

import numpy

import theano
import theano.tensor as T


from logistic_sgd import LogisticRegression, load_data
```

```
class HiddenLayer(object):
    def __init__(self, rng, input, n_in, n_out, W=None, b=None,
                 activation=T.tanh):
        """
        Typical hidden layer of a MLP: units are fully-connected and have
        sigmoidal activation function. Weight matrix W is of shape (n_in,n_out)
        and the bias vector b is of shape (n_out,).

        NOTE : The nonlinearity used here is tanh

        Hidden unit activation is given by: tanh(dot(input,W) + b)

        :type rng: numpy.random.RandomState
        :param rng: a random number generator used to initialize weights

        :type input: theano.tensor.dmatrix
        :param input: a symbolic tensor of shape (n_examples, n_in)

        :type n_in: int
        :param n_in: dimensionality of input

        :type n_out: int
        :param n_out: number of hidden units

        :type activation: theano.Op or function
        :param activation: Non linearity to be applied in the hidden
                           layer
        """
        self.input = input

        # `W` is initialized with `W_values` which is uniformely sampled
        # from sqrt(-6./(n_in+n_hidden)) and sqrt(6./(n_in+n_hidden))
        # for tanh activation function
        # the output of uniform if converted using asarray to dtype
        # theano.config.floatX so that the code is runable on GPU
        # Note : optimal initialization of weights is dependent on the
        #        activation function used (among other things).
        #        For example, results presented in [Xavier10] suggest that you
        #        should use 4 times larger initial weights for sigmoid
        #        compared to tanh
        #        We have no info for other function, so we use the same as
        #        tanh.
        if W is None:
            W_values = numpy.asarray(rng.uniform(
                    low=-numpy.sqrt(6. / (n_in + n_out)),
                    high=numpy.sqrt(6. / (n_in + n_out)),
                    size=(n_in, n_out)), dtype=theano.config.floatX)
            if activation == theano.tensor.nnet.sigmoid:
                W_values *= 4

            W = theano.shared(value=W_values, name='W', borrow=True)

        if b is None:
```

```
            b_values = numpy.zeros((n_out,), dtype=theano.config.floatX)
            b = theano.shared(value=b_values, name='b', borrow=True)

        self.W = W
        self.b = b

        lin_output = T.dot(input, self.W) + self.b
        self.output = (lin_output if activation is None
                       else activation(lin_output))
        # parameters of the model
        self.params = [self.W, self.b]


class MLP(object):
    """Multi-Layer Perceptron Class

    A multilayer perceptron is a feedforward artificial neural network model
    that has one layer or more of hidden units and nonlinear activations.
    Intermediate layers usually have as activation function thanh or the
    sigmoid function (defined here by a ''SigmoidalLayer'' class)  while the
    top layer is a softamx layer (defined here by a ''LogisticRegression''
    class).
    """

    def __init__(self, rng, input, n_in, n_hidden, n_out):
        """Initialize the parameters for the multilayer perceptron

        :type rng: numpy.random.RandomState
        :param rng: a random number generator used to initialize weights

        :type input: theano.tensor.TensorType
        :param input: symbolic variable that describes the input of the
        architecture (one minibatch)

        :type n_in: int
        :param n_in: number of input units, the dimension of the space in
        which the datapoints lie

        :type n_hidden: int
        :param n_hidden: number of hidden units

        :type n_out: int
        :param n_out: number of output units, the dimension of the space in
        which the labels lie

        """

        # Since we are dealing with a one hidden layer MLP, this will
        # translate into a TanhLayer connected to the LogisticRegression
        # layer; this can be replaced by a SigmoidalLayer, or a layer
        # implementing any other nonlinearity
        self.hiddenLayer = HiddenLayer(rng=rng, input=input,
                                       n_in=n_in, n_out=n_hidden,
```

```
                                        activation=T.tanh)

        # The logistic regression layer gets as input the hidden units
        # of the hidden layer
        self.logRegressionLayer = LogisticRegression(
            input=self.hiddenLayer.output,
            n_in=n_hidden,
            n_out=n_out)

        # L1 norm ; one regularization option is to enforce L1 norm to
        # be small
        self.L1 = abs(self.hiddenLayer.W).sum() \
                + abs(self.logRegressionLayer.W).sum()

        # square of L2 norm ; one regularization option is to enforce
        # square of L2 norm to be small
        self.L2_sqr = (self.hiddenLayer.W ** 2).sum() \
                    + (self.logRegressionLayer.W ** 2).sum()

        # negative log likelihood of the MLP is given by the negative
        # log likelihood of the output of the model, computed in the
        # logistic regression layer
        self.negative_log_likelihood = self.logRegressionLayer.negative_log_likelihood
        # same holds for the function computing the number of errors
        self.errors = self.logRegressionLayer.errors

        # the parameters of the model are the parameters of the two layer it is
        # made out of
        self.params = self.hiddenLayer.params + self.logRegressionLayer.params


def test_mlp(learning_rate=0.01, L1_reg=0.00, L2_reg=0.0001, n_epochs=1000,
             dataset='mnist.pkl.gz', batch_size=20, n_hidden=500):
    """
    Demonstrate stochastic gradient descent optimization for a multilayer
    perceptron

    This is demonstrated on MNIST.

    :type learning_rate: float
    :param learning_rate: learning rate used (factor for the stochastic
    gradient

    :type L1_reg: float
    :param L1_reg: L1-norm's weight when added to the cost (see
    regularization)

    :type L2_reg: float
    :param L2_reg: L2-norm's weight when added to the cost (see
    regularization)

    :type n_epochs: int
    :param n_epochs: maximal number of epochs to run the optimizer
```

```
    :type dataset: string
    :param dataset: the path of the MNIST dataset file from
                 http://www.iro.umontreal.ca/~lisa/deep/data/mnist/mnist.pkl.gz


    """
    datasets = load_data(dataset)

    train_set_x, train_set_y = datasets[0]
    valid_set_x, valid_set_y = datasets[1]
    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] / batch_size
    n_valid_batches = valid_set_x.get_value(borrow=True).shape[0] / batch_size
    n_test_batches = test_set_x.get_value(borrow=True).shape[0] / batch_size

    ######################
    # BUILD ACTUAL MODEL #
    ######################
    print '... building the model'

    # 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
    y = T.ivector('y')  # the labels are presented as 1D vector of
                        # [int] labels

    rng = numpy.random.RandomState(1234)

    # construct the MLP class
    classifier = MLP(rng=rng, input=x, n_in=28 * 28,
                     n_hidden=n_hidden, n_out=10)

    # the cost we minimize during training is the negative log likelihood of
    # the model plus the regularization terms (L1 and L2); cost is expressed
    # here symbolically
    cost = classifier.negative_log_likelihood(y) \
         + L1_reg * classifier.L1 \
         + L2_reg * classifier.L2_sqr

    # compiling a Theano function that computes the mistakes that are made
    # by the model on a minibatch
    test_model = theano.function(inputs=[index],
            outputs=classifier.errors(y),
            givens={
                x: test_set_x[index * batch_size:(index + 1) * batch_size],
                y: test_set_y[index * batch_size:(index + 1) * batch_size]})

    validate_model = theano.function(inputs=[index],
            outputs=classifier.errors(y),
            givens={
                x: valid_set_x[index * batch_size:(index + 1) * batch_size],
```

```
            y: valid_set_y[index * batch_size:(index + 1) * batch_size]})

    # compute the gradient of cost with respect to theta (sotred in params)
    # the resulting gradients will be stored in a list gparams
    gparams = []
    for param in classifier.params:
        gparam = T.grad(cost, param)
        gparams.append(gparam)

    # specify how to update the parameters of the model as a list of
    # (variable, update expression) pairs
    updates = []
    # given two list the zip A = [a1, a2, a3, a4] and B = [b1, b2, b3, b4] of
    # same length, zip generates a list C of same size, where each element
    # is a pair formed from the two lists :
    #    C = [(a1, b1), (a2, b2), (a3, b3), (a4, b4)]
    for param, gparam in zip(classifier.params, gparams):
        updates.append((param, param - learning_rate * gparam))

    # compiling a Theano function `train_model` that returns the cost, but
    # in the same time updates the parameter of the model based on the rules
    # defined in `updates`
    train_model = theano.function(inputs=[index], outputs=cost,
            updates=updates,
            givens={
                x: train_set_x[index * batch_size:(index + 1) * batch_size],
                y: train_set_y[index * batch_size:(index + 1) * batch_size]})

    ###############
    # TRAIN MODEL #
    ###############
    print '... training'

    # early-stopping parameters
    patience = 10000  # look as this many examples regardless
    patience_increase = 2  # wait this much longer when a new best is
                           # found
    improvement_threshold = 0.995  # a relative improvement of this much is
                                   # considered significant
    validation_frequency = min(n_train_batches, patience / 2)
                                  # go through this many
                                  # minibatche before checking the network
                                  # on the validation set; in this case we
                                  # check every epoch

    best_params = None
    best_validation_loss = numpy.inf
    best_iter = 0
    test_score = 0.
    start_time = time.clock()

    epoch = 0
    done_looping = False
```

```
    while (epoch < n_epochs) and (not done_looping):
        epoch = epoch + 1
        for minibatch_index in xrange(n_train_batches):

            minibatch_avg_cost = train_model(minibatch_index)
            # iteration number
            iter = (epoch - 1) * n_train_batches + minibatch_index

            if (iter + 1) % validation_frequency == 0:
                # compute zero-one loss on validation set
                validation_losses = [validate_model(i) for i
                                     in xrange(n_valid_batches)]
                this_validation_loss = numpy.mean(validation_losses)

                print('epoch %i, minibatch %i/%i, validation error %f %%' %
                      (epoch, minibatch_index + 1, n_train_batches,
                       this_validation_loss * 100.))

                # if we got the best validation score until now
                if this_validation_loss < best_validation_loss:
                    #improve patience if loss improvement is good enough
                    if this_validation_loss < best_validation_loss *  \
                           improvement_threshold:
                        patience = max(patience, iter * patience_increase)

                    best_validation_loss = this_validation_loss
                    best_iter = iter

                    # test it on the test set
                    test_losses = [test_model(i) for i
                                   in xrange(n_test_batches)]
                    test_score = numpy.mean(test_losses)

                    print(('     epoch %i, minibatch %i/%i, test error of '
                           'best model %f %%') %
                          (epoch, minibatch_index + 1, n_train_batches,
                           test_score * 100.))

            if patience <= iter:
                    done_looping = True
                    break

    end_time = time.clock()
    print(('Optimization complete. Best validation score of %f %% '
           'obtained at iteration %i, with test performance %f %%') %
          (best_validation_loss * 100., best_iter + 1, test_score * 100.))
    print >> sys.stderr, ('The code for file ' +
                          os.path.split(__file__)[1] +
                          ' ran for %.2fm' % ((end_time - start_time) / 60.))


if __name__ == '__main__':
    test_mlp()
```

The user can then run the code by calling :

```
python code/mlp.py
```

The output one should expect is of the form :

```
Optimization complete. Best validation score of 1.690000 % obtained at iteration 2070000, w
The code for file mlp.py ran for 97.34m
```

On an Intel(R) Core(TM) i7-2600K CPU @ 3.40GHz the code runs with approximately 10.3 epoch/minute and it took 828 epochs to reach a test error of 1.65%.

To put this into perspective, we refer the reader to the results section of this page.

5.4 Tips and Tricks for training MLPs

There are several hyper-parameters in the above code, which are not (and, generally speaking, cannot be) optimized by gradient descent. Strictly speaking, finding an optimal set of values for these hyper-parameters is not a feasible problem. First, we can't simply optimize each of them independently. Second, we cannot readily apply gradient techniques that we described previously (partly because some parameters are discrete values and others are real-valued). Third, the optimization problem is not convex and finding a (local) minimum would involve a non-trivial amount of work.

The good news is that over the last 25 years, researchers have devised various rules of thumb for choosing hyper-parameters in a neural network. A very good overview of these tricks can be found in Efficient BackProp by Yann LeCun, Leon Bottou, Genevieve Orr, and Klaus-Robert Mueller. In here, we summarize the same issues, with an emphasis on the parameters and techniques that we actually used in our code.

5.4.1 Nonlinearity

Two of the most common ones are the $sigmoid$ and the $tanh$ function. For reasons explained in Section 4.4, nonlinearities that are symmetric around the origin are preferred because they tend to produce zero-mean inputs to the next layer (which is a desirable property). Empirically, we have observed that the $tanh$ has better convergence properties.

5.4.2 Weight initialization

At initialization we want the weights to be small enough around the origin so that the activation function operates in its linear regime, where gradients are the largest. Other desirable properties, especially for deep networks, are to conserve variance of the activation as well as variance of back-propagated gradients from layer to layer. This allows information to flow well upward and downward in the network and reduces discrepancies between layers. Under some assumptions, a compromise between these two constraints leads to the following initialization: $uniform[-\frac{6}{\sqrt{fan_{in}+fan_{out}}}, \frac{6}{\sqrt{fan_{in}+fan_{out}}}]$ for tanh and $uniform[-4*\frac{6}{\sqrt{fan_{in}+fan_{out}}}, 4*\frac{6}{\sqrt{fan_{in}+fan_{out}}}]$ for sigmoid. Where fan_{in} is the number of inputs and fan_{out} the number of hidden units. For mathematical considerations please refer to [Xavier10].

5.4.3 Learning rate

There is a great deal of literature on choosing a good learning rate. The simplest solution is to simply have a constant rate. Rule of thumb: try several log-spaced values ($10^{-1}, 10^{-2}, \ldots$) and narrow the (logarithmic) grid search to the region where you obtain the lowest validation error.

Decreasing the learning rate over time is sometimes a good idea. One simple rule for doing that is $\frac{\mu_0}{1+d\times t}$ where μ_0 is the initial rate (chosen, perhaps, using the grid search technique explained above), d is a so-called "decrease constant" which controls the rate at which the learning rate decreases (typically, a smaller positive number, 10^{-3} and smaller) and t is the epoch/stage.

Section 4.7 details procedures for choosing a learning rate for each parameter (weight) in our network and for choosing them adaptively based on the error of the classifier.

5.4.4 Number of hidden units

This hyper-parameter is very much dataset-dependent. Vaguely speaking, the more complicated the input distribution is, the more capacity the network will require to model it, and so the larger the number of hidden units that will be needed (note that the number of weights in a layer, perhaps a more direct measure of capacity, is $D \times D_h$ (recall D is the number of inputs and D_h is the number of hidden units).

Unless we employ some regularization scheme (early stopping or L1/L2 penalties), a typical number of hidden units vs. generalization performance graph will be U-shaped.

5.4.5 Regularization parameter

Typical values to try for the L1/L2 regularization parameter λ are $10^{-2}, 10^{-3}, \ldots$. In the framework that we described so far, optimizing this parameter will not lead to significantly better solutions, but is worth exploring nonetheless.

CHAPTER

SIX

CONVOLUTIONAL NEURAL NETWORKS (LENET)

Note: This section assumes the reader has already read through *Classifying MNIST digits using Logistic Regression* and *Multilayer Perceptron*. Additionally, it uses the following new Theano functions and concepts: T.tanh, shared variables, basic arithmetic ops, T.grad, floatX, downsample , conv2d, dimshuffle. If you intend to run the code on GPU also read GPU.

To run this example on a GPU, you need a good GPU. First, it need at least 1G of GPU RAM and possibly more if your monitor is connected to the GPU.

Second, when the GPU is connected to the monitor, there is a limit of a few seconds for each GPU function call. This is needed as current GPU can't be used for the monitor while doing computation. If there wasn't this limit, the screen would freeze for too long and this look as if the computer froze. User don't like this. This example hit this limit with medium GPU. When the GPU isn't connected to a monitor, there is no time limit. You can lower the batch size to fix the time out problem.

Note: The code for this section is available for download here.

6.1 Motivation

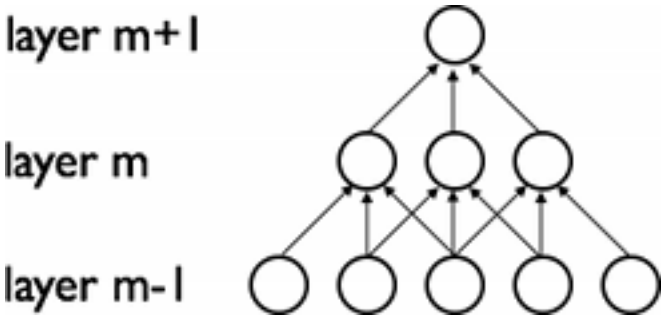
Convolutional Neural Networks (CNN) are variants of MLPs which are inspired from biology. From Hubel and Wiesel's early work on the cat's visual cortex [Hubel68], we know there exists a complex arrangement of cells within the visual cortex. These cells are sensitive to small sub-regions of the input space, called a **receptive field**, and are tiled in such a way as to cover the entire visual field. These filters are local in input space and are thus better suited to exploit the strong spatially local correlation present in natural images.

Additionally, two basic cell types have been identified: simple cells (S) and complex cells (C). Simple cells (S) respond maximally to specific edge-like stimulus patterns within their receptive field. Complex cells (C) have larger receptive fields and are locally invariant to the exact position of the stimulus.

The visual cortex being the most powerful "vision" system in existence, it seems natural to emulate its behavior. Many such neurally inspired models can be found in the litterature. To name a few: the NeoCognitron [Fukushima], HMAX [Serre07] and LeNet-5 [LeCun98], which will be the focus of this tutorial.

6.2 Sparse Connectivity

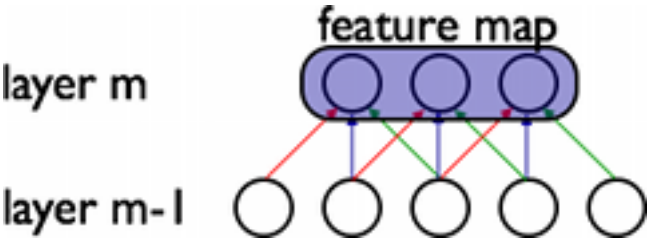
CNNs exploit spatially local correlation by enforcing a local connectivity pattern between neurons of adjacent layers. The input hidden units in the m-th layer are connected to a local subset of units in the (m-1)-th layer, which have spatially contiguous receptive fields. We can illustrate this graphically as follows:



Imagine that layer **m-1** is the input retina. In the above, units in layer **m** have receptive fields of width 3 with respect to the input retina and are thus only connected to 3 adjacent neurons in the layer below (the retina). Units in layer **m** have a similar connectivity with the layer below. We say that their receptive field with respect to the layer below is also 3, but their receptive field with respect to the input is larger (it is 5). The architecture thus confines the learnt "filters" (corresponding to the input producing the strongest response) to be a spatially local pattern (since each unit is unresponsive to variations outside of its receptive field with respect to the retina). As shown above, stacking many such layers leads to "filters" (not anymore linear) which become increasingly "global" however (i.e spanning a larger region of pixel space). For example, the unit in hidden layer **m+1** can encode a non-linear feature of width 5 (in terms of pixel space).

6.3 Shared Weights

In CNNs, each sparse filter h_i is additionally replicated across the entire visual field. These "replicated" units form a **feature map**, which share the same parametrization, i.e. the same weight vector and the same bias.



In the above figure, we show 3 hidden units belonging to the same feature map. Weights of the same color are shared, i.e. are constrained to be identical. Gradient descent can still be used to learn such shared parameters, and requires only a small change to the original algorithm. The gradient of a shared weight is simply the sum of the gradients of the parameters being shared.

Why are shared weights interesting ? Replicating units in this way allows for features to be detected regardless of their position in the visual field. Additionally, weight sharing offers a very efficient way to do this,

since it greatly reduces the number of free parameters to learn. By controlling model capacity, CNNs tend to achieve better generalization on vision problems.

6.4 Details and Notation

Conceptually, a feature map is obtained by convolving the input image with a linear filter, adding a bias term and then applying a non-linear function. If we denote the k-th feature map at a given layer as h^k, whose filters are determined by the weights W^k and bias b_k, then the feature map h^k is obtained as follows (for $tanh$ non-linearities):

$$h^k_{ij} = \tanh((W^k * x)_{ij} + b_k).$$

Note: Recall the following definition of convolution for a 1D signal. $o[n] = f[n] * g[n] = \sum_{u=-\infty}^{\infty} f[u]g[u-n] = \sum_{u=-\infty}^{\infty} f[n-u]g[u]$.

This can be extended to 2D as follows: $o[m,n] = f[m,n] * g[m,n] = \sum_{u=-\infty}^{\infty} \sum_{v=-\infty}^{\infty} f[u,v]g[u-m, v-n]$.

To form a richer representation of the data, hidden layers are composed of a set of multiple feature maps, $\{h^{(k)}, k = 0..K\}$. The weights W of this layer can be parametrized as a 4D tensor (destination feature map index, source feature map index, source vertical position index, source horizontal position index) and the biases b as a vector (one element per destination feature map index). We illustrate this graphically as follows:

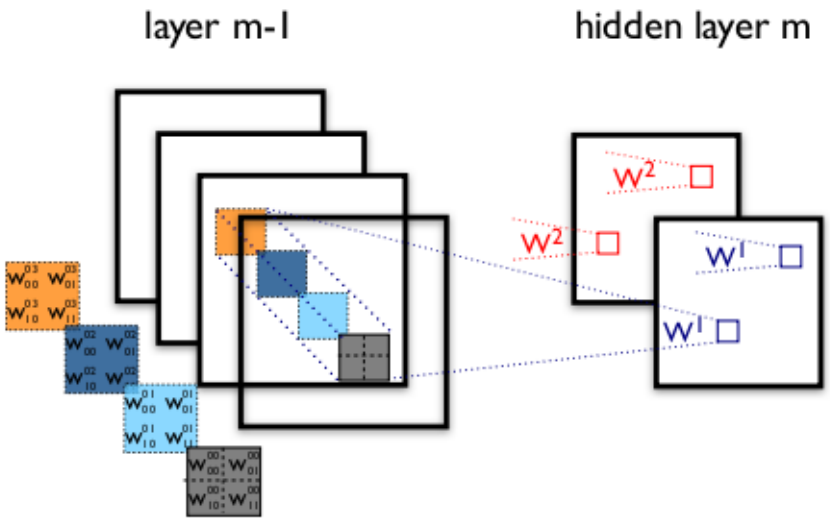


Figure 6.1: **Figure 1**: example of a convolutional layer

Here, we show two layers of a CNN, containing 4 feature maps at layer (m-1) and 2 feature maps (h^0 and h^1)

at layer m. Pixels (neuron outputs) in h^0 and h^1 (outlined as blue and red squares) are computed from pixels of layer (m-1) which fall within their 2x2 receptive field in the layer below (shown as colored rectangles). Notice how the receptive field spans all four input feature maps. The weights W^0 and W^1 of h^0 and h^1 are thus 3D weight tensors. The leading dimension indexes the input feature maps, while the other two refer to the pixel coordinates.

Putting it all together, W_{ij}^{kl} denotes the weight connecting each pixel of the k-th feature map at layer m, with the pixel at coordinates (i,j) of the l-th feature map of layer (m-1).

6.5 The ConvOp

ConvOp is the main workhorse for implementing a convolutional layer in Theano. It is meant to replicate the behaviour of scipy.signal.convolve2d. Conceptually, the ConvOp (once instantiated) takes two symbolic inputs:

- a 4D tensor corresponding to a mini-batch of input images. The shape of the tensor is as follows: [mini-batch size, number of input feature maps, image height, image width].
- a 4D tensor corresponding to the weight matrix W. The shape of the tensor is: [number of feature maps at layer m, number of feature maps at layer m-1, filter height, filter width]

Below is the Theano code for implementing a convolutional layer similar to the one of Figure 1. The input consists of 3 features maps (an RGB color image) of size 120x160. We use two convolutional filters with 9x9 receptive fields.

```
from theano.tensor.nnet import conv
rng = numpy.random.RandomState(23455)

# instantiate 4D tensor for input
input = T.tensor4(name='input')

# initialize shared variable for weights.
w_shp = (2, 3, 9, 9)
w_bound = numpy.sqrt(3 * 9 * 9)
W = theano.shared( numpy.asarray(
            rng.uniform(
                low=-1.0 / w_bound,
                high=1.0 / w_bound,
                size=w_shp),
            dtype=input.dtype), name ='W')

# initialize shared variable for bias (1D tensor) with random values
# IMPORTANT: biases are usually initialized to zero. However in this
# particular application, we simply apply the convolutional layer to
# an image without learning the parameters. We therefore initialize
# them to random values to "simulate" learning.
b_shp = (2,)
b = theano.shared(numpy.asarray(
            rng.uniform(low=-.5, high=.5, size=b_shp),
            dtype=input.dtype), name ='b')

# build symbolic expression that computes the convolution of input with filters in w
```

```
conv_out = conv.conv2d(input, W)

# build symbolic expression to add bias and apply activation function, i.e. produce neural
# A few words on ''dimshuffle'' :
#   ''dimshuffle'' is a powerful tool in reshaping a tensor;
#   what it allows you to do is to shuffle dimension around
#   but also to insert new ones along which the tensor will be
#   broadcastable;
#   dimshuffle('x', 2, 'x', 0, 1)
#   This will work on 3d tensors with no broadcastable
#   dimensions. The first dimension will be broadcastable,
#   then we will have the third dimension of the input tensor as
#   the second of the resulting tensor, etc. If the tensor has
#   shape (20, 30, 40), the resulting tensor will have dimensions
#   (1, 40, 1, 20, 30). (AxBxC tensor is mapped to 1xCx1xAxB tensor)
#   More examples:
#    dimshuffle('x') -> make a 0d (scalar) into a 1d vector
#    dimshuffle(0, 1) -> identity
#    dimshuffle(1, 0) -> inverts the first and second dimensions
#    dimshuffle('x', 0) -> make a row out of a 1d vector (N to 1xN)
#    dimshuffle(0, 'x') -> make a column out of a 1d vector (N to Nx1)
#    dimshuffle(2, 0, 1) -> AxBxC to CxAxB
#    dimshuffle(0, 'x', 1) -> AxB to Ax1xB
#    dimshuffle(1, 'x', 0) -> AxB to Bx1xA
output = T.nnet.sigmoid(conv_out + b.dimshuffle('x', 0, 'x', 'x'))

# create theano function to compute filtered images
f = theano.function([input], output)
```

Let's have a little bit of fun with this...

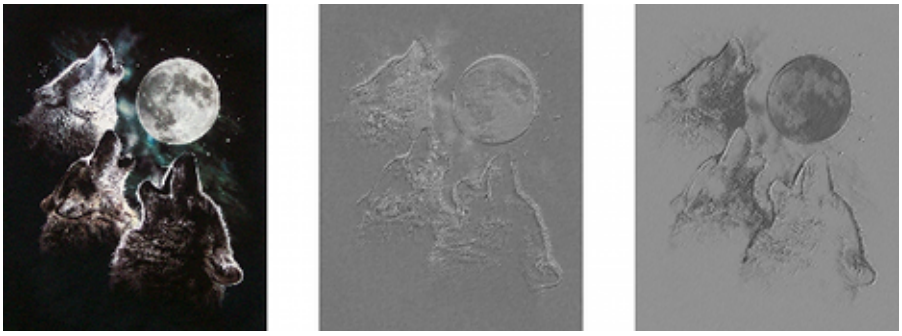
```
import pylab
from PIL import Image

# open random image of dimensions 639x516
img = Image.open(open('images/3wolfmoon.jpg'))
img = numpy.asarray(img, dtype='float64') / 256.

# put image in 4D tensor of shape (1, 3, height, width)
img_ = img.swapaxes(0, 2).swapaxes(1, 2).reshape(1, 3, 639, 516)
filtered_img = f(img_)

# plot original image and first and second components of output
pylab.subplot(1, 3, 1); pylab.axis('off'); pylab.imshow(img)
pylab.gray();
# recall that the convOp output (filtered image) is actually a "minibatch",
# of size 1 here, so we take index 0 in the first dimension:
pylab.subplot(1, 3, 2); pylab.axis('off'); pylab.imshow(filtered_img[0, 0, :, :])
pylab.subplot(1, 3, 3); pylab.axis('off'); pylab.imshow(filtered_img[0, 1, :, :])
pylab.show()
```

This should generate the following output.



Notice that a randomly initialized filter acts very much like an edge detector!

Also of note, remark that we use the same weight initialization formula as with the MLP. Weights are sampled randomly from a uniform distribution in the range [-1/fan-in, 1/fan-in], where fan-in is the number of inputs to a hidden unit. For MLPs, this was the number of units in the layer below. For CNNs however, we have to take into account the number of input feature maps and the size of the receptive fields.

6.6 MaxPooling

Another important concept of CNNs is that of max-pooling, which is a form of non-linear down-sampling. Max-pooling partitions the input image into a set of non-overlapping rectangles and, for each such sub-region, outputs the maximum value.

Max-pooling is useful in vision for two reasons: (1) it reduces the computational complexity for upper layers and (2) it provides a form of translation invariance. To understand the invariance argument, imagine cascading a max-pooling layer with a convolutional layer. There are 8 directions in which one can translate the input image by a single pixel. If max-pooling is done over a 2x2 region, 3 out of these 8 possible configurations will produce exactly the same output at the convolutional layer. For max-pooling over a 3x3 window, this jumps to 5/8.

Since it provides additional robustness to position, max-pooling is thus a "smart" way of reducing the dimensionality of intermediate representations.

Max-pooling is done in Theano by way of `theano.tensor.signal.downsample.max_pool_2d`. This function takes as input an N dimensional tensor (with N >= 2), a downscaling factor and performs max-pooling over the 2 trailing dimensions of the tensor.

An example is worth a thousand words:

```
from theano.tensor.signal import downsample

input = T.dtensor4('input')
maxpool_shape = (2, 2)
pool_out = downsample.max_pool_2d(input, maxpool_shape, ignore_border=True)
f = theano.function([input],pool_out)

invals = numpy.random.RandomState(1).rand(3, 2, 5, 5)
print 'With ignore_border set to True:'
print 'invals[0, 0, :, :] =\n', invals[0, 0, :, :]
print 'output[0, 0, :, :] =\n', f(invals)[0, 0, :, :]
```

```
pool_out = downsample.max_pool_2d(input, maxpool_shape, ignore_border=False)
f = theano.function([input],pool_out)
print 'With ignore_border set to False:'
print 'invals[1, 0, :, :] =\n ', invals[1, 0, :, :]
print 'output[1, 0, :, :] =\n ', f(invals)[1, 0, :, :]
```

This should generate the following output:

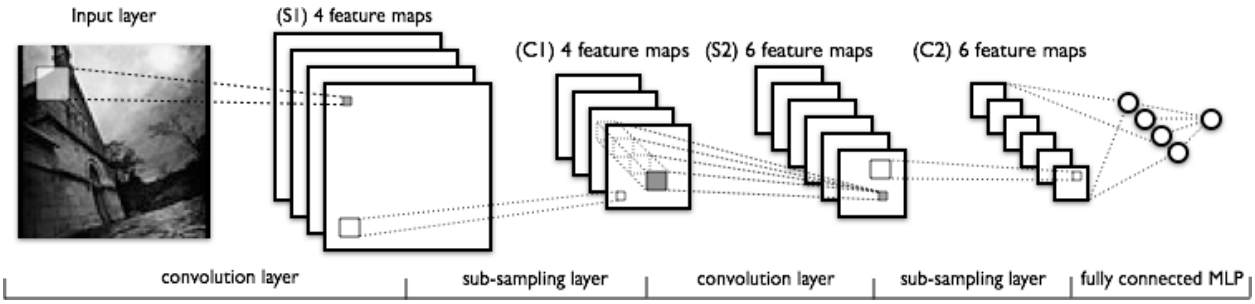
```
With ignore_border set to True:
    invals[0, 0, :, :] =
    [[  4.17022005e-01   7.20324493e-01   1.14374817e-04   3.02332573e-01 1.46755891e-01]
     [  9.23385948e-02   1.86260211e-01   3.45560727e-01   3.96767474e-01 5.38816734e-01]
     [  4.19194514e-01   6.85219500e-01   2.04452250e-01   8.78117436e-01 2.73875932e-02]
     [  6.70467510e-01   4.17304802e-01   5.58689828e-01   1.40386939e-01 1.98101489e-01]
     [  8.00744569e-01   9.68261576e-01   3.13424178e-01   6.92322616e-01 8.76389152e-01]]
    output[0, 0, :, :] =
    [[ 0.72032449  0.39676747]
     [ 0.6852195   0.87811744]]

With ignore_border set to False:
    invals[1, 0, :, :] =
    [[ 0.01936696  0.67883553  0.21162812  0.26554666  0.49157316]
     [ 0.05336255  0.57411761  0.14672857  0.58930554  0.69975836]
     [ 0.10233443  0.41405599  0.69440016  0.41417927  0.04995346]
     [ 0.53589641  0.66379465  0.51488911  0.94459476  0.58655504]
     [ 0.90340192  0.1374747   0.13927635  0.80739129  0.39767684]]
    output[1, 0, :, :] =
    [[ 0.67883553  0.58930554  0.69975836]
     [ 0.66379465  0.94459476  0.58655504]
     [ 0.90340192  0.80739129  0.39767684]]
```

Note that contrary to most Theano code, the `max_pool_2d` operation is a little *special*. It requires the downscaling factor `ds` (tuple of length 2 containing downscaling factors for image width and height) to be known at graph build time. This may change in the near future.

6.7 The Full Model: LeNet

Sparse, convolutional layers and max-pooling are at the heart of the LeNet family of models. While the exact details of the model will vary greatly, the figure below shows a graphical depiction of a LeNet model.



The lower-layers are composed to alternating convolution and max-pooling layers. The upper-layers how-

ever are fully-connected and correspond to a traditional MLP (hidden layer + logistic regression). The input to the first fully-connected layer is the set of all features maps at the layer below.

From an implementation point of view, this means lower-layers operate on 4D tensors. These are then flattened to a 2D matrix of rasterized feature maps, to be compatible with our previous MLP implementation.

6.8 Putting it All Together

We now have all we need to implement a LeNet model in Theano. We start with the LeNetConvPoolLayer class, which implements a {convolution + max-pooling} layer.

```
class LeNetConvPoolLayer(object):

    def __init__(self, rng, input, filter_shape, image_shape, poolsize=(2, 2)):
        """
        Allocate a LeNetConvPoolLayer with shared variable internal parameters.

        :type rng: numpy.random.RandomState
        :param rng: a random number generator used to initialize weights

        :type input: theano.tensor.dtensor4
        :param input: symbolic image tensor, of shape image_shape

        :type filter_shape: tuple or list of length 4
        :param filter_shape: (number of filters, num input feature maps,
                              filter height,filter width)

        :type image_shape: tuple or list of length 4
        :param image_shape: (batch size, num input feature maps,
                             image height, image width)

        :type poolsize: tuple or list of length 2
        :param poolsize: the downsampling (pooling) factor (#rows,#cols)
        """
        assert image_shape[1] == filter_shape[1]
        self.input = input

        # initialize weight values: the fan-in of each hidden neuron is
        # restricted by the size of the receptive fields.
        fan_in =  numpy.prod(filter_shape[1:])
        W_values = numpy.asarray(rng.uniform(
              low=-numpy.sqrt(3./fan_in),
              high=numpy.sqrt(3./fan_in),
              size=filter_shape), dtype=theano.config.floatX)
        self.W = theano.shared(value=W_values, name='W')

        # the bias is a 1D tensor -- one bias per output feature map
        b_values = numpy.zeros((filter_shape[0],), dtype=theano.config.floatX)
        self.b = theano.shared(value=b_values, name='b')

        # convolve input feature maps with filters
        conv_out = conv.conv2d(input, self.W,
```

```
                filter_shape=filter_shape, image_shape=image_shape)

        # downsample each feature map individually, using maxpooling
        pooled_out = downsample.max_pool_2d(conv_out, poolsize, ignore_border=True)

        # add the bias term. Since the bias is a vector (1D array), we first
        # reshape it to a tensor of shape (1, n_filters, 1, 1). Each bias will thus
        # be broadcasted across mini-batches and feature map width & height
        self.output = T.tanh(pooled_out + self.b.dimshuffle('x', 0, 'x', 'x'))

        # store parameters of this layer
        self.params = [self.W, self.b]
```

Notice that when initializing the weight values, the fan-in is determined by the size of the receptive fields and the number of input feature maps.

Finally, using the LogisticRegression class defined in *Classifying MNIST digits using Logistic Regression* and the HiddenLayer class defined in *Multilayer Perceptron* , we can instantiate the network as follows.

```
learning_rate = 0.1
rng = numpy.random.RandomState(23455)

ishape = (28, 28)  # this is the size of MNIST images
batch_size = 20  # sized of the minibatch

# allocate symbolic variables for the data
x = theano.floatX.xmatrix(theano.config.floatX)  # rasterized images
y = T.lvector()  # the labels are presented as 1D vector of [long int] labels

##############################
# BEGIN BUILDING ACTUAL MODE
##############################

# Reshape matrix of rasterized images of shape (batch_size,28*28)
# to a 4D tensor, compatible with our LeNetConvPoolLayer
layer0_input = x.reshape((batch_size,1,28,28))

# Construct the first convolutional pooling layer:
# filtering reduces the image size to (28-5+1,28-5+1)=(24,24)
# maxpooling reduces this further to (24/2,24/2) = (12,12)
# 4D output tensor is thus of shape (20,20,12,12)
layer0 = LeNetConvPoolLayer(rng, input=layer0_input,
        image_shape=(batch_size, 1, 28, 28),
        filter_shape=(20, 1, 5, 5), poolsize=(2, 2))

# Construct the second convolutional pooling layer
# filtering reduces the image size to (12 - 5 + 1, 12 - 5 + 1)=(8, 8)
# maxpooling reduces this further to (8/2,8/2) = (4, 4)
# 4D output tensor is thus of shape (20,50,4,4)
layer1 = LeNetConvPoolLayer(rng, input=layer0.output,
        image_shape=(batch_size, 20, 12, 12),
        filter_shape=(50, 20, 5, 5), poolsize=(2, 2))
```

```
# the SigmoidalLayer being fully-connected, it operates on 2D matrices of
# shape (batch_size,num_pixels) (i.e matrix of rasterized images).
# This will generate a matrix of shape (20, 32 * 4 * 4) = (20, 512)
layer2_input = layer1.output.flatten(2)

# construct a fully-connected sigmoidal layer
layer2 = HiddenLayer(rng, input=layer2_input,
                     n_in=50 * 4 * 4, n_out=500,
                     activation=T.tanh    )

# classify the values of the fully-connected sigmoidal layer
layer3 = LogisticRegression(input=layer2.output, n_in=500, n_out=10)


# the cost we minimize during training is the NLL of the model
cost = layer3.negative_log_likelihood(y)

# create a function to compute the mistakes that are made by the model
test_model = theano.function([x, y], layer3.errors(y))

# create a list of all model parameters to be fit by gradient descent
params = layer3.params + layer2.params + layer1.params + layer0.params

# create a list of gradients for all model parameters
grads = T.grad(cost, params)

# train_model is a function that updates the model parameters by SGD
# Since this model has many parameters, it would be tedious to manually
# create an update rule for each model parameter. We thus create the updates
# dictionary by automatically looping over all (params[i],grads[i])  pairs.
updates = []
for param_i, grad_i in zip(params, grads):
    updates.append((param_i, param_i - learning_rate * grad_i))
train_model = theano.function([index], cost, updates = updates,
        givens={
            x: train_set_x[index * batch_size: (index + 1) * batch_size],
            y: train_set_y[index * batch_size: (index + 1) * batch_size]})
```

We leave out the code, which performs the actual training and early-stopping, since it is exactly the same as with an MLP. The interested reader can nevertheless access the code in the 'code' folder of DeepLearning-Tutorials.

6.9 Running the Code

The user can then run the code by calling:

```
python code/convolutional_mlp.py
```

The following output was obtained with the default parameters on a Core i7-2600K CPU clocked at 3.40GHz and using flags 'floatX=float32':

```
Optimization complete.
Best validation score of 0.910000 % obtained at iteration 17800,with test
performance 0.920000 %
The code for file convolutional_mlp.py ran for 380.28m
```

Using a GeForce GTX 285, we obtained the following:

```
Optimization complete.
Best validation score of 0.910000 % obtained at iteration 15500,with test
performance 0.930000 %
The code for file convolutional_mlp.py ran for 46.76m
```

And similarly on a GeForce GTX 480:

```
Optimization complete.
Best validation score of 0.910000 % obtained at iteration 16400,with test
performance 0.930000 %
The code for file convolutional_mlp.py ran for 32.52m
```

Note that the discrepancies in validation and test error (as well as iteration count) are due to different implementations of the rounding mechanism in hardware. They can be safely ignored.

6.10 Tips and Tricks

6.10.1 Choosing Hyperparameters

CNNs are especially tricky to train, as they add even more hyper-parameters than a standard MLP. While the usual rules of thumb for learning rates and regularization constants still apply, the following should be kept in mind when optimizing CNNs.

Number of filters

When choosing the number of filters per layer, keep in mind that computing the activations of a single convolutional filter is much more expensive than with traditional MLPs !

Assume layer $(l-1)$ contains K^{l-1} feature maps and $M \times N$ pixel positions (i.e., number of positions times number of feature maps), and there are K^l filters at layer l of shape $m \times n$. Then computing a feature map (applying an $m \times n$ filter at all $(M-m) \times (N-n)$ pixel positions where the filter can be applied) costs $(M-m) \times (N-n) \times m \times n \times K^{l-1}$. The total cost is K^l times that. Things may be more complicated if not all features at one level are connected to all features at the previous one.

For a standard MLP, the cost would only be $K^l \times K^{l-1}$ where there are K^l different neurons at level l. As such, the number of filters used in CNNs is typically much smaller than the number of hidden units in MLPs and depends on the size of the feature maps (itself a function of input image size and filter shapes).

Since feature map size decreases with depth, layers near the input layer will tend to have fewer filters while layers higher up can have much more. In fact, to equalize computation at each layer, the product of the number of features and the number of pixel positions is typically picked to be roughly constant across layers. To preserve the information about the input would require keeping the total number of activations

(number of feature maps times number of pixel positions) to be non-decreasing from one layer to the next (of course we could hope to get away with less when we are doing supervised learning). The number of feature maps directly controls capacity and so that depends on the number of available examples and the complexity of the task.

Filter Shape

Common filter shapes found in the litterature vary greatly, usually based on the dataset. Best results on MNIST-sized images (28x28) are usually in the 5x5 range on the first layer, while natural image datasets (often with hundreds of pixels in each dimension) tend to use larger first-layer filters of shape 12x12 or 15x15.

The trick is thus to find the right level of "granularity" (i.e. filter shapes) in order to create abstractions at the proper scale, given a particular dataset.

Max Pooling Shape

Typical values are 2x2 or no max-pooling. Very large input images may warrant 4x4 pooling in the lower-layers. Keep in mind however, that this will reduce the dimension of the signal by a factor of 16, and may result in throwing away too much information.

Tips

If you want to try this model on a new dataset, here are a few tips that can help you get better results:

- Whitening the data (e.g. with PCA)
- Decay the learning rate in each epoch

CHAPTER

SEVEN

DENOISING AUTOENCODERS (DA)

Note: This section assumes the reader has already read through *Classifying MNIST digits using Logistic Regression* and *Multilayer Perceptron*. Additionally it uses the following Theano functions and concepts : T.tanh, shared variables, basic arithmetic ops, T.grad, Random numbers, floatX. If you intend to run the code on GPU also read GPU.

Note: The code for this section is available for download here.

The Denoising Autoencoder (dA) is an extension of a classical autoencoder and it was introduced as a building block for deep networks in [Vincent08]. We will start the tutorial with a short discussion on *Autoencoders*.

7.1 Autoencoders

See section 4.6 of [Bengio09] for an overview of auto-encoders. An autoencoder takes an input $\mathbf{x} \in [0,1]^d$ and first maps it (with an *encoder*) to a hidden representation $\mathbf{y} \in [0,1]^{d'}$ through a deterministic mapping, e.g.:

$$\mathbf{y} = s(\mathbf{W}\mathbf{x} + \mathbf{b})$$

Where s is a non-linearity such as the sigmoid. The latent representation $\mathbf{y}$, or **code** is then mapped back (with a *decoder*) into a **reconstruction** $\mathbf{z}$ of same shape as $\mathbf{x}$ through a similar transformation, e.g.:

$$\mathbf{z} = s(\mathbf{W}'\mathbf{y} + \mathbf{b}')$$

where ' does not indicate transpose, and $\mathbf{z}$ should be seen as a prediction of $\mathbf{x}$, given the code $\mathbf{y}$. The weight matrix $\mathbf{W}'$ of the reverse mapping may be optionally constrained by $\mathbf{W}' = \mathbf{W}^T$, which is an instance of *tied weights*. The parameters of this model (namely $\mathbf{W}$, $\mathbf{b}$, $\mathbf{b}'$ and, if one doesn't use tied weights, also $\mathbf{W}'$) are optimized such that the average reconstruction error is minimized. The reconstruction error can be measured in many ways, depending on the appropriate distributional assumptions on the input given the code, e.g., using the traditional *squared error* $L(\mathbf{x}, \mathbf{z}) = ||\mathbf{x} - \mathbf{z}||^2$, or if the input is interpreted as either bit vectors or vectors of bit probabilities by the reconstruction *cross-entropy* defined as :

$$L_H(\mathbf{x}, \mathbf{z}) = -\sum_{k=1}^{d} [\mathbf{x}_k \log \mathbf{z}_k + (1 - \mathbf{x}_k) \log(1 - \mathbf{z}_k)]$$

The hope is that the code $\mathbf{y}$ is a distributed representation that captures the coordinates along the main factors of variation in the data (similarly to how the projection on principal components captures the main factors of variation in the data). Because $\mathbf{y}$ is viewed as a lossy compression of $\mathbf{x}$, it cannot be a good compression (with small loss) for all $\mathbf{x}$, so learning drives it to be one that is a good compression in particular for training examples, and hopefully for others as well, but not for arbitrary inputs. That is the sense in which an auto-encoder generalizes: it gives low reconstruction error to test examples from the same distribution as the training examples, but generally high reconstruction error to uniformly chosen configurations of the input vector.

If there is one linear hidden layer (the code) and the mean squared error criterion is used to train the network, then the k hidden units learn to project the input in the span of the first k principal components of the data. If the hidden layer is non-linear, the auto-encoder behaves differently from PCA, with the ability to capture multi-modal aspects of the input distribution. The departure from PCA becomes even more important when we consider *stacking multiple encoders* (and their corresponding decoders) when building a deep auto-encoder [Hinton06].

We want to implement an auto-encoder using Theano, in the form of a class, that could be afterwards used in constructing a stacked autoencoder. The first step is to create shared variables for the parameters of the autoencoder ($\mathbf{W}$, $\mathbf{b}$ and $\mathbf{b}'$, since we are using tied weights in this tutorial):

```
class AutoEncoder(object):

  def __init__(self, numpy_rng, input=None, n_visible=784, n_hidden=500,
               W=None, bhid=None, bvis=None):
    """

    :type numpy_rng: numpy.random.RandomState
    :param numpy_rng: number random generator used to generate weights


    :type input: theano.tensor.TensorType
    :paran input: a symbolic description of the input or None for standalone
                  dA

    :type n_visible: int
    :param n_visible: number of visible units

    :type n_hidden: int
    :param n_hidden:  number of hidden units

    :type W: theano.tensor.TensorType
    :param W: Theano variable pointing to a set of weights that should be
              shared belong the dA and another architecture; if dA should
              be standalone set this to None

    :type bhid: theano.tensor.TensorType
    :param bhid: Theano variable pointing to a set of biases values (for
                 hidden units) that should be shared belong dA and another
                 architecture; if dA should be standalone set this to None

    :type bvis: theano.tensor.TensorType
    :param bvis: Theano variable pointing to a set of biases values (for
                 visible units) that should be shared belong dA and another
```

```
                architecture; if dA should be standalone set this to None

    """
    self.n_visible = n_visible
    self.n_hidden = n_hidden


    # note : W' was written as `W_prime` and b' as `b_prime`
    if not W:
        # 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)
        W = theano.shared(value=initial_W, name='W')

    if not bvis:
        bvis = theano.shared(value=numpy.zeros(n_visible,
                                       dtype=theano.config.floatX), name='bvis')

    if not bhid:
        bhid = theano.shared(value=numpy.zeros(n_hidden,
                                            dtype=theano.config.floatX), name='bhid')


    self.W = W
    # b corresponds to the bias of the hidden
    self.b = bhid
    # b_prime corresponds to the bias of the visible
    self.b_prime = bvis
    # tied weights, therefore W_prime is W transpose
    self.W_prime = self.W.T
    # if no input is given, generate a variable representing the input
    if input == None:
        # we use a matrix because we expect a minibatch of several examples,
        # each example being a row
        self.x = T.dmatrix(name='input')
    else:
        self.x = input

    self.params = [self.W, self.b, self.b_prime]
```

Note that we pass the symbolic `input` to the autoencoder as a parameter. This is such that later we can concatenate layers of autoencoders to form a deep network: the symbolic output (the $\mathbf{y}$ above) of the k-th layer will be the symbolic input of the (k+1)-th.

Now we can express the computation of the latent representation and of the reconstructed signal:

```
def get_hidden_values(self, input):
    """ Computes the values of the hidden layer """
    return T.nnet.sigmoid(T.dot(input, self.W) + self.b)

def get_reconstructed_input(self, hidden):
    """ Computes the reconstructed input given the values of the hidden layer """
    return  T.nnet.sigmoid(T.dot(hidden, self.W_prime) + self.b_prime)
```

And using these function we can compute the cost and the updates of one stochastic gradient descent step :

```
def get_cost_updates(self, learning_rate):
    """ This function computes the cost and the updates for one trainng
    step """

    y = self.get_hidden_values(self.x)
    z = self.get_reconstructed_input(y)
    # note : we sum over the size of a datapoint; if we are using minibatches,
    #        L will  be a vector, with one entry per example in minibatch
    L = -T.sum(self.x * T.log(z) + (1 - self.x) * T.log(1 - z), axis=1)
    # note : L is now a vector, where each element is the cross-entropy cost
    #        of the reconstruction of the corresponding example of the
    #        minibatch. We need to compute the average of all these to get
    #        the cost of the minibatch
    cost = T.mean(L)

    # compute the gradients of the cost of the `dA` with respect
    # to its parameters
    gparams = T.grad(cost, self.params)
    # generate the list of updates
    updates = []
    for param, gparam in zip(self.params, gparams):
        updates.append((param, param - learning_rate * gparam))

    return (cost, updates)
```

We can now define a function that applied iteratively will update the parameters `W`, `b` and `b_prime` such that the reconstruction cost is approximately minimized.

```
autoencoder = AutoEncoder(numpy_rng=numpy.random.RandomState(1234), n_visible=784, n_hidde
cost, updates = autoencoder.get_cost_updates(learning_rate=0.1)
train = theano.function([x], cost, updates=updates)
```

One serious potential issue with auto-encoders is that if there is no other constraint besides minimizing the reconstruction error, then an auto-encoder with n inputs and an encoding of dimension at least n could potentially just learn the identity function, for which many encodings would be useless (e.g., just copying the input), i.e., the autoencoder would not differentiate test examples (from the training distribution) from other input configurations. Surprisingly, experiments reported in [Bengio07] nonetheless suggest that in practice, when trained with stochastic gradient descent, non-linear auto-encoders with more hidden units than inputs (called overcomplete) yield useful representations (in the sense of classification error measured on a network taking this representation in input). A simple explanation is based on the observation that stochastic gradient descent with early stopping is similar to an L2 regularization of the parameters. To achieve perfect reconstruction of continuous inputs, a one-hidden layer auto-encoder with non-linear hidden

units (exactly like in the above code) needs very small weights in the first (encoding) layer (to bring the non-linearity of the hidden units in their linear regime) and very large weights in the second (decoding) layer. With binary inputs, very large weights are also needed to completely minimize the reconstruction error. Since the implicit or explicit regularization makes it difficult to reach large-weight solutions, the optimization algorithm finds encodings which only work well for examples similar to those in the training set, which is what we want. It means that the representation is exploiting statistical regularities present in the training set, rather than learning to replicate the identity function.

There are different ways that an auto-encoder with more hidden units than inputs could be prevented from learning the identity, and still capture something useful about the input in its hidden representation. One is the addition of sparsity (forcing many of the hidden units to be zero or near-zero), and it has been exploited very successfully by many [Ranzato07] [Lee08]. Another is to add randomness in the transformation from input to reconstruction. This is exploited in Restricted Boltzmann Machines (discussed later in *Restricted Boltzmann Machines (RBM)*), as well as in Denoising Auto-Encoders, discussed below.

7.2 Denoising Autoencoders

The idea behind denoising autoencoders is simple. In order to force the hidden layer to discover more robust features and prevent it from simply learning the identity, we train the autoencoder to *reconstruct the input from a corrupted version of it*.

The denoising auto-encoder is a stochastic version of the auto-encoder. Intuitively, a denoising auto-encoder does two things: try to encode the input (preserve the information about the input), and try to undo the effect of a corruption process stochastically applied to the input of the auto-encoder. The latter can only be done by capturing the statistical dependencies between the inputs. The denoising auto-encoder can be understood from different perspectives (the manifold learning perspective, stochastic operator perspective, bottom-up – information theoretic perspective, top-down – generative model perspective), all of which are explained in [Vincent08]. See also section 7.2 of [Bengio09] for an overview of auto-encoders.

In [Vincent08], the stochastic corruption process consists in randomly setting some of the inputs (as many as half of them) to zero. Hence the denoising auto-encoder is trying to *predict the corrupted (i.e. missing) values from the uncorrupted (i.e., non-missing) values*, for randomly selected subsets of missing patterns. Note how being able to predict any subset of variables from the rest is a sufficient condition for completely capturing the joint distribution between a set of variables (this is how Gibbs sampling works).

To convert the autoencoder class into a denoising autoencoder class, all we need to do is to add a stochastic corruption step operating on the input. The input can be corrupted in many ways, but in this tutorial we will stick to the original corruption mechanism of randomly masking entries of the input by making them zero. The code below does just that :

```
from theano.tensor.shared_randomstreams import RandomStreams

def get_corrupted_input(self, input, corruption_level):
      """ This function keeps ``1-corruption_level`` entries of the inputs the same
      and zero-out randomly selected subset of size ``coruption_level``
      Note : first argument of theano.rng.binomial is the shape(size) of
             random numbers that it should produce
             second argument is the number of trials
             third argument is the probability of success of any trial
```

```
            this will produce an array of 0s and 1s where 1 has a probability of
            1 - ''corruption_level'' and 0 with ''corruption_level''
        """
        return  self.theano_rng.binomial(size=input.shape, n=1, p=1 - corruption_level) * inp
```

In the stacked autoencoder class (*Stacked Autoencoders*) the weights of the `dA` class have to be shared with those of an corresponding sigmoid layer. For this reason, the constructor of the `dA` also gets Theano variables pointing to the shared parameters. If those parameters are left to `None`, new ones will be constructed.

The final denoising autoencoder class becomes :

```
class dA(object):
    """Denoising Auto-Encoder class (dA)

    A denoising autoencoders tries to reconstruct the input from a corrupted
    version of it by projecting it first in a latent space and reprojecting
    it afterwards back in the input space. Please refer to Vincent et al.,2008
    for more details. If x is the input then equation (1) computes a partially
    destroyed version of x by means of a stochastic mapping q_D. Equation (2)
    computes the projection of the input into the latent space. Equation (3)
    computes the reconstruction of the input, while equation (4) computes the
    reconstruction error.

    .. math::

        \tilde{x} ~ q_D(\tilde{x}|x)                                    (1)

        y = s(W \tilde{x} + b)                                          (2)

        x = s(W' y  + b')                                               (3)

        L(x,z) = -sum_{k=1}^d [x_k \log z_k + (1-x_k) \log( 1-z_k)]     (4)

    """

    def __init__(self, numpy_rng, theano_rng=None, input=None, n_visible=784, n_hidden=500,
                 W=None, bhid=None, bvis=None):
        """
        Initialize the dA class by specifying the number of visible units (the
        dimension d of the input ), the number of hidden units ( the dimension
        d' of the latent or hidden space ) and the corruption level. The
        constructor also receives symbolic variables for the input, weights and
        bias. Such a symbolic variables are useful when, for example the input is
        the result of some computations, or when weights are shared between the
        dA and an MLP layer. When dealing with SdAs this always happens,
        the dA on layer 2 gets as input the output of the dA on layer 1,
        and the weights of the dA are used in the second stage of training
        to construct an MLP.

        :type numpy_rng: numpy.random.RandomState
        :param numpy_rng: number random generator used to generate weights

        :type theano_rng: theano.tensor.shared_randomstreams.RandomStreams
```

```
        :param theano_rng: Theano random generator; if None is given one is generated
                    based on a seed drawn from 'rng'

        :type input: theano.tensor.TensorType
        :paran input: a symbolic description of the input or None for standalone
                     dA

        :type n_visible: int
        :param n_visible: number of visible units

        :type n_hidden: int
        :param n_hidden:  number of hidden units

        :type W: theano.tensor.TensorType
        :param W: Theano variable pointing to a set of weights that should be
                  shared belong the dA and another architecture; if dA should
                  be standalone set this to None

        :type bhid: theano.tensor.TensorType
        :param bhid: Theano variable pointing to a set of biases values (for
                     hidden units) that should be shared belong dA and another
                     architecture; if dA should be standalone set this to None

        :type bvis: theano.tensor.TensorType
        :param bvis: Theano variable pointing to a set of biases values (for
                     visible units) that should be shared belong dA and another
                     architecture; if dA should be standalone set this to None


        """
        self.n_visible = n_visible
        self.n_hidden = n_hidden

        # create a Theano random generator that gives symbolic random values
        if not theano_rng :
            theano_rng = RandomStreams(rng.randint(2 ** 30))

        # note : W' was written as 'W_prime' and b' as 'b_prime'
        if not W:
            # 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)
            W = theano.shared(value=initial_W, name='W')

        if not bvis:
            bvis = theano.shared(value = numpy.zeros(n_visible,
                                       dtype=theano.config.floatX), name='bvis')
```

```
        if not bhid:
            bhid = theano.shared(value=numpy.zeros(n_hidden,
                                                   dtype=theano.config.floatX), name='bhid')

        self.W = W
        # b corresponds to the bias of the hidden
        self.b = bhid
        # b_prime corresponds to the bias of the visible
        self.b_prime = bvis
        # tied weights, therefore W_prime is W transpose
        self.W_prime = self.W.T
        self.theano_rng = theano_rng
        # if no input is given, generate a variable representing the input
        if input == None:
            # we use a matrix because we expect a minibatch of several examples,
            # each example being a row
            self.x = T.dmatrix(name='input')
        else:
            self.x = input

        self.params = [self.W, self.b, self.b_prime]

    def get_corrupted_input(self, input, corruption_level):
        """ This function keeps ``1-corruption_level`` entries of the inputs the same
        and zero-out randomly selected subset of size ``coruption_level``
        Note : first argument of theano.rng.binomial is the shape(size) of
               random numbers that it should produce
               second argument is the number of trials
               third argument is the probability of success of any trial

                this will produce an array of 0s and 1s where 1 has a probability of
                1 - ``corruption_level`` and 0 with ``corruption_level``
        """
        return  self.theano_rng.binomial(size=input.shape, n=1, p=1 - corruption_level) * in


    def get_hidden_values(self, input):
        """ Computes the values of the hidden layer """
        return T.nnet.sigmoid(T.dot(input, self.W) + self.b)

    def get_reconstructed_input(self, hidden ):
        """ Computes the reconstructed input given the values of the hidden layer """
        return  T.nnet.sigmoid(T.dot(hidden, self.W_prime) + self.b_prime)

    def get_cost_updates(self, corruption_level, learning_rate):
        """ This function computes the cost and the updates for one trainng
        step of the dA """

        tilde_x = self.get_corrupted_input(self.x, corruption_level)
        y = self.get_hidden_values( tilde_x)
        z = self.get_reconstructed_input(y)
        # note : we sum over the size of a datapoint; if we are using minibatches,
        #        L will  be a vector, with one entry per example in minibatch
```

```
        L = -T.sum(self.x * T.log(z) + (1 - self.x) * T.log(1 - z), axis=1 )
        # note : L is now a vector, where each element is the cross-entropy cost
        #        of the reconstruction of the corresponding example of the
        #        minibatch. We need to compute the average of all these to get
        #        the cost of the minibatch
        cost = T.mean(L)

        # compute the gradients of the cost of the `dA` with respect
        # to its parameters
        gparams = T.grad(cost, self.params)
        # generate the list of updates
        updates = []
        for param, gparam in zip(self.params, gparams):
            updates.append((param, param - learning_rate * gparam))

        return (cost, updates)
```

7.3 Putting it All Together

It is easy now to construct an instance of our `dA` class and train it.

```
# 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

######################
# BUILDING THE MODEL #
######################

rng = numpy.random.RandomState(123)
theano_rng = RandomStreams(rng.randint(2 ** 30))

da = dA(numpy_rng=rng, theano_rng=theano_rng, input=x,
        n_visible=28 * 28, n_hidden=500)

cost, updates = da.get_cost_updates(corruption_level=0.2,
                            learning_rate=learning_rate)


train_da = theano.function([index], cost, updates=updates,
     givens = {x: train_set_x[index * batch_size: (index + 1) * batch_size]})

start_time = time.clock()

############
# TRAINING #
############

# go through training epochs
for epoch in xrange(training_epochs):
    # go through trainng set
```

```
    c = []
    for batch_index in xrange(n_train_batches):
        c.append(train_da(batch_index))

    print 'Training epoch %d, cost ' % epoch, numpy.mean(c)

end_time = time.clock

training_time = (end_time - start_time)

print ('Training took %f minutes' % (pretraining_time / 60.))
```

In order to get a feeling of what the network learned we are going to plot the filters (defined by the weight matrix). Bare in mind however, that this does not provide the entire story, since we neglect the biases and plot the weights up to a multiplicative constant (weights are converted to values between 0 and 1).

To plot our filters we will need the help of `tile_raster_images` (see *Plotting Samples and Filters*) so we urge the reader to familiarize himself with it. Also using the help of PIL library, the following lines of code will save the filters as an image :

```
image = PIL.Image.fromarray(tile_raster_images(X=da.W.get_value(borrow=True).T,
             img_shape=(28, 28), tile_shape=(10, 10),
             tile_spacing=(1, 1)))
image.save('filters_corruption_30.png')
```

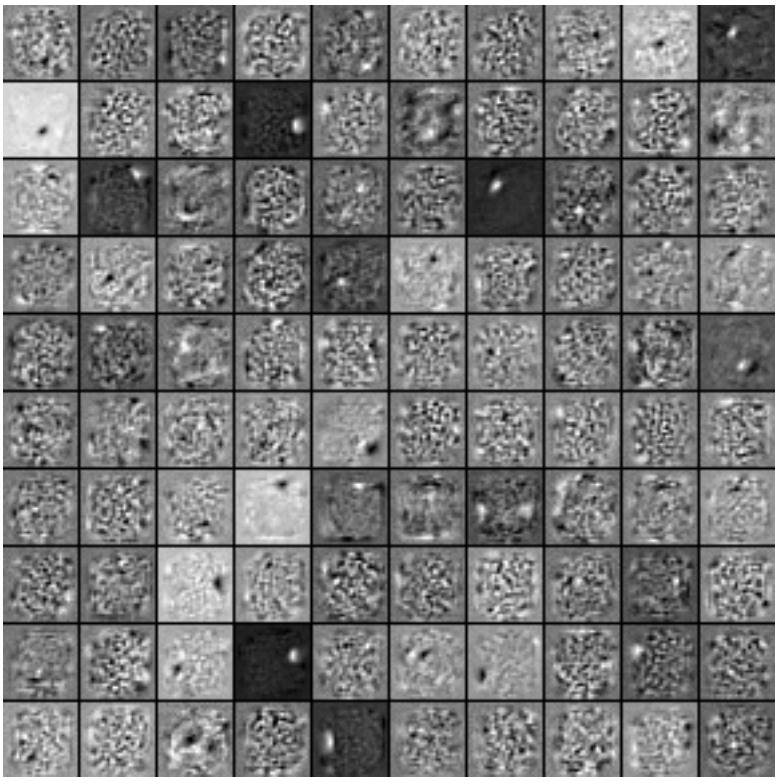
7.4 Running the Code

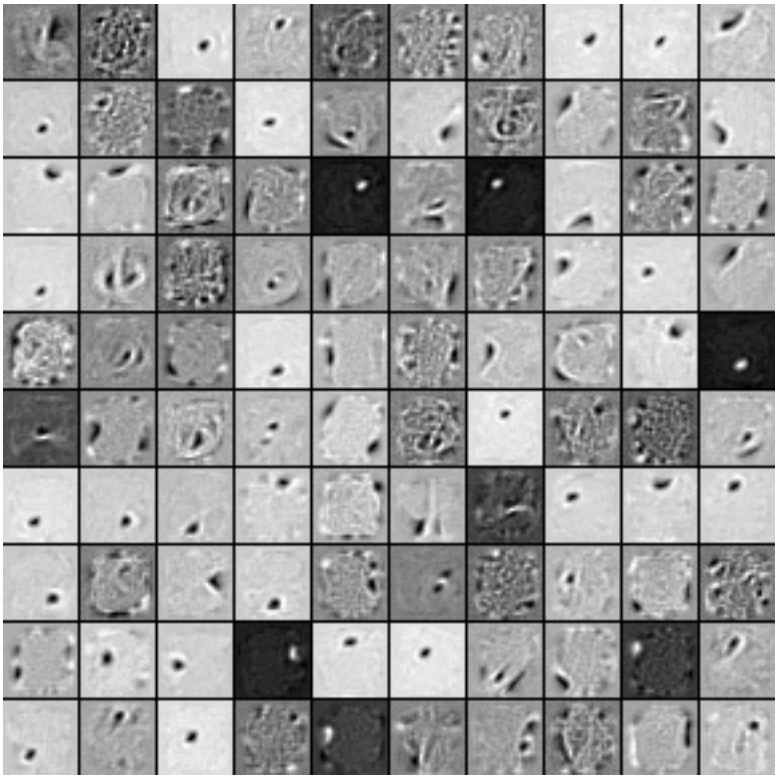
To run the code :

```
python dA.py
```

The resulted filters when we do not use any noise are :

The filters for 30 percent noise :





CHAPTER

EIGHT

STACKED DENOISING AUTOENCODERS (SDA)

Note: This section assumes the reader has already read through *Classifying MNIST digits using Logistic Regression* and *Multilayer Perceptron*. Additionally it uses the following Theano functions and concepts : T.tanh, shared variables, basic arithmetic ops, T.grad, Random numbers, floatX. If you intend to run the code on GPU also read GPU.

Note: The code for this section is available for download here.

The Stacked Denoising Autoencoder (SdA) is an extension of the stacked autoencoder [Bengio07] and it was introduced in [Vincent08].

This tutorial builds on the previous tutorial *Denoising Autoencoders* and we recommend, especially if you do not have experience with autoencoders, to read it before going any further.

8.1 Stacked Autoencoders

The denoising autoencoders can be stacked to form a deep network by feeding the latent representation (output code) of the denoising auto-encoder found on the layer below as input to the current layer. The **unsupervised pre-training** of such an architecture is done one layer at a time. Each layer is trained as a denoising auto-encoder by minimizing the reconstruction of its input (which is the output code of the previous layer). Once the first k layers are trained, we can train the $k+1$-th layer because we can now compute the code or latent representation from the layer below. Once all layers are pre-trained, the network goes through a second stage of training called **fine-tuning**. Here we consider **supervised fine-tuning** where we want to minimize prediction error on a supervised task. For this we first add a logistic regression layer on top of the network (more precisely on the output code of the output layer). We then train the entire network as we would train a multilayer perceptron. At this point, we only consider the encoding parts of each auto-encoder. This stage is supervised, since now we use the target class during training (see the *Multilayer Perceptron* for details on the multilayer perceptron).

This can be easily implemented in Theano, using the class defined before for a denoising autoencoder. We can see the stacked denoising autoencoder as having two facades, one is a list of autoencoders, the other is an MLP. During pre-training we use the first facade, i.e we treat our model as a list of autoencoders, and train each autoencoder seperately. In the second stage of training, we use the second facade. These two facedes are linked by the fact that the autoencoders and the sigmoid layers of the MLP share parameters, and the fact that autoencoders get as input latent representations of intermediate layers of the MLP.

```
class SdA(object):

  def __init__(self, numpy_rng, theano_rng=None, n_ins=784,
               hidden_layers_sizes=[500, 500], n_outs=10,
               corruption_levels=[0.1, 0.1]):
      """ This class is made to support a variable number of layers.

      :type numpy_rng: numpy.random.RandomState
      :param numpy_rng: numpy random number generator used to draw initial
                  weights

      :type theano_rng: theano.tensor.shared_randomstreams.RandomStreams
      :param theano_rng: Theano random generator; if None is given one is
                         generated based on a seed drawn from 'rng'

      :type n_ins: int
      :param n_ins: dimension of the input to the sdA

      :type n_layers_sizes: list of ints
      :param n_layers_sizes: intermediate layers size, must contain
                             at least one value

      :type n_outs: int
      :param n_outs: dimension of the output of the network

      :type corruption_levels: list of float
      :param corruption_levels: amount of corruption to use for each
                                layer
      """

      self.sigmoid_layers = []
      self.dA_layers = []
      self.params = []
      self.n_layers = len(hidden_layers_sizes)

      assert self.n_layers > 0

      if not theano_rng:
          theano_rng = RandomStreams(numpy_rng.randint(2 ** 30))
      # allocate symbolic variables for the data
      self.x = T.matrix('x')  # the data is presented as rasterized images
      self.y = T.ivector('y')  # the labels are presented as 1D vector of
                               # [int] labels
```

`self.sigmoid_layers` will store the sigmoid layers of the MLP facade, while `self.dA_layers` will store the denoising autoencoder associated with the layers of the MLP.

Next step, we construct `n_layers` sigmoid layers (we use the `SigmoidalLayer` class introduced in *Multilayer Perceptron*, with the only modification that we replaced the non-linearity from `tanh` to the logistic function $s(x) = \frac{1}{1+e^{-x}}$) and `n_layers` denoising autoencoders, where `n_layers` is the depth of our model. We link the sigmoid layers such that they form an MLP, and construct each denoising autoencoder such that they share the weight matrix and the bias of the encoding part with its corresponding sigmoid layer.

```
for i in xrange(self.n_layers):
    # construct the sigmoidal layer

    # the size of the input is either the number of hidden units of
    # the layer below or the input size if we are on the first layer
    if i == 0:
        input_size = n_ins
    else:
        input_size = hidden_layers_sizes[i - 1]

    # the input to this layer is either the activation of the hidden
    # layer below or the input of the SdA if you are on the first
    # layer
    if i == 0:
        layer_input = self.x
    else:
        layer_input = self.sigmoid_layers[-1].output

    sigmoid_layer = SigmoidalLayer(rng=rng,
                                   input=layer_input,
                                   n_in=input_size,
                                   n_out=hidden_layers_sizes[i])
    # add the layer to our list of layers
    self.sigmoid_layers.append(sigmoid_layer)

    # its arguably a philosophical question...
    # but we are going to only declare that the parameters of the
    # sigmoid_layers are parameters of the StackedDAA
    # the visible biases in the dA are parameters of those
    # dA, but not the SdA
    self.params.extend(sigmoid_layer.params)

    # Construct a denoising autoencoder that shared weights with this
    # layer
    dA_layer = dA(rng=rng, trng=trng, input=layer_input,
                  n_visible=input_size,
                  n_hidden=hidden_layers_sizes[i],
                  corruption_level=corruption_levels[0],
                  W=sigmoid_layer.W,
                  bhid=sigmoid_layer.b)
    self.dA_layers.append(dA_layer)
```

All we need now is to add the logistic layer on top of the sigmoid layers such that we have an MLP. We will use the `LogisticRegression` class introduced in *Classifying MNIST digits using Logistic Regression*.

```
# We now need to add a logistic layer on top of the MLP
self.logLayer = LogisticRegression(
                 input=self.sigmoid_layers[-1].output,
                 n_in=hidden_layers_sizes[-1], n_out=n_outs)

self.params.extend(self.logLayer.params)
# construct a function that implements one step of finetunining
```

```
# compute the cost for second phase of training,
# defined as the negative log likelihood
self.finetune_cost = self.logLayer.negative_log_likelihood(self.y)
# compute the gradients with respect to the model parameters
# symbolic variable that points to the number of errors made on the
# minibatch given by self.x and self.y
self.errors = self.logLayer.errors(self.y)
```

The class also provides a method that generates training functions for each of the denoising autoencoder associated with the different layers. They are returned as a list, where element i is a function that implements one step of training the `dA` correspoinding to layer i.

```
def pretraining_functions(self, train_set_x, batch_size):
    ''' Generates a list of functions, each of them implementing one
    step in trainnig the dA corresponding to the layer with same index.
    The function will require as input the minibatch index, and to train
    a dA you just need to iterate, calling the corresponding function on
    all minibatch indexes.

    :type train_set_x: theano.tensor.TensorType
    :param train_set_x: Shared variable that contains all datapoints used
                        for training the dA

    :type batch_size: int
    :param batch_size: size of a [mini]batch

    :type learning_rate: float
    :param learning_rate: learning rate used during training for any of
                          the dA layers
    '''

    # index to a [mini]batch
    index = T.lscalar('index')  # index to a minibatch
```

In order to be able to change the corruption level or the learning rate during training we associate a Theano variable to them.

```
corruption_level = T.scalar('corruption')  # amount of corruption to use
learning_rate = T.scalar('lr')  # learning rate to use
# number of batches
n_batches = train_set_x.get_value(borrow=True).shape[0] / batch_size
# begining of a batch, given `index`
batch_begin = index * batch_size
# ending of a batch given `index`
batch_end = batch_begin + batch_size

pretrain_fns = []
for dA in self.dA_layers:
    # get the cost and the updates list
    cost, updates = dA.get_cost_updates(corruption_level, learning_rate)
    # compile the theano function
    fn = theano.function(inputs=[index,
                      theano.Param(corruption_level, default=0.2),
```

```
                    theano.Param(learning_rate, default=0.1)],
            outputs=cost,
            updates=updates,
            givens={self.x: train_set_x[batch_begin:batch_end]})
    # append `fn` to the list of functions
    pretrain_fns.append(fn)

return pretrain_fns
```

Now any function `pretrain_fns[i]` takes as arguments `index` and optionally `corruption` – the corruption level or `lr` – the learning rate. Note that the name of the parameters are the name given to the Theano variables when they are constructed, not the name of the python variables (`learning_rate` or `corruption_level`). Keep this in mind when working with Theano.

In the same fashion we build a method for constructing function required during finetuning (a `train_model`, a `validate_model` and a `test_model` function).

```
def build_finetune_functions(self, datasets, batch_size, learning_rate):
    '''Generates a function `train` that implements one step of
    finetuning, a function `validate` that computes the error on
    a batch from the validation set, and a function `test` that
    computes the error on a batch from the testing set

    :type datasets: list of pairs of theano.tensor.TensorType
    :param datasets: It is a list that contain all the datasets;
                     the has to contain three pairs, `train`,
                     `valid`, `test` in this order, where each pair
                     is formed of two Theano variables, one for the
                     datapoints, the other for the labels

    :type batch_size: int
    :param batch_size: size of a minibatch

    :type learning_rate: float
    :param learning_rate: learning rate used during finetune stage
    '''

    (train_set_x, train_set_y) = datasets[0]
    (valid_set_x, valid_set_y) = datasets[1]
    (test_set_x, test_set_y) = datasets[2]

    # compute number of minibatches for training, validation and testing
    n_valid_batches = valid_set_x.get_value(borrow=True).shape[0] / batch_size
    n_test_batches = test_set_x.get_value(borrow=True).shape[0] / batch_size

    index = T.lscalar('index')  # index to a [mini]batch

    # compute the gradients with respect to the model parameters
    gparams = T.grad(self.finetune_cost, self.params)

    # compute list of fine-tuning updates
    updates = []
    for param, gparam in zip(self.params, gparams):
```

```
        updates.append((param, param - gparam * learning_rate))

    train_fn = theano.function(inputs=[index],
          outputs=self.finetune_cost,
          updates=updates,
          givens={
            self.x: train_set_x[index * batch_size: (index + 1) * batch_size],
            self.y: train_set_y[index * batch_size: (index + 1) * batch_size]})

    test_score_i = theano.function([index], self.errors,
             givens={
               self.x: test_set_x[index * batch_size: (index+1) * batch_size],
               self.y: test_set_y[index * batch_size: (index+1) * batch_size]})

    valid_score_i = theano.function([index], self.errors,
          givens={
             self.x: valid_set_x[index * batch_size: (index + 1) * batch_size],
             self.y: valid_set_y[index * batch_size: (index + 1) * batch_size]})

    # Create a function that scans the entire validation set
    def valid_score():
        return [valid_score_i(i) for i in xrange(n_valid_batches)]

    # Create a function that scans the entire test set
    def test_score():
        return [test_score_i(i) for i in xrange(n_test_batches)]

    return train_fn, valid_score, test_score
```

Note that the returned `valid_score` and `test_score` are not Theano functions, but rather python functions that also loop over the entire validation set and the entire test set producing a list of the losses over these sets.

8.2 Putting it all together

The few lines of code below constructs the stacked denoising autoencoder :

```
numpy_rng = numpy.random.RandomState(123)
print '... building the model'
# construct the stacked denoising autoencoder class
sda = SdA(numpy_rng=numpy_rng, n_ins=28 * 28,
          hidden_layers_sizes=[100, 100, 100],
          n_outs=10)
```

There are two stages in training this network, a layer-wise pre-training and fine-tuning afterwards.

For the pre-training stage, we will loop over all the layers of the network. For each layer we will use the compiled theano function that implements a SGD step towards optimizing the weights for reducing the reconstruction cost of that layer. This function will be applied to the training set for a fixed number of epochs given by `pretraining_epochs`.

```
########################
# PRETRAINING THE MODEL #
########################
print '... getting the pretraining functions'
pretraining_fns = sda.pretraining_functions(
                                    train_set_x=train_set_x,
                                    batch_size=batch_size)

print '... pre-training the model'
start_time = time.clock()
## Pre-train layer-wise
for i in xrange(sda.n_layers):
    # go through pretraining epochs
    for epoch in xrange(pretraining_epochs):
        # go through the training set
        c = []
        for batch_index in xrange(n_train_batches):
            c.append( pretraining_fns[i](index=batch_index,
                     corruption=0.2, lr=pretrain_lr ) )
        print 'Pre-training layer %i, epoch %d, cost '%(i,epoch), numpy.mean(c)

end_time = time.clock()

print ('Pretraining took %f minutes' %((end_time - start_time) / 60.))
```

The fine-tuning loop is very similar with the one in the *Multilayer Perceptron*, the only difference is that we will use now the functions given by `build_finetune_functions` .

8.3 Running the Code

The user can run the code by calling:

```
python code/SdA.py
```

By default the code runs 15 pre-training epochs for each layer, with a batch size of 1. The corruption level for the first layer is 0.1, for the second 0.2 and 0.3 for the third. The pretraining learning rate is was 0.001 and the finetuning learning rate is 0.1. Pre-training takes 585.01 minutes, with an average of 13 minutes per epoch. Fine-tuning is completed after 36 epochs in 444.2 minutes, with an average of 12.34 minutes per epoch. The final validation score is 1.39% with a testing score of 1.3%. These results were obtained on a machine with an Intel Xeon E5430 @ 2.66GHz CPU, with a single-threaded GotoBLAS.

8.4 Tips and Tricks

One way to improve the running time of your code (given that you have sufficient memory available), is to compute how the network, up to layer $k-1$, transforms your data. Namely, you start by training your first layer dA. Once it is trained, you can compute the hidden units values for every datapoint in your dataset and store this as a new dataset that you will use to train the dA corresponding to layer 2. Once you trained the dA for layer 2, you compute, in a similar fashion, the dataset for layer 3 and so on. You can see now, that at this

point, the dAs are trained individually, and they just provide (one to the other) a non-linear transformation of the input. Once all dAs are trained, you can start fine-tunning the model.

CHAPTER

NINE

RESTRICTED BOLTZMANN MACHINES (RBM)

Note: This section assumes the reader has already read through *Classifying MNIST digits using Logistic Regression* and *Multilayer Perceptron*. Additionally it uses the following Theano functions and concepts : T.tanh, shared variables, basic arithmetic ops, T.grad, Random numbers, floatX and scan. If you intend to run the code on GPU also read GPU.

Note: The code for this section is available for download here.

9.1 Energy-Based Models (EBM)

Energy-based models associate a scalar energy to each configuration of the variables of interest. Learning corresponds to modifying that energy function so that its shape has desirable properties. For example, we would like plausible or desirable configurations to have low energy. Energy-based probabilistic models define a probability distribution through an energy function, as follows:

$$p(x) = \frac{e^{-E(x)}}{Z}. \tag{9.1}$$

The normalizing factor Z is called the **partition function** by analogy with physical systems.

$$Z = \sum_x e^{-E(x)}$$

An energy-based model can be learnt by performing (stochastic) gradient descent on the empirical negative log-likelihood of the training data. As for the logistic regression we will first define the log-likelihood and then the loss function as being the negative log-likelihood.

$$\mathcal{L}(\theta, \mathcal{D}) = \frac{1}{N} \sum_{x^{(i)} \in \mathcal{D}} \log\ p(x^{(i)})$$
$$\ell(\theta, \mathcal{D}) = -\mathcal{L}(\theta, \mathcal{D})$$

using the stochastic gradient $-\frac{\partial \log p(x^{(i)})}{\partial \theta}$, where θ are the parameters of the model.

EBMs with Hidden Units

In many cases of interest, we do not observe the example x fully, or we want to introduce some non-observed variables to increase the expressive power of the model. So we consider an observed part (still denoted x here) and a **hidden** part h. We can then write:

$$P(x) = \sum_h P(x, h) = \sum_h \frac{e^{-E(x,h)}}{Z}. \tag{9.2}$$

In such cases, to map this formulation to one similar to Eq. (9.1), we introduce the notation (inspired from physics) of **free energy**, defined as follows:

$$\mathcal{F}(x) = -\log \sum_h e^{-E(x,h)} \tag{9.3}$$

which allows us to write,

$$P(x) = \frac{e^{-\mathcal{F}(x)}}{Z} \text{ with } Z = \sum_x e^{-\mathcal{F}(x)}.$$

The data negative log-likelihood gradient then has a particularly interesting form.

$$-\frac{\partial \log p(x)}{\partial \theta} = \frac{\partial \mathcal{F}(x)}{\partial \theta} - \sum_{\tilde{x}} p(\tilde{x}) \frac{\partial \mathcal{F}(\tilde{x})}{\partial \theta}. \tag{9.4}$$

Notice that the above gradient contains two terms, which are referred to as the **positive** and **negative phase**. The terms positive and negative do not refer to the sign of each term in the equation, but rather reflect their effect on the probability density defined by the model. The first term increases the probability of training data (by reducing the corresponding free energy), while the second term decreases the probability of samples generated by the model.

It is usually difficult to determine this gradient analytically, as it involves the computation of $E_P[\frac{\partial \mathcal{F}(x)}{\partial \theta}]$. This is nothing less than an expectation over all possible configurations of the input x (under the distribution P formed by the model) !

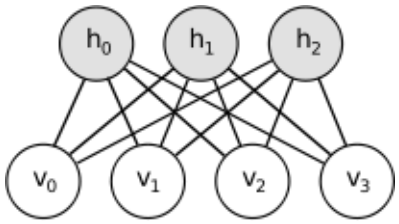
The first step in making this computation tractable is to estimate the expectation using a fixed number of model samples. Samples used to estimate the negative phase gradient are referred to as **negative particles**, which are denoted as $\mathcal{N}$. The gradient can then be written as:

$$-\frac{\partial \log p(x)}{\partial \theta} \approx \frac{\partial \mathcal{F}(x)}{\partial \theta} - \frac{1}{|\mathcal{N}|} \sum_{\tilde{x} \in \mathcal{N}} \frac{\partial \mathcal{F}(\tilde{x})}{\partial \theta}. \tag{9.5}$$

where we would ideally like elements $\tilde{x}$ of $\mathcal{N}$ to be sampled according to P (i.e. we are doing Monte-Carlo). With the above formula, we almost have a pratical, stochastic algorithm for learning an EBM. The only missing ingredient is how to extract these negative particles $\mathcal{N}$. While the statistical literature abounds with sampling methods, Markov Chain Monte Carlo methods are especially well suited for models such as the Restricted Boltzmann Machines (RBM), a specific type of EBM.

9.2 Restricted Boltzmann Machines (RBM)

Boltzmann Machines (BMs) are a particular form of log-linear Markov Random Field (MRF), i.e., for which the energy function is linear in its free parameters. To make them powerful enough to represent complicated distributions (i.e., go from the limited parametric setting to a non-parametric one), we consider that some of the variables are never observed (they are called hidden). By having more hidden variables (also called hidden units), we can increase the modeling capacity of the Boltzmann Machine (BM). Restricted Boltzmann Machines further restrict BMs to those without visible-visible and hidden-hidden connections. A graphical depiction of an RBM is shown below.



The energy function $E(v, h)$ of an RBM is defined as:

$$E(v, h) = -b'v - c'h - h'Wv \tag{9.6}$$

where W represents the weights connecting hidden and visible units and b, c are the offsets of the visible and hidden layers respectively.

This translates directly to the following free energy formula:

$$\mathcal{F}(v) = -b'v - \sum_i \log \sum_{h_i} e^{h_i(c_i + W_i v)}.$$

Because of the specific structure of RBMs, visible and hidden units are conditionally independent given one-another. Using this property, we can write:

$$p(h|v) = \prod_i p(h_i|v)$$
$$p(v|h) = \prod_j p(v_j|h).$$

RBMs with binary units

In the commonly studied case of using binary units (where v_j and $h_i \in \{0, 1\}$), we obtain from Eq. (9.6) and (9.2), a probabilistic version of the usual neuron activation function:

$$P(h_i = 1|v) = sigm(c_i + W_i v) \tag{9.7}$$

$$P(v_j = 1|h) = sigm(b_j + W'_j h) \tag{9.8}$$

The free energy of an RBM with binary units further simplifies to:

$$\mathcal{F}(v) = -b'v - \sum_i \log(1 + e^{(c_i + W_i v)}). \tag{9.9}$$

Update Equations with Binary Units

Combining Eqs. (9.5) with (9.9), we obtain the following log-likelihood gradients for an RBM with binary units:

$$
\begin{aligned}
-\frac{\partial \log p(v)}{\partial W_{ij}} &= E_v[p(h_i|v) \cdot v_j] - v_j^{(i)} \cdot sigm(W_i \cdot v^{(i)} + c_i) \\
-\frac{\partial \log p(v)}{\partial c_i} &= E_v[p(h_i|v)] - sigm(W_i \cdot v^{(i)}) \\
-\frac{\partial \log p(v)}{\partial b_j} &= E_v[p(v_j|h)] - v_j^{(i)}
\end{aligned}
\tag{9.10}
$$

For a more detailed derivation of these equations, we refer the reader to the following page, or to section 5 of Learning Deep Architectures for AI. We will however not use these formulas, but rather get the gradient using Theano T.grad from equation (9.4).

9.3 Sampling in an RBM

Samples of $p(x)$ can be obtained by running a Markov chain to convergence, using Gibbs sampling as the transition operator.

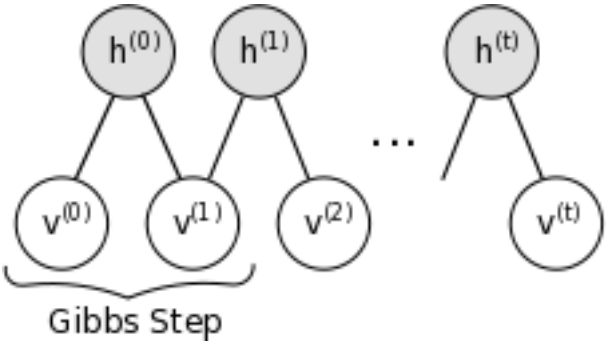
Gibbs sampling of the joint of N random variables $S = (S_1, ..., S_N)$ is done through a sequence of N sampling sub-steps of the form $S_i \sim p(S_i|S_{-i})$ where S_{-i} contains the $N - 1$ other random variables in S excluding S_i.

For RBMs, S consists of the set of visible and hidden units. However, since they are conditionally independent, one can perform block Gibbs sampling. In this setting, visible units are sampled simultaneously given fixed values of the hidden units. Similarly, hidden units are sampled simultaneously given the visibles. A step in the Markov chain is thus taken as follows:

$$
\begin{aligned}
h^{(n+1)} &\sim sigm(W' v^{(n)} + c) \\
v^{(n+1)} &\sim sigm(W h^{(n+1)} + b),
\end{aligned}
$$

where $h^{(n)}$ refers to the set of all hidden units at the n-th step of the Markov chain. What it means is that, for example, $h_i^{(n+1)}$ is randomly chosen to be 1 (versus 0) with probability $sigm(W_i' v^{(n)} + c_i)$, and similarly, $v_j^{(n+1)}$ is randomly chosen to be 1 (versus 0) with probability $sigm(W_{\cdot j} h^{(n+1)} + b_j)$.

This can be illustrated graphically:



As $t \to \infty$, samples $(v^{(t)}, h^{(t)})$ are guaranteed to be accurate samples of $p(v, h)$.

In theory, each parameter update in the learning process would require running one such chain to convergence. It is needless to say that doing so would be prohibitively expensive. As such, several algorithms have been devised for RBMs, in order to efficiently sample from $p(v, h)$ during the learning process.

9.3.1 Contrastive Divergence (CD-k)

Contrastive Divergence uses two tricks to speed up the sampling process:

- since we eventually want $p(v) \approx p_{train}(v)$ (the true, underlying distribution of the data), we initialize the Markov chain with a training example (i.e., from a distribution that is expected to be close to p, so that the chain will be already close to having converged to its final distribution p).
- CD does not wait for the chain to converge. Samples are obtained after only k-steps of Gibbs sampling. In pratice, $k = 1$ has been shown to work surprisingly well.

9.3.2 Persistent CD

Persistent CD [Tieleman08] uses another approximation for sampling from $p(v, h)$. It relies on a single Markov chain, which has a persistent state (i.e., not restarting a chain for each observed example). For each parameter update, we extract new samples by simply running the chain for k-steps. The state of the chain is then preserved for subsequent updates.

The general intuition is that if parameter updates are small enough compared to the mixing rate of the chain, the Markov chain should be able to "catch up" to changes in the model.

9.4 Implementation

We construct an `RBM` class. The parameters of the network can either be initialized by the constructor or can be passed as arguments. This option is useful when an RBM is used as the building block of a deep network, in which case the weight matrix and the hidden layer bias is shared with the corresponding sigmoidal layer of an MLP network.

```
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-versa),
      as well as for performing CD updates.

      :param input: None for standalone RBMs or symbolic variable if RBM is
      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 to a
        shared weight matrix in case RBM is part of a DBN network; in a DBN,
        the weights are shared between RBMs and layers of a MLP

        :param hbias: None for standalone RBMs or symbolic variable pointing
        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.random.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')

        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')

        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')


        # initialize input layer for standalone RBM or layer0 of DBN
        self.input = input if input else T.dmatrix('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]
```

Next step is to define functions which construct the symbolic graph associated with Eqs. (9.7) - (9.8). The code is as follows:

```
def propup(self, vis):
    ''' This function propagates the visible units activation upwards to
    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 optimization and
    stability this symbolic variable will be needed to write down a more
    stable graph (see details in the reconstruction cost function)
    '''
    pre_sigmoid_activation = T.dot(vis, self.W) + self.hbias
    return [pre_sigmoid_activation, T.nnet.sigmoid(pre_sigmoid_activation)]

def sample_h_given_v(self, v0_sample):
    ''' This function infers state of hidden units given visible units '''
    # 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 dtype
    # int64 by default. If we want to keep our computations in floatX
    # 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 downwards to
    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 optimization and
    stability this symbolic variable will be needed to write down a more
    stable 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_activation)]

def sample_v_given_h(self, h0_sample):
    ''' This function infers state of visible units given hidden units '''
    # 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 dtype
    # int64 by default. If we want to keep our computations in floatX
```

```
    # 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]
```

We can then use these functions to define the symbolic graph for a Gibbs sampling step. We define two functions:

- `gibbs_vhv` which performs a step of Gibbs sampling starting from the visible units. As we shall see, this will be useful for sampling from the RBM.
- `gibbs_hvh` which performs a step of Gibbs sampling starting from the hidden units. This function will be useful for performing CD and PCD updates.

The code is as follows:

```
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_sample)
    pre_sigmoid_h1, h1_mean, h1_sample = self.sample_h_given_v(v1_sample)
    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_sample)
    pre_sigmoid_v1, v1_mean, v1_sample = self.sample_v_given_h(h1_sample)
    return [pre_sigmoid_h1, h1_mean, h1_sample, pre_sigmoid_v1, v1_mean, v1_sample]
```

Note that we also return the pre-sigmoid activation. 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.

The class also has a function that computes the free energy of the model, needed for computing the gradient of the parameters (see Eq. (9.4)). Note that we also return the pre-sigmoid

```
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
```

We then add a `get_cost_updates` method, whose purpose is to generate the symbolic gradients for CD-k and PCD-k updates.

```
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 persistent
    chain, if one is used.
    """

    # compute positive phase
    pre_sigmoid_ph, ph_mean, ph_sample = self.sample_h_given_v(self.input)

    # 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
```

Note that `get_cost_updates` takes as argument a variable called `persistent`. This allows us to use the same code to implement both CD and PCD. To use PCD, `persistent` should refer to a shared variable which contains the state of the Gibbs chain from the previous iteration.

If `persistent` is `None`, we initialize the Gibbs chain with the hidden sample generated during the positive phase, therefore implementing CD. Once we have established the starting point of the chain, we can then compute the sample at the end of the Gibbs chain, sample that we need for getting the gradient (see Eq. (9.4)). To do so, we will use the `scan` op provided by Theano, therefore we urge the reader to look it up by following this link.

```
# 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, None, chain_start],
            n_steps=k)
```

Once we have the generated the chain we take the sample at the end of the chain to get the free energy of the negative phase. Note that the `chain_end` is a symbolical Theano variable expressed in terms of the model parameters, and if we would apply `T.grad` naively, the function will try to go through the Gibbs chain to get the gradients. This is not what we want (it will mess up our gradients) and therefire we need to indicate to `T.grad` that `chain_end` is a constant. We do this by using the argument `consider_constant` of `T.grad`.

```
# 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])
```

Finally, we add to the updates dictionary returned by scan (which contains updates rules for random states of `theano_rng`) to contain the parameter updates. In the case of PCD, these should also update the shared variable containing the state of the Gibbs chain.

```
# 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 - gparam * T.cast(lr, dtype=theano.config.floatX)
if persistent:
    # Note that this works only if persistent is a shared variable
    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_nvs[-1])

return monitoring_cost, updates
```

9.4.1 Tracking Progress

RBMs are particularly tricky to train. Because of the partition function Z of Eq. (9.1), we cannot estimate the log-likelihood $\log(P(x))$ during training. We therefore have no direct useful metric for choosing the optimal hyperparameters.

Several options are available to the user.

Inspection of Negative Samples

Negative samples obtained during training can be visualized. As training progresses, we know that the model defined by the RBM becomes closer to the true underlying distribution, $p_{train}(x)$. Negative samples should thus look like samples from the training set. Obviously bad hyperparameters can be discarded in this fashion.

Visual Inspection of Filters

The filters learnt by the model can be visualized. This amounts to plotting the weights of each unit as a gray-scale image (after reshaping to a square matrix). Filters should pick out strong features in the data. While it is not clear for an arbitrary dataset, what these features should look like, training on MNIST usually results in filters which act as stroke detectors, while training on natural images lead to Gabor like filters if trained in conjunction with a sparsity criteria.

Proxies to Likelihood

Other, more tractable functions can be used as a proxy to the likelihood. When training an RBM with PCD, one can use pseudo-likelihood as the proxy. Pseudo-likelihood (PL) is much less expensive to compute, as it assumes that all bits are independent. Therefore,

$$PL(x) = \prod_i P(x_i|x_{-i}) \text{ and}$$
$$\log PL(x) = \sum_i \log P(x_i|x_{-i})$$

Here x_{-i} denotes the set of all bits of x except bit i. The log-PL is therefore the sum of the log-probabilities of each bit x_i, conditionned on the state of all other bits. For MNIST, this would involve summing over the 784 input dimensions, which remains rather expensive. For this reason, we use the following stochastic approximation to log-PL:

$$g = N \cdot \log P(x_i|x_{-i}), \text{ where } i \sim U(0, N), \text{, and}$$
$$E[g] = \log PL(x)$$

where the expectation is taken over the uniform random choice of index i, and N is the number of visible units. In order to work with binary units, we further introduce the notation $\tilde{x}_i$ to refer to x with bit-i being flipped (1->0, 0->1). The log-PL for an RBM with binary units is then written as:

$$\log PL(x) \approx N \cdot \log \frac{e^{-FE(x)}}{e^{-FE(x)} + e^{-FE(\tilde{x}_i)}}$$
$$\approx N \cdot \log[sigm(FE(\tilde{x}_i) - FE(x))]$$

We therefore return this cost as well as the RBM updates in the `get_cost_updates` function of the `RBM` class. Notice that we modify the updates dictionary to increment the index of bit i. This will result in bit i cycling over all possible values $\{0, 1, ..., N\}$, from one update to another.

Note that for CD training the cost-entropy cost between the input and the reconstruction(the same as the one used for the de-noising autoencoder) is more reliable then the pseudo-loglikelihood. Here is the code we use to compute the pseudo-likelihood:

```
def get_pseudo_likelihood_cost(self, updates):
    """Stochastic approximation to the pseudo-likelihood"""

    # index of bit i in expression p(x_i | x_{\i})
    bit_i_idx = theano.shared(value=0, name='bit_i_idx')
```

```
    # binarize the input image by rounding to nearest integer
    xi = T.iround(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 assigns
    # 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)

    # equivalent to e^(-FE(x_i)) / (e^(-FE(x_i)) + e^(-FE(x_{\i})))
    cost = T.mean(self.n_visible * T.log(T.nnet.sigmoid(fe_xi_flip - fe_xi)))

    # increment bit_i_idx % number as part of updates
    updates[bit_i_idx] = (bit_i_idx + 1) % self.n_visible

    return cost
```

9.4.2 Main Loop

We now have all the necessary ingredients to start training our network.

Before going over the training loop however, the reader should familiarize himself with the function `tile_raster_images` (see *Plotting Samples and Filters*). Since RBMs are generative models, we are interested in sampling from them and plotting/visualizing these samples. We also want to visualize the filters (weights) learnt by the RBM, to gain insights into what the RBM is actually doing. Bear in mind however, that this does not provide the entire story, since we neglect the biases and plot the weights up to a multiplicative constant (weights are converted to values between 0 and 1).

Having these utility functions, we can start training the RBM and plot/save the filters after each training epoch. We train the RBM using PCD, as it has been shown to lead to a better generative model ([Tieleman08]).

```
# 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]})

plotting_time = 0.
start_time = time.clock()


# go through training epochs
for epoch in xrange(training_epochs):

    # go through the training set
```

```
    mean_cost = []
    for batch_index in xrange(n_train_batches):
       mean_cost += [train_rbm(batch_index)]

    print 'Training epoch %d, cost is '%epoch, numpy.mean(mean_cost)

    # Plot filters after each training epoch
    plotting_start = time.clock()
    # Construct image from the weight matrix
    image = PIL.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 = time.clock()
    plotting_time += (plotting_stop - plotting_start)

end_time = time.clock()

pretraining_time = (end_time - start_time) - plotting_time

print ('Training took %f minutes' % (pretraining_time / 60.))
```

Once the RBM is trained, we can then use the `gibbs_vhv` function to implement the Gibbs chain required for sampling. We initialize the Gibbs chain starting from test examples (although we could as well pick it from the training set) in order to speed up convergence and avoid problems with random initialization. We again use Theano's `scan` op to do 1000 steps before each plotting.

```
#################################
#     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 chain
test_idx = rng.randint(number_of_test_samples - 20)
persistent_vis_chain = theano.shared(numpy.asarray(
    test_set_x.get_value(borrow=True)[test_idx: test_idx + 20],
    dtype=theano.config.floatX))
```

Next we create the 20 persistent chains in parallel to get our samples. To do so, we compile a theano function which performs one Gibbs step and updates the state of the persistent chain with the new visible sample. We apply this function iteratively for a large number of steps, plotting the samples at every 1000 steps.

```
# find out the number of test
number_of_test_samples = test_set_x.get_value(borrow=True).shape[0]

# pick random test examples, with which to initialize the persistent chain
test_idx = rng.randint(number_of_test_samples-n_chains)
persistent_vis_chain = theano.shared(numpy.array(
    test_set_x.get_value(borrow=True)[test_idx:test_idx + 100],
    dtype=theano.config.floatX))
```

```
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, None, persistent_vis_chai
                            n_steps=plot_every)

# add to updates the shared variable that takes care of our persistent
# 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 actual samples for
# reinitializing the state of our persistent chain
sample_fn = theano.function([], [vis_mfs[-1], vis_samples[-1]],
                            updates=updates)

# sample the RBM, plotting at least 'n_samples'
n_samples = 10
# 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 xrange(n_samples):
    # generate 'plot_every' intermediate samples that we discard, because successive sample
    vis_mf, vis_sample = sample_fn()
    image_data[29 * idx: 29 * idx + 28, :] = tile_raster_images(
            X=vis_mf,
            img_shape=(28, 28),
            tile_shape=(1, batch_size),
            tile_spacing=(1, 1))
    # construct image

image = PIL.Image.fromarray(image_data)
print ' ... plotting sample ', idx
image.save('samples.png')
```

9.5 Results

We ran the code with PCD-15, learning rate of 0.1 and a batch size of 20, for 15 epochs. Training the model takes 122.466 minutes on a Intel Xeon E5430 @ 2.66GHz CPU, with a single-threaded GotoBLAS.

The output was the following:

```
... loading data
Training epoch 0, cost is  -90.6507246003
Training epoch 1, cost is  -81.235857373
Training epoch 2, cost is  -74.9120966945
Training epoch 3, cost is  -73.0213216101
Training epoch 4, cost is  -68.4098570497
Training epoch 5, cost is  -63.2693021647
```

```
Training epoch 6, cost is  -65.99578971
Training epoch 7, cost is  -68.1236650015
Training epoch 8, cost is  -68.3207365087
Training epoch 9, cost is  -64.2949797113
Training epoch 10, cost is  -61.5194867893
Training epoch 11, cost is  -61.6539369402
Training epoch 12, cost is  -63.5465278086
Training epoch 13, cost is  -63.3787093527
Training epoch 14, cost is  -62.755739271
Training took 122.466000 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
```

The pictures below show the filters after 15 epochs :

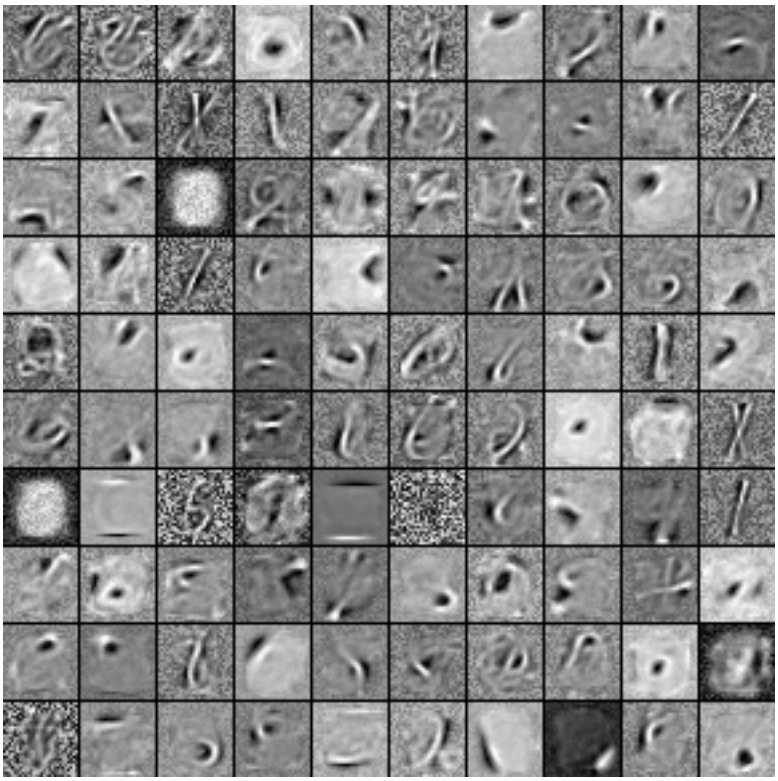
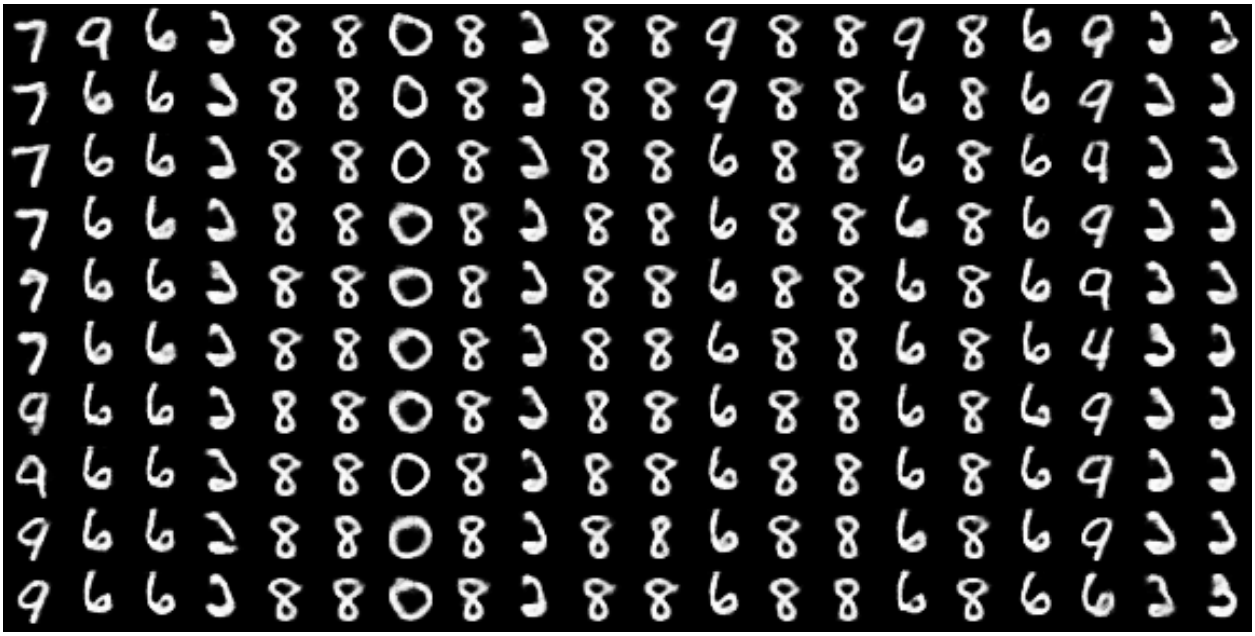


Figure 9.1: Filters obtained after 15 epochs.

Here are the samples generated by the RBM after training. Each row represents a mini-batch of negative particles (samples from independent Gibbs chains). 1000 steps of Gibbs sampling were taken between each

of those rows.



CHAPTER

TEN

DEEP BELIEF NETWORKS

Note: This section assumes the reader has already read through *Classifying MNIST digits using Logistic Regression* and *Multilayer Perceptron* and *Restricted Boltzmann Machines (RBM)*. Additionally it uses the following Theano functions and concepts : T.tanh, shared variables, basic arithmetic ops, T.grad, Random numbers, floatX. If you intend to run the code on GPU also read GPU.

Note: The code for this section is available for download here.

10.1 Deep Belief Networks

[Hinton06] showed that RBMs can be stacked and trained in a greedy manner to form so-called Deep Belief Networks (DBN). DBNs are graphical models which learn to extract a deep hierarchical representation of the training data. They model the joint distribution between observed vector x and the ℓ hidden layers h^k as follows:

$$P(x, h^1, \ldots, h^\ell) = \left(\prod_{k=0}^{\ell-2} P(h^k | h^{k+1}) \right) P(h^{\ell-1}, h^\ell) \tag{10.1}$$

where $x = h^0$, $P(h^{k-1}|h^k)$ is a conditional distribution for the visible units conditioned on the hidden units of the RBM at level k, and $P(h^{\ell-1}, h^\ell)$ is the visible-hidden joint distribution in the top-level RBM. This is illustrated in the figure below.

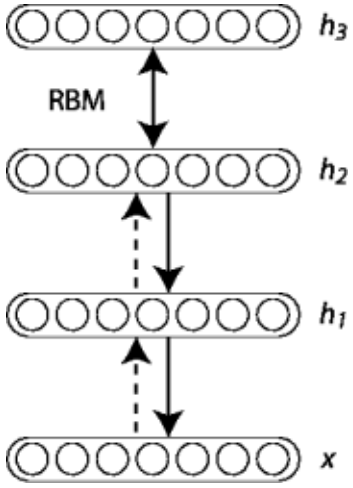
The principle of greedy layer-wise unsupervised training can be applied to DBNs with RBMs as the building blocks for each layer [Hinton06], [Bengio07]. The process is as follows:

1. Train the first layer as an RBM that models the raw input $x = h^{(0)}$ as its visible layer.

2. Use that first layer to obtain a representation of the input that will be used as data for the second layer. Two common solutions exist. This representation can be chosen as being the mean activations $p(h^{(1)} = 1|h^{(0)})$ or samples of $p(h^{(1)}|h^{(0)})$.

3. Train the second layer as an RBM, taking the transformed data (samples or mean activations) as training examples (for the visible layer of that RBM).

4. Iterate (2 and 3) for the desired number of layers, each time propagating upward either samples or mean values.



5. Fine-tune all the parameters of this deep architecture with respect to a proxy for the DBN log- likelihood, or with respect to a supervised training criterion (after adding extra learning machinery to convert the learned representation into supervised predictions, e.g. a linear classifier).

In this tutorial, we focus on fine-tuning via supervised gradient descent. Specifically, we use a logistic regression classifier to classify the input x based on the output of the last hidden layer $h^{(l)}$ of the DBN. Fine-tuning is then performed via supervised gradient descent of the negative log-likelihood cost function. Since the supervised gradient is only non-null for the weights and hidden layer biases of each layer (i.e. null for the visible biases of each RBM), this procedure is equivalent to initializing the parameters of a deep MLP with the weights and hidden layer biases obtained with the unsupervised training strategy.

10.2 Justifying Greedy-Layer Wise Pre-Training

Why does such an algorithm work ? Taking as example a 2-layer DBN with hidden layers $h^{(1)}$ and $h^{(2)}$ (with respective weight parameters $W^{(1)}$ and $W^{(2)}$), [Hinton06] established (see also Bengio09]_ for a detailed derivation) that $\log p(x)$ can be rewritten as,

$$\begin{aligned}\log p(x) =& KL(Q(h^{(1)}|x)||p(h^{(1)}|x)) + H_{Q(h^{(1)}|x)} + \\ & \sum_h Q(h^{(1)}|x)(\log p(h^{(1)}) + \log p(x|h^{(1)})).\end{aligned} \tag{10.2}$$

$KL(Q(h^{(1)}|x)||p(h^{(1)}|x))$ represents the KL divergence between the posterior $Q(h^{(1)}|x)$ of the first RBM if it were standalone, and the probability $p(h^{(1)}|x)$ for the same layer but defined by the entire DBN (i.e. taking into account the prior $p(h^{(1)}, h^{(2)})$ defined by the top-level RBM). $H_{Q(h^{(1)}|x)}$ is the entropy of the distribution $Q(h^{(1)}|x)$.

It can be shown that if we initialize both hidden layers such that $W^{(2)} = {W^{(1)}}^T$, $Q(h^{(1)}|x) = p(h^{(1)}|x)$ and the KL divergence term is null. If we learn the first level RBM and then keep its parameters $W^{(1)}$ fixed, optimizing Eq. (10.2) with respect to $W^{(2)}$ can thus only increase the likelihood $p(x)$.

Also, notice that if we isolate the terms which depend only on $W^{(2)}$, we get:

$$\sum_h Q(h^{(1)}|x)p(h^{(1)})$$

Optimizing this with respect to $W^{(2)}$ amounts to training a second-stage RBM, using the output of $Q(h^{(1)}|x)$ as the training distribution, when x is sampled from the training distribution for the first RBM.

10.3 Implementation

To implement DBNs in Theano, we will use the class defined in the *Restricted Boltzmann Machines (RBM)* tutorial. One can also observe that the code for the DBN is very similar with the one for SdA, because both involve the principle of unsupervised layer-wise pre-training followed by supervised fine-tuning as a deep MLP. The main difference is that we use the RBM class instead of the dA class.

We start off by defining the DBN class which will store the layers of the MLP, along with their associated RBMs. Since we take the viewpoint of using the RBMs to initialize an MLP, the code will reflect this by seperating as much as possible the RBMs used to initialize the network and the MLP used for classification.

```
class DBN(object):

    def __init__(self, numpy_rng, theano_rng=None, n_ins=784,
                 hidden_layers_sizes=[500, 500], n_outs=10):
        """This class is made to support a variable number of layers.

        :type numpy_rng: numpy.random.RandomState
        :param numpy_rng: numpy random number generator used to draw initial
                weights

        :type theano_rng: theano.tensor.shared_randomstreams.RandomStreams
        :param theano_rng: Theano random generator; if None is given one is
                           generated based on a seed drawn from `rng`

        :type n_ins: int
        :param n_ins: dimension of the input to the DBN

        :type n_layers_sizes: list of ints
        :param n_layers_sizes: intermediate layers size, must contain
                               at least one value

        :type n_outs: int
        :param n_outs: dimension of the output of the network
        """

        self.sigmoid_layers = []
        self.rbm_layers = []
        self.params = []
        self.n_layers = len(hidden_layers_sizes)

        assert self.n_layers > 0
```

```
        if not theano_rng:
            theano_rng = RandomStreams(numpy_rng.randint(2 ** 30))

        # allocate symbolic variables for the data
        self.x = T.matrix('x')  # the data is presented as rasterized images
        self.y = T.ivector('y')  # the labels are presented as 1D vector of
                                 # [int] labels
```

`self.sigmoid_layers` will store the feed-forward graphs which together form the MLP, while `self.rbm_layers` will store the RBMs used to pretrain each layer of the MLP.

Next step, we construct `n_layers` sigmoid layers (we use the `SigmoidalLayer` class introduced in *Multilayer Perceptron*, with the only modification that we replaced the non-linearity from `tanh` to the logistic function $s(x) = \frac{1}{1+e^{-x}}$) and `n_layers` RBMs, where `n_layers` is the depth of our model. We link the sigmoid layers such that they form an MLP, and construct each RBM such that they share the weight matrix and the hidden bias with its corresponding sigmoid layer.

```
for i in xrange(self.n_layers):
    # construct the sigmoidal layer

    # the size of the input is either the number of hidden units of the
    # layer below or the input size if we are on the first layer
    if i == 0:
        input_size = n_ins
    else:
        input_size = hidden_layers_sizes[i - 1]

    # the input to this layer is either the activation of the hidden
    # layer below or the input of the DBN if you are on the first layer
    if i == 0:
        layer_input = self.x
    else:
        layer_input = self.sigmoid_layers[-1].output

    sigmoid_layer = HiddenLayer(rng=numpy_rng,
                                input=layer_input,
                                n_in=input_size,
                                n_out=hidden_layers_sizes[i],
                                activation=T.nnet.sigmoid)

    # add the layer to our list of layers
    self.sigmoid_layers.append(sigmoid_layer)

    # its arguably a philosophical question...  but we are going to only declare that
    # the parameters of the sigmoid_layers are parameters of the DBN. The visible
    # biases in the RBM are parameters of those RBMs, but not of the DBN.
    self.params.extend(sigmoid_layer.params)

    # Construct an RBM that shared weights with this layer
    rbm_layer = RBM(numpy_rng=numpy_rng,
                    theano_rng=theano_rng,
                    input=layer_input,
                    n_visible=input_size,
```

```
                    n_hidden=hidden_layers_sizes[i],
                    W=sigmoid_layer.W,
                    hbias=sigmoid_layer.b)
    self.rbm_layers.append(rbm_layer)
```

All that is left is to stack one last logistic regression layer in order to form an MLP. We will use the `LogisticRegression` class introduced in *Classifying MNIST digits using Logistic Regression*.

```
# We now need to add a logistic layer on top of the MLP
self.logLayer = LogisticRegression(
                 input=self.sigmoid_layers[-1].output,
                 n_in=hidden_layers_sizes[-1], n_out=n_outs)
self.params.extend(self.logLayer.params)

# construct a function that implements one step of fine-tuning compute
# the cost for second phase of training, defined as the negative log
# likelihood of the logistic regression (output) layer
self.finetune_cost = self.logLayer.negative_log_likelihood(self.y)

# compute the gradients with respect to the model parameters
# symbolic variable that points to the number of errors made on the
# minibatch given by self.x and self.y
self.errors = self.logLayer.errors(self.y)
```

The class also provides a method which generates training functions for each of the RBMs. They are returned as a list, where element i is a function which implements one step of training for the `RBM` at layer i.

```
def pretraining_functions(self, train_set_x, batch_size, k):
    ''' Generates a list of functions, for performing one step of gradient descent at a
    given layer. The function will require as input the minibatch index, and to train an
    RBM you just need to iterate, calling the corresponding function on all minibatch
    indexes.

    :type train_set_x: theano.tensor.TensorType
    :param train_set_x: Shared var. that contains all datapoints used for training the RBM
    :type batch_size: int
    :param batch_size: size of a [mini]batch
    :param k: number of Gibbs steps to do in CD-k / PCD-k
    '''

    # index to a [mini]batch
    index = T.lscalar('index')  # index to a minibatch
```

In order to be able to change the learning rate during training, we associate a Theano variable to it that has a default value.

```
learning_rate = T.scalar('lr')  # learning rate to use

# number of batches
n_batches = train_set_x.get_value(borrow=True).shape[0] / batch_size
# begining of a batch, given `index`
batch_begin = index * batch_size
# ending of a batch given `index`
batch_end = batch_begin + batch_size
```

```
pretrain_fns = []
for rbm in self.rbm_layers:

    # get the cost and the updates list
    # using CD-k here (persisent=None) for training each RBM.
    # TODO: change cost function to reconstruction error
    cost, updates = rbm.cd(learning_rate, persistent=None, k)

    # compile the Theano function; check if k is also a Theano
    # variable, if so added to the inputs of the function
    if isinstance(k, theano.Variable):
        inputs = [index, theano.Param(learning_rate, default=0.1), k]
    else:
        inputs =  index, theano.Param(learning_rate, default=0.1)]
    fn = theano.function(inputs=inputs,
                         outputs=cost,
                         updates=updates,
                         givens={self.x: train_set_x[batch_begin:
                                                     batch_end]})
    # append `fn` to the list of functions
    pretrain_fns.append(fn)

return pretrain_fns
```

Now any function `pretrain_fns[i]` takes as arguments `index` and optionally `lr` – the learning rate. Note that the names of the parameters are the names given to the Theano variables (e.g. `lr`) when they are constructed and not the name of the python variables (e.g. `learning_rate`). Keep this in mind when working with Theano. Optionally, if you provide `k` (the number of Gibbs steps to perform in CD or PCD) this will also become an argument of your function.

In the same fashion, the DBN class includes a method for building the functions required for finetuning (a `train_model`, a `validate_model` and a `test_model` function).

```
def build_finetune_functions(self, datasets, batch_size, learning_rate):
    '''Generates a function `train` that implements one step of finetuning, a function
    `validate` that computes the error on a batch from the validation set, and a function
    `test` that computes the error on a batch from the testing set

    :type datasets: list of pairs of theano.tensor.TensorType
    :param datasets: It is a list that contain all the datasets;  the has to contain three
    pairs, `train`, `valid`, `test` in this order, where each pair is formed of two Theano
    variables, one for the datapoints, the other for the labels
    :type batch_size: int
    :param batch_size: size of a minibatch
    :type learning_rate: float
    :param learning_rate: learning rate used during finetune stage
    '''

    (train_set_x, train_set_y) = datasets[0]
    (valid_set_x, valid_set_y) = datasets[1]
    (test_set_x, test_set_y) = datasets[2]

    # compute number of minibatches for training, validation and testing
```

```
    n_valid_batches = valid_set_x.get_value(borrow=True).shape[0] / batch_size
    n_test_batches  = test_set_x.get_value(borrow=True).shape[0]  / batch_size

    index   = T.lscalar('index')    # index to a [mini]batch

    # compute the gradients with respect to the model parameters
    gparams = T.grad(self.finetune_cost, self.params)

    # compute list of fine-tuning updates
    updates = []
    for param, gparam in zip(self.params, gparams):
        updates.append((param, param - gparam * learning_rate))

    train_fn = theano.function(inputs=[index],
          outputs= self.finetune_cost,
          updates=updates,
          givens={
            self.x: train_set_x[index * batch_size: (index + 1) * batch_size],
            self.y: train_set_y[index * batch_size: (index + 1) * batch_size]})

    test_score_i = theano.function([index], self.errors,
             givens={
               self.x: test_set_x[index * batch_size: (index + 1) * batch_size],
               self.y: test_set_y[index * batch_size: (index + 1) * batch_size]})

    valid_score_i = theano.function([index], self.errors,
          givens={
             self.x: valid_set_x[index * batch_size: (index + 1) * batch_size],
             self.y: valid_set_y[index * batch_size: (index + 1) * batch_size]})

    # Create a function that scans the entire validation set
    def valid_score():
        return [valid_score_i(i) for i in xrange(n_valid_batches)]

    # Create a function that scans the entire test set
    def test_score():
        return [test_score_i(i) for i in xrange(n_test_batches)]

    return train_fn, valid_score, test_score
```

Note that the returned `valid_score` and `test_score` are not Theano functions, but rather Python functions. These loop over the entire validation set and the entire test set to produce a list of the losses obtained over these sets.

10.4 Putting it all together

The few lines of code below constructs the deep belief network :

```
numpy_rng = numpy.random.RandomState(123)
print '... building the model'
# construct the Deep Belief Network
```

```
dbn = DBN(numpy_rng=numpy_rng, n_ins=28 * 28,
          hidden_layers_sizes=[1000, 1000, 1000],
          n_outs=10)
```

There are two stages in training this network: (1) a layer-wise pre-training and (2) a fine-tuning stage.

For the pre-training stage, we loop over all the layers of the network. For each layer, we use the compiled theano function which determines the input to the `i`-th level RBM and performs one step of CD-k within this RBM. This function is applied to the training set for a fixed number of epochs given by `pretraining_epochs`.

```
########################
# PRETRAINING THE MODEL #
########################
print '... getting the pretraining functions'
# We are using CD-1 here
pretraining_fns = dbn.pretraining_functions(
        train_set_x=train_set_x,
        batch_size=batch_size,
        k=k)

print '... pre-training the model'
start_time = time.clock()
## Pre-train layer-wise
for i in xrange(dbn.n_layers):
    # go through pretraining epochs
    for epoch in xrange(pretraining_epochs):
        # go through the training set
        c = []
        for batch_index in xrange(n_train_batches):
            c.append(pretraining_fns[i](index=batch_index,
                                        lr=pretrain_lr))
        print 'Pre-training layer %i, epoch %d, cost '%(i,epoch),numpy.mean(c)

end_time = time.clock()
```

The fine-tuning loop is very similar to the one in the *Multilayer Perceptron* tutorial, the only difference being that we now use the functions given by `build_finetune_functions`.

10.5 Running the Code

The user can run the code by calling:

```
python code/DBN.py
```

With the default parameters, the code runs for 100 pre-training epochs with mini-batches of size 10. This corresponds to performing 500,000 unsupervised parameter updates. We use an unsupervised learning rate of 0.01, with a supervised learning rate of 0.1. The DBN itself consists of three hidden layers with 1000 units per layer. With early-stopping, this configuration achieved a minimal validation error of 1.27 with corresponding test error of 1.34 after 46 supervised epochs.

On an Intel(R) Xeon(R) CPU X5560 running at 2.80GHz, using a multi-threaded MKL library (running on 4 cores), pretraining took 615 minutes with an average of 2.05 mins/(layer * epoch). Fine-tuning took only 101 minutes or approximately 2.20 mins/epoch.

Hyper-parameters were selected by optimizing on the validation error. We tested unsupervised learning rates in $\{10^{-1}, ..., 10^{-5}\}$ and supervised learning rates in $\{10^{-1}, ..., 10^{-4}\}$. We did not use any form of regularization besides early-stopping, nor did we optimize over the number of pretraining updates.

10.6 Tips and Tricks

One way to improve the running time of your code (given that you have sufficient memory available), is to compute the representation of the entire dataset at layer `i` in a single pass, once the weights of the $i-1$-th layers have been fixed. Namely, start by training your first layer RBM. Once it is trained, you can compute the hidden units values for every example in the dataset and store this as a new dataset which is used to train the 2nd layer RBM. Once you trained the RBM for layer 2, you compute, in a similar fashion, the dataset for layer 3 and so on. This avoids calculating the intermediate (hidden layer) representations, `pretraining_epochs` times at the expense of increased memory usage.

CHAPTER

ELEVEN

HYBRID MONTE-CARLO SAMPLING

Note: This is an advanced tutorial, which shows how one can implemented Hybrid Monte-Carlo (HMC) sampling using Theano. We assume the reader is already familiar with Theano and energy-based models such as the RBM.

Note: The code for this section is available for download here.

11.1 Theory

Maximum likelihood learning of energy-based models requires a robust algorithm to sample negative phase particles (see Eq.(4) of the *Restricted Boltzmann Machines (RBM)* tutorial). When training RBMs with CD or PCD, this is typically done with block Gibbs sampling, where the conditional distributions $p(h|v)$ and $p(v|h)$ are used as the transition operators of the Markov chain.

In certain cases however, these conditional distributions might be difficult to sample from (i.e. requiring expensive matrix inversions, as in the case of the "mean-covariance RBM"). Also, even if Gibbs sampling can be done efficiently, it nevertheless operates via a random walk which might not be statistically efficient for some distributions. In this context, and when sampling from continuous variables, Hybrid Monte Carlo (HMC) can prove to be a powerful tool [Duane87]. It avoids random walk behavior by simulating a physical system governed by Hamiltonian dynamics, potentially avoiding tricky conditional distributions in the process.

In HMC, model samples are obtained by simulating a physical system, where particles move about a high-dimensional landscape, subject to potential and kinetic energies. Adapting the notation from [Neal93], particles are characterized by a position vector or state $s \in \mathcal{R}^D$ and velocity vector $\phi \in \mathcal{R}^D$. The combined state of a particle is denoted as $\chi = (s, \phi)$. The Hamiltonian is then defined as the sum of potential energy $E(s)$ (same energy function defined by energy-based models) and kinetic energy $K(\phi)$, as follows:

$$\mathcal{H}(s, \phi) = E(s) + K(\phi) = E(s) + \frac{1}{2} \sum_i \phi_i^2$$

Instead of sampling $p(s)$ directly, HMC operates by sampling from the canonical distribution $p(s, \phi) = \frac{1}{Z} \exp(-\mathcal{H}(s, \phi)) = p(s)p(\phi)$. Because the two variables are independent, marginalizing over ϕ is trivial and recovers the original distribution of interest.

Hamiltonian Dynamics

State s and velocity ϕ are modified such that $\mathcal{H}(s, \phi)$ remains constant throughout the simulation. The differential equations are given by:

$$\begin{aligned} \frac{ds_i}{dt} &= \frac{\partial \mathcal{H}}{\partial \phi_i} = \phi_i \\ \frac{d\phi_i}{dt} &= -\frac{\partial \mathcal{H}}{\partial s_i} = -\frac{\partial E}{\partial s_i} \end{aligned} \tag{11.1}$$

As shown in [Neal93], the above transformation preserves volume and is reversible. The above dynamics can thus be used as transition operators of a Markov chain and will leave $p(s, \phi)$ invariant. That chain by itself is not ergodic however, since simulating the dynamics maintains a fixed Hamiltonian $\mathcal{H}(s, \phi)$. HMC thus alternates hamiltonian dynamic steps, with Gibbs sampling of the velocity. Because $p(s)$ and $p(\phi)$ are independent, sampling $\phi_{new} \sim p(\phi|s)$ is trivial since $p(\phi|s) = p(\phi)$, where $p(\phi)$ is often taken to be the uni-variate Gaussian.

The Leap-Frog Algorithm

In practice, we cannot simulate Hamiltonian dynamics exactly because of the problem of time discretization. There are several ways one can do this. To maintain invariance of the Markov chain however, care must be taken to preserve the properties of volume conservation and time reversibility. The **leap-frog algorithm** maintains these properties and operates in 3 steps:

$$\begin{aligned} \phi_i(t + \epsilon/2) &= \phi_i(t) - \frac{\epsilon}{2} \frac{\partial}{\partial s_i} E(s(t)) \\ s_i(t + \epsilon) &= s_i(t) + \epsilon \phi_i(t + \epsilon/2) \\ \phi_i(t + \epsilon) &= \phi_i(t + \epsilon/2) - \frac{\epsilon}{2} \frac{\partial}{\partial s_i} E(s(t + \epsilon)) \end{aligned} \tag{11.2}$$

We thus perform a half-step update of the velocity at time $t + \epsilon/2$, which is then used to compute $s(t + \epsilon)$ and $\phi(t + \epsilon)$.

Accept / Reject

In practice, using finite stepsizes ϵ will not preserve $\mathcal{H}(s, \phi)$ exactly and will introduce bias in the simulation. Also, rounding errors due to the use of floating point numbers means that the above transformation will not be perfectly reversible.

HMC cancels these effects **exactly** by adding a Metropolis accept/reject stage, after n leapfrog steps. The new state $\chi' = (s', \phi')$ is accepted with probability $p_{acc}(\chi, \chi')$, defined as:

$$p_{acc}(\chi, \chi') = min\left(1, \frac{\exp(-\mathcal{H}(s', \phi')}{\exp(-\mathcal{H}(s, \phi)}\right)$$

HMC Algorithm

In this tutorial, we obtain a new HMC sample as follows:

1. sample a new velocity from a univariate Gaussian distribution
2. perform n leapfrog steps to obtain the new state χ'
3. perform accept/reject move of χ'

11.2 Implementing HMC Using Theano

In Theano, update dictionaries and shared variables provide a natural way to implement a sampling algorithm. The current state of the sampler can be represented as a Theano shared variable, with HMC updates being implemented by the updates list of a Theano function.

We breakdown the HMC algorithm into the following sub-components:

- $simulate\_dynamics$: a symbolic Python function which, given an initial position and velocity, will perform n_steps leapfrog updates and return the symbolic variables for the proposed state χ'.
- hmc_move: a symbolic Python function which given a starting position, generates χ by randomly sampling a velocity vector. It then calls $simulate\_dynamics$ and determines whether the transition $\chi \to \chi'$ is to be accepted.
- $hmc\_updates$: a Python function which, given the symbolic outputs of hmc_move, generates the list of updates for a single iteration of HMC.
- $HMC\_sampler$: a Python helper class which wraps everything together.

simulate_dynamics

To perform n leapfrog steps, we first need to define a function over which $Scan$ can iterate over. Instead of implementing Eq. (11.2) verbatim, notice that we can obtain $s(t+n\epsilon)$ and $\phi(t+n\epsilon)$ by performing an initial half-step update for ϕ, followed by n full-step updates for s, ϕ and one last half-step update for ϕ. In loop form, this gives:

$$
\begin{aligned}
&\phi_i(t+\epsilon/2) = \phi_i(t) - \frac{\epsilon}{2}\frac{\partial}{\partial s_i}E(s(t)) \\
&s_i(t+\epsilon) = s_i(t) + \epsilon\phi_i(t+\epsilon/2) \\
&\text{For } m \in [2, n], \text{ perform full updates:} \\
&\quad \phi_i(t+(m-1/2)\epsilon) = \phi_i(t+(m-3/2)\epsilon) - \epsilon\frac{\partial}{\partial s_i}E(s(t+(m-1)\epsilon)) \\
&\quad s_i(t+m\epsilon) = s_i(t) + \epsilon\phi_i(t+(m-1/2)\epsilon) \\
&\phi_i(t+n\epsilon) = \phi_i(t+(n-1/2)\epsilon) - \frac{\epsilon}{2}\frac{\partial}{\partial s_i}E(s(t+n\epsilon))
\end{aligned}
\tag{11.3}
$$

The inner-loop defined above is implemented by the following $leapfrog$ function, with pos, vel and $step$ replacing s, ϕ and ϵ respectively.

```
def leapfrog(pos, vel, step):
    """
    Inside loop of Scan. Performs one step of leapfrog update, using
    Hamiltonian dynamics.

    Parameters
    ----------
    pos: theano matrix
        in leapfrog update equations, represents pos(t), position at time t
    vel: theano matrix
        in leapfrog update equations, represents vel(t - stepsize/2),
        velocity at time (t - stepsize/2)
```

```
    step: theano scalar
        scalar value controlling amount by which to move

    Returns
    -------
    rval1: [theano matrix, theano matrix]
        Symbolic theano matrices for new position pos(t + stepsize), and
        velocity vel(t + stepsize/2)
    rval2: List of (variable, update expr) pairs
        List of updates for the Scan Op
    """
    # from pos(t) and vel(t - eps/2), compute vel(t + eps / 2)
    dE_dpos = TT.grad(energy_fn(pos).sum(), pos)
    new_vel = vel - step * dE_dpos
    # from vel(t + eps / 2) compute pos(t + eps)
    new_pos = pos + step * new_vel

    return [new_pos, new_vel],{}
```

The $simulate_dynamics$ function performs the full algorithm of Eqs. (11.3). We start with the initial half-step update of ϕ and full-step of s, and then scan over the $leapfrog$ method $n\_steps - 1$ times.

```
def simulate_dynamics(initial_pos, initial_vel, stepsize, n_steps, energy_fn):
    """
    Return final (position, velocity) obtained after an `n_steps` leapfrog
    updates, using Hamiltonian dynamics.

    Parameters
    ----------
    initial_pos: shared theano matrix
        Initial position at which to start the simulation
    initial_vel: shared theano matrix
        Initial velocity of particles
    stepsize: shared theano scalar
        Scalar value controlling amount by which to move
    energy_fn: python function
        Python function, operating on symbolic theano variables, used to compute
        the potential energy at a given position.

    Returns
    -------
    rval1: theano matrix
        Final positions obtained after simulation
    rval2: theano matrix
        Final velocity obtained after simulation
    """

    def leapfrog(pos, vel, step):
        """ ... """

    # compute velocity at time-step: t + stepsize / 2
    initial_energy = energy_fn(initial_pos)
    dE_dpos = TT.grad(initial_energy.sum(), initial_pos)
```

```
    vel_half_step = initial_vel - 0.5 * stepsize * dE_dpos

    # compute position at time-step: t + stepsize
    pos_full_step = initial_pos + stepsize * vel_half_step

    # perform leapfrog updates: the scan op is used to repeatedly compute
    # vel(t + (m-1/2)*stepsize) and pos(t + m*stepsize) for m in [2,n_steps].
    (final_pos, final_vel), scan_updates = theano.scan(leapfrog,
            outputs_info=[
                dict(initial=pos_full_step, return_steps=1),
                dict(initial=vel_half_step, return_steps=1),
                ],
            non_sequences=[stepsize],
            n_steps=n_steps-1)

    # NOTE: Scan always returns an updates dictionary, in case the scanned function draws
    # samples from a RandomStream. These updates must then be used when compiling the Thea
    # function, to avoid drawing the same random numbers each time the function is called.
    # this case however, we consciously ignore "scan_updates" because we know it is empty.
    assert not scan_updates

    # The last velocity returned by scan is vel(t + (n_steps-1/2)*stepsize)
    # We therefore perform one more half-step to return vel(t + n_steps*stepsize)
    energy = energy_fn(final_pos)
    final_vel = final_vel - 0.5 * stepsize * TT.grad(energy.sum(), final_pos)

    # return new proposal state
    return final_pos, final_vel
```

A final half-step is performed to compute $\phi(t + n\epsilon)$, and the final proposed state χ' is returned.

hmc_move

The hmc_move function implements the remaining steps (steps 1 and 3) of an HMC move proposal (while wrapping the $simulate\_dynamics$ function). Given a matrix of initial states $s \in \mathcal{R}^{N \times D}$ ($positions$) and energy function $E(s)$ ($energy\_fn$), it defines the symbolic graph for computing n_steps of HMC, using a given $stepsize$. The function prototype is as follows:

```
def hmc_move(s_rng, positions, energy_fn, stepsize, n_steps):
    """
    This function performs one-step of Hybrid Monte-Carlo sampling. We start by
    sampling a random velocity from a univariate Gaussian distribution, perform
    `n_steps` leap-frog updates using Hamiltonian dynamics and accept-reject
    using Metropolis-Hastings.

    Parameters
    ----------
    s_rng: theano shared random stream
        Symbolic random number generator used to draw random velocity and
        perform accept-reject move.
    positions: shared theano matrix
        Symbolic matrix whose rows are position vectors.
    energy_fn: python function
        Python function, operating on symbolic theano variables, used to compute
```

```
        the potential energy at a given position.
    stepsize:  shared theano scalar
        Shared variable containing the stepsize to use for `n_steps` of HMC
        simulation steps.
    n_steps: integer
        Number of HMC steps to perform before proposing a new position.

    Returns
    -------
    rval1: boolean
        True if move is accepted, False otherwise
    rval2: theano matrix
        Matrix whose rows contain the proposed "new position"
    """
```

We start by sampling random velocities, using the provided shared RandomStream object. Velocities are sampled independently for each dimension and for each particle under simulation, yielding a $N \times D$ matrix.

```
# sample random velocity for `batchsize` particles
initial_vel = s_rng.normal(size=positions.shape)
```

Since we now have an initial position and velocity, we can now call the $simulate\_dynamics$ to obtain the proposal for the new state χ'.

```
# perform simulation of particles subject to Hamiltonian dynamics
final_pos, final_vel = simulate_dynamics(
        initial_pos = positions,
        initial_vel = initial_vel,
        stepsize = stepsize,
        n_steps = n_steps,
        energy_fn = energy_fn)
```

We then accept/reject the proposed state based on the Metropolis algorithm.

```
# accept/reject the proposed move based on the joint distribution
accept = metropolis_hastings_accept(
        energy_prev=hamiltonian(positions, initial_vel, energy_fn),
        energy_next=hamiltonian(final_pos, final_vel, energy_fn),
        s_rng=s_rng)
```

where $metropolis\_hastings\_accept$ and $hamiltonian$ are helper functions, defined as follows.

```
def metropolis_hastings_accept(energy_prev, energy_next, s_rng):
    """
    Performs a Metropolis-Hastings accept-reject move.

    Parameters
    ----------
    energy_prev: theano vector
        Symbolic theano tensor which contains the energy associated with the
        configuration at time-step t.
    energy_next: theano vector
        Symbolic theano tensor which contains the energy associated with the
        proposed configuration at time-step t+1.
```

```
    s_rng: theano.tensor.shared_randomstreams.RandomStreams
        Theano shared random stream object used to generate the random number
        used in proposal.

    Returns
    -------
    return: boolean
        True if move is accepted, False otherwise
    """
    ediff = energy_prev - energy_next
    return (TT.exp(ediff) - s_rng.uniform(size=energy_prev.shape)) >= 0


def hamiltonian(pos, vel, energy_fn):
    """ ... """
    # assuming mass is 1
    return energy_fn(pos) + kinetic_energy(vel)

def kinetic_energy(vel):
    """ ... """
    return 0.5 * (vel ** 2).sum(axis=1)
```

hmc_move finally returns the tuple $(accept, final\_pos)$. $accept$ is a symbolic boolean variable indicating whether or not the new state $final_pos$ should be used or not.

hmc_updates

The purpose of $hmc\_updates$ is to generate the list of updates to perform, whenever our HMC sampling function is called. $hmc\_updates$ thus receives as parameters, a series of shared variables to update ($positions$, $stepsize$ and $avg\_acceptance\_rate$), and the parameters required to compute their new state.

```
def hmc_updates(positions, stepsize, avg_acceptance_rate, final_pos, accept,
                target_acceptance_rate, stepsize_inc, stepsize_dec,
                stepsize_min, stepsize_max, avg_acceptance_slowness):

    ## POSITION UPDATES ##
    # broadcast `accept` scalar to tensor with the same dimensions as final_pos.
    accept_matrix = accept.dimshuffle(0, *(('x',) * (final_pos.ndim - 1)))
    # if accept is True, update to `final_pos` else stay put
    new_positions = TT.switch(accept_matrix, final_pos, positions)
```

Using the above code, the dictionary $positions : new\_positions$ can be used to update the state of the sampler with either (1) the new state $final\_pos$ if $accept$ is True, or (2) the old state if $accept$ is False. This conditional assignment is performed by the switch op.

$switch$ expects as its first argument, a boolean mask with the same broadcastable dimensions as the second and third argument. Since $accept$ is scalar-valued, we must first use dimshuffle to transform it to a tensor with $final\_pos.ndim$ broadcastable dimensions ($accept\_matrix$).

$hmc\_updates$ additionally implements an adaptive version of HMC, as implemented in the accompanying code to [Ranzato10]. We start by tracking the average acceptance rate of the HMC move proposals (across many simulations), using an exponential moving average with time constant $1 - avg\_acceptance\_slowness$.

```
## ACCEPT RATE UPDATES ##
# perform exponential moving average
new_acceptance_rate = TT.add(
        avg_acceptance_slowness * avg_acceptance_rate,
        (1.0 - avg_acceptance_slowness) * accept.mean())
```

If the average acceptance rate is larger than the $target\_acceptance\_rate$, we increase the $stepsize$ by a factor of $stepsize\_inc$ in order to increase the mixing rate of our chain. If the average acceptance rate is too low however, $stepsize$ is decreased by a factor of $stepsize\_dec$, yielding a more conservative mixing rate. The clip op allows us to maintain the $stepsize$ in the range [$stepsize\_min$, $stepsize\_max$].

```
## STEPSIZE UPDATES ##
# if acceptance rate is too low, our sampler is too "noisy" and we reduce
# the stepsize. If it is too high, our sampler is too conservative, we can
# get away with a larger stepsize (resulting in better mixing).
_new_stepsize = TT.switch(avg_acceptance_rate > target_acceptance_rate,
                          stepsize * stepsize_inc, stepsize * stepsize_dec)
# maintain stepsize in [stepsize_min, stepsize_max]
new_stepsize = TT.clip(_new_stepsize, stepsize_min, stepsize_max)
```

The final updates list is then returned:

```
return [(positions, new_positions),
        (stepsize, new_stepsize),
        (avg_acceptance_rate, new_acceptance_rate)]
```

HMC_sampler

We finally tie everything together using the $HMC\_Sampler$ class. Its main elements are:

- $new\_from\_shared\_positions$: a constructor method which allocates various shared variables and strings together the calls to hmc_move and $hmc\_updates$. It also builds the theano function $simulate$, whose sole purpose is to execute the updates generated by $hmc\_updates$.
- $draw$: a convenience method which calls the Theano function $simulate$ and returns a copy of the contents of the shared variable $self.positions$.

```
class HMC_sampler(object):
    """
    Convenience wrapper for performing Hybrid Monte Carlo (HMC). It creates the
    symbolic graph for performing an HMC simulation (using `hmc_move` and
    `hmc_updates`). The graph is then compiled into the `simulate` function, a
    theano function which runs the simulation and updates the required shared
    variables.

    Users should interface with the sampler thorugh the `draw` function which
    advances the markov chain and returns the current sample by calling
    `simulate` and `get_position` in sequence.

    The hyper-parameters are the same as those used by Marc'Aurelio's
    'train_mcRBM.py' file (available on his personal home page).
    """

    def __init__(self, **kwargs):
```

```
        self.__dict__.update(kwargs)

    @classmethod
    def new_from_shared_positions(cls, shared_positions, energy_fn,
            initial_stepsize=0.01, target_acceptance_rate=.9, n_steps=20,
            stepsize_dec=0.98,
            stepsize_min=0.001,
            stepsize_max=0.25,
            stepsize_inc=1.02,
            avg_acceptance_slowness=0.9, # used in geometric avg. 1.0 would be not moving a
            seed=12345):
        """
        :param shared_positions: theano ndarray shared var with many particle [initial] pos
        :param energy_fn:
            callable such that energy_fn(positions)
            returns theano vector of energies.
            The len of this vector is the batchsize.

            The sum of this energy vector must be differentiable (with theano.tensor.grad)
            respect to the positions for HMC sampling to work.
        """
        batchsize = shared_positions.shape[0]

        # allocate shared variables
        stepsize = sharedX(initial_stepsize, 'hmc_stepsize')
        avg_acceptance_rate = sharedX(target_acceptance_rate, 'avg_acceptance_rate')
        s_rng = TT.shared_randomstreams.RandomStreams(seed)

        # define graph for an `n_steps` HMC simulation
        accept, final_pos = hmc_move(
                s_rng,
                shared_positions,
                energy_fn,
                stepsize,
                n_steps)

        # define the list of updates, to apply on every `simulate` call
        simulate_updates = hmc_updates(
                shared_positions,
                stepsize,
                avg_acceptance_rate,
                final_pos=final_pos,
                accept=accept,
                stepsize_min=stepsize_min,
                stepsize_max=stepsize_max,
                stepsize_inc=stepsize_inc,
                stepsize_dec=stepsize_dec,
                target_acceptance_rate=target_acceptance_rate,
                avg_acceptance_slowness=avg_acceptance_slowness)

        # compile theano function
        simulate = function([], [], updates=simulate_updates)
```

```
        # create HMC_sampler object with the following attributes ...
        return cls(
                positions=shared_positions,
                stepsize=stepsize,
                stepsize_min=stepsize_min,
                stepsize_max=stepsize_max,
                avg_acceptance_rate=avg_acceptance_rate,
                target_acceptance_rate=target_acceptance_rate,
                s_rng=s_rng,
                _updates=simulate_updates,
                simulate=simulate)

    def draw(self, **kwargs):
        """
        Returns a new position obtained after `n_steps` of HMC simulation.

        Parameters
        ----------
        kwargs: dictionary
            The `kwargs` dictionary is passed to the shared variable
            (self.positions) `get_value()` function.  For example, to avoid
            copying the shared variable value, consider passing `borrow=True`.

        Returns
        -------
        rval: numpy matrix
            Numpy matrix whose of dimensions similar to `initial_position`.
       """
        self.simulate()
        return self.positions.get_value(borrow=False)
```

11.3 Testing our Sampler

We test our implementation of HMC by sampling from a multi-variate Gaussian distribution. We start by generating a random mean vector mu and covariance matrix cov, which allows us to define the energy function of the corresponding Gaussian distribution: $gaussian\_energy$. We then initialize the state of the sampler by allocating a $position$ shared variable. It is passed to the constructor of $HMC\_sampler$ along with our target energy function.

Following a burn-in period, we then generate a large number of samples and compare the empirical mean and covariance matrix to their true values.

```
def sampler_on_nd_gaussian(sampler_cls, burnin, n_samples, dim=10):
    batchsize=3

    rng = np.random.RandomState(123)

    # Define a covariance and mu for a gaussian
    mu  = np.array(rng.rand(dim) * 10, dtype=theano.config.floatX)
    cov = np.array(rng.rand(dim, dim), dtype=theano.config.floatX)
    cov = (cov + cov.T) / 2.
```

```
    cov[numpy.arange(dim), numpy.arange(dim)] = 1.0
    cov_inv = linalg.inv(cov)

    # Define energy function for a multi-variate Gaussian
    def gaussian_energy(x):
        return 0.5 * (TT.dot((x - mu), cov_inv) * (x - mu)).sum(axis=1)

    # Declared shared random variable for positions
    position = shared(rng.randn(batchsize, dim).astype(theano.config.floatX))

    # Create HMC sampler
    sampler = sampler_cls(position, gaussian_energy,
            initial_stepsize=1e-3, stepsize_max=0.5)

    # Start with a burn-in process
    garbage = [sampler.draw() for r in xrange(burnin)]  #burn-in
    # Draw `n_samples`: result is a 3D tensor of dim [n_samples, batchsize, dim]
    _samples = np.asarray([sampler.draw() for r in xrange(n_samples)])
    # Flatten to [n_samples * batchsize, dim]
    samples = _samples.T.reshape(dim, -1).T

    print '****** TARGET VALUES ******'
    print 'target mean:', mu
    print 'target cov:\n', cov

    print '****** EMPIRICAL MEAN/COV USING HMC ******'
    print 'empirical mean: ', samples.mean(axis=0)
    print 'empirical_cov:\n', np.cov(samples.T)

    print '****** HMC INTERNALS ******'
    print 'final stepsize', sampler.stepsize.get_value()
    print 'final acceptance_rate', sampler.avg_acceptance_rate.get_value()

    return sampler

def test_hmc():
    sampler = sampler_on_nd_gaussian(HMC_sampler.new_from_shared_positions,
            burnin=1000, n_samples=1000, dim=5)
    assert abs(sampler.avg_acceptance_rate.get_value() -
               sampler.target_acceptance_rate) < .1
    assert sampler.stepsize.get_value() >= sampler.stepsize_min
    assert sampler.stepsize.get_value() <= sampler.stepsize_max
```

The above code can be run using the command: "nosetests -s code/hmc/test_hmc.py". The output is as follows:

```
[desjagui@atchoum hmc]$ python test_hmc.py

****** TARGET VALUES ******
target mean: [ 6.96469186  2.86139335  2.26851454  5.51314769  7.1946897 ]
target cov:
[[ 1.          0.66197111  0.71141257  0.55766643  0.35753822]
 [ 0.66197111  1.          0.31053199  0.45455485  0.37991646]
```

```
 [ 0.71141257  0.31053199  1.          0.62800335  0.38004541]
 [ 0.55766643  0.45455485  0.62800335  1.          0.50807871]
 [ 0.35753822  0.37991646  0.38004541  0.50807871  1.        ]]

****** EMPIRICAL MEAN/COV USING HMC ******
empirical mean:  [ 6.94155164  2.81526039  2.26301715  5.46536853  7.19414496]
empirical_cov:
[[ 1.05152997  0.68393537  0.76038645  0.59930252  0.37478746]
 [ 0.68393537  0.97708159  0.37351422  0.48362404  0.3839558 ]
 [ 0.76038645  0.37351422  1.03797111  0.67342957  0.41529132]
 [ 0.59930252  0.48362404  0.67342957  1.02865056  0.53613649]
 [ 0.37478746  0.3839558   0.41529132  0.53613649  0.98721449]]

****** HMC INTERNALS ******
final stepsize 0.460446628091
final acceptance_rate 0.922502043428
```

As can be seen above, the samples generated by our HMC sampler yield an empirical mean and covariance matrix, which are very close to the true underlying parameters. The adaptive algorithm also seemed to work well as the final acceptance rate is close to our target of 0.9.

11.4 References

CHAPTER

TWELVE

MODELING AND GENERATING SEQUENCES OF POLYPHONIC MUSIC WITH THE RNN-RBM

Note: This tutorial demonstrates a basic implementation of the RNN-RBM as described in [Boulanger-Lewandowski12] (pdf). We assume the reader is familiar with recurrent neural networks using the scan op and restricted Boltzmann machines (RBM).

Note: The code for this section is available for download here: rnnrbm.py.

You will need the modified Python MIDI package (GPL license) in your `$PYTHONPATH` or in the working directory in order to convert MIDI files to and from piano-rolls. The script also assumes that the content of the Nottingham Database of folk tunes has been extracted in the `../data` directory. Alternative MIDI datasets are available here.

Note that both dependencies above can be setup automatically by running the `download.sh` script in the `../data` directory.

Caution: Depending on your locally installed Theano version, you may have problems running this script. If this is the case, please use the 'bleeding-edge' developer version from github.

12.1 The RNN-RBM

The RNN-RBM is an energy-based model for density estimation of temporal sequences, where the feature vector $v^{(t)}$ at time step t may be high-dimensional. It allows to describe multimodal conditional distributions of $v^{(t)}|\mathcal{A}^{(t)}$, where $\mathcal{A}^{(t)} \equiv \{v_\tau|\tau < t\}$ denotes the *sequence history* at time t, via a series of conditional RBMs (one a each time step) whose parameters $b_v^{(t)}, b_h^{(t)}$ depend on the output of a deterministic RNN with hidden units $u^{(t)}$:

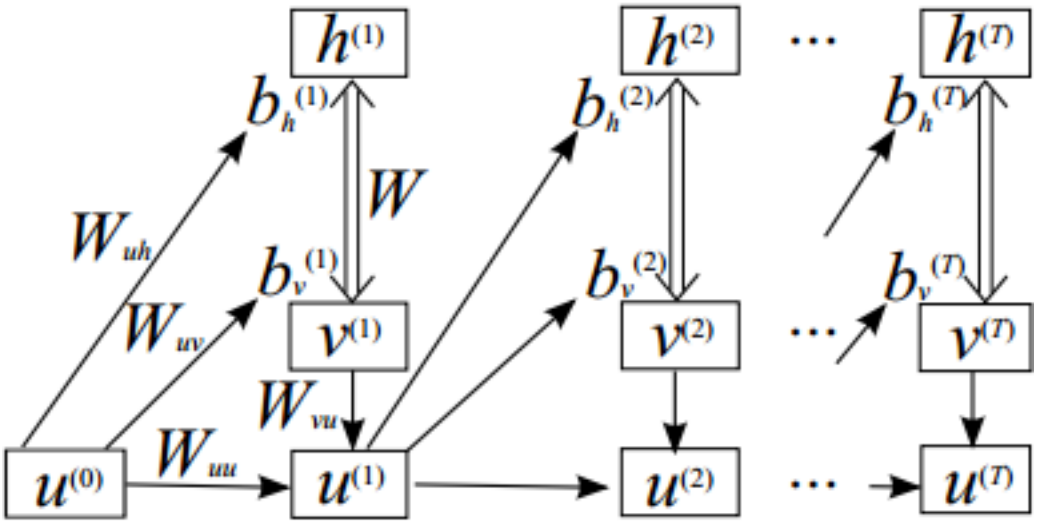
$$b_v^{(t)} = b_v + W_{uv}u^{(t-1)} \tag{12.1}$$

$$b_h^{(t)} = b_h + W_{uh}u^{(t-1)} \tag{12.2}$$

and the single-layer RNN recurrence relation is defined by:

$$u^{(t)} = \tanh(b_u + W_{uu}u^{(t-1)} + W_{vu}v^{(t)}) \tag{12.3}$$

The resulting model is unrolled in time in the following figure:



The overall probability distribution is given by the sum over the T time steps in a given sequence:

$$P(\{v^{(t)}\}) = \sum_{t=1}^{T} P(v^{(t)}|\mathcal{A}^{(t)}) \tag{12.4}$$

where the right-hand side multiplicand is the marginalized probability of the t^{th} RBM.

Note that for clarity of the implementation, contrarily to [BoulangerLewandowski12], we use the obvious naming convention for weight matrices and we use $u^{(t)}$ instead of $\hat{h}^{(t)}$ for the recurrent hidden units.

12.2 Implementation

We wish to construct two Theano functions: one to train the RNN-RBM, and one to generate sample sequences from it.

For *training*, i.e. given $\{v^{(t)}\}$, the RNN hidden state $\{u^{(t)}\}$ and the associated $\{b_v^{(t)}, b_h^{(t)}\}$ parameters are deterministic and can be readily computed for each training sequence. A stochastic gradient descent (SGD) update on the parameters can then be estimated via contrastive divergence (CD) on the individual time steps of a sequence in the same way that individual training examples are treated in a mini-batch for regular RBMs.

Sequence generation is similar except that the $v^{(t)}$ must be sampled sequentially at each time step with a separate (non-batch) Gibbs chain before being passed down to the recurrence and the sequence history.

12.2.1 The RBM layer

The `build_rbm` function shown below builds a Gibbs chain from an input mini-batch (a binary matrix) via the CD approximation. Note that it also supports a single frame (a binary vector) in the non-batch case.

```
def build_rbm(v, W, bv, bh, k):
    '''Construct a k-step Gibbs chain starting at v for an RBM.

v : Theano vector or matrix
  If a matrix, multiple chains will be run in parallel (batch).
W : Theano matrix
  Weight matrix of the RBM.
bv : Theano vector
  Visible bias vector of the RBM.
bh : Theano vector
  Hidden bias vector of the RBM.
k : scalar or Theano scalar
  Length of the Gibbs chain.

Return a (v_sample, cost, monitor, updates) tuple:

v_sample : Theano vector or matrix with the same shape as `v`
  Corresponds to the generated sample(s).
cost : Theano scalar
  Expression whose gradient with respect to W, bv, bh is the CD-k approximation
  to the log-likelihood of `v` (training example) under the RBM.
  The cost is averaged in the batch case.
monitor: Theano scalar
  Pseudo log-likelihood (also averaged in the batch case).
updates: dictionary of Theano variable -> Theano variable
  The `updates` object returned by scan.'''

    def gibbs_step(v):
        mean_h = T.nnet.sigmoid(T.dot(v, W) + bh)
        h = rng.binomial(size=mean_h.shape, n=1, p=mean_h,
                         dtype=theano.config.floatX)
        mean_v = T.nnet.sigmoid(T.dot(h, W.T) + bv)
        v = rng.binomial(size=mean_v.shape, n=1, p=mean_v,
                         dtype=theano.config.floatX)
        return mean_v, v

    chain, updates = theano.scan(lambda v: gibbs_step(v)[1], outputs_info=[v],
                                 n_steps=k)
    v_sample = chain[-1]

    mean_v = gibbs_step(v_sample)[0]
    monitor = T.xlogx.xlogy0(v, mean_v) + T.xlogx.xlogy0(1 - v, 1 - mean_v)
    monitor = monitor.sum() / v.shape[0]

    def free_energy(v):
        return -(v * bv).sum() - T.log(1 + T.exp(T.dot(v, W) + bh)).sum()
    cost = (free_energy(v) - free_energy(v_sample)) / v.shape[0]

    return v_sample, cost, monitor, updates
```

12.2.2 The RNN layer

The `build_rnnrbm` function defines the RNN recurrence relation to obtain the RBM parameters; the recurrence function is flexible enough to serve both in the training scenario where $v^{(t)}$ is given and the "batch" RBM is constructed at the end on the whole sequence at once, and in the generation scenario where $v^{(t)}$ is sampled separately at each time step using the Gibbs chain defined above.

```
def build_rnnrbm(n_visible, n_hidden, n_hidden_recurrent):
    '''Construct a symbolic RNN-RBM and initialize parameters.

n_visible : integer
  Number of visible units.
n_hidden : integer
  Number of hidden units of the conditional RBMs.
n_hidden_recurrent : integer
  Number of hidden units of the RNN.

Return a (v, v_sample, cost, monitor, params, updates_train, v_t,
          updates_generate) tuple:

v : Theano matrix
  Symbolic variable holding an input sequence (used during training)
v_sample : Theano matrix
  Symbolic variable holding the negative particles for CD log-likelihood
  gradient estimation (used during training)
cost : Theano scalar
  Expression whose gradient (considering v_sample constant) corresponds to the
  LL gradient of the RNN-RBM (used during training)
monitor : Theano scalar
  Frame-level pseudo-likelihood (useful for monitoring during training)
params : tuple of Theano shared variables
  The parameters of the model to be optimized during training.
updates_train : dictionary of Theano variable -> Theano variable
  Update object that should be passed to theano.function when compiling the
  training function.
v_t : Theano matrix
  Symbolic variable holding a generated sequence (used during sampling)
updates_generate : dictionary of Theano variable -> Theano variable
  Update object that should be passed to theano.function when compiling the
  generation function.'''

    W = shared_normal(n_visible, n_hidden, 0.01)
    bv = shared_zeros(n_visible)
    bh = shared_zeros(n_hidden)
    Wuh = shared_normal(n_hidden_recurrent, n_hidden, 0.0001)
    Wuv = shared_normal(n_hidden_recurrent, n_visible, 0.0001)
    Wvu = shared_normal(n_visible, n_hidden_recurrent, 0.0001)
    Wuu = shared_normal(n_hidden_recurrent, n_hidden_recurrent, 0.0001)
    bu = shared_zeros(n_hidden_recurrent)

    params = W, bv, bh, Wuh, Wuv, Wvu, Wuu, bu  # learned parameters as shared
                                                # variables
```

```
    v = T.matrix()  # a training sequence
    u0 = T.zeros((n_hidden_recurrent,))  # initial value for the RNN hidden
                                         # units

    # If `v_t` is given, deterministic recurrence to compute the variable
    # biases bv_t, bh_t at each time step. If `v_t` is None, same recurrence
    # but with a separate Gibbs chain at each time step to sample (generate)
    # from the RNN-RBM. The resulting sample v_t is returned in order to be
    # passed down to the sequence history.
    def recurrence(v_t, u_tm1):
        bv_t = bv + T.dot(u_tm1, Wuv)
        bh_t = bh + T.dot(u_tm1, Wuh)
        generate = v_t is None
        if generate:
            v_t, _, _, updates = build_rbm(T.zeros((n_visible,)), W, bv_t,
                                           bh_t, k=25)
        u_t = T.tanh(bu + T.dot(v_t, Wvu) + T.dot(u_tm1, Wuu))
        return ([v_t, u_t], updates) if generate else [u_t, bv_t, bh_t]

    # For training, the deterministic recurrence is used to compute all the
    # {bv_t, bh_t, 1 <= t <= T} given v. Conditional RBMs can then be trained
    # in batches using those parameters.
    (u_t, bv_t, bh_t), updates_train = theano.scan(
        lambda v_t, u_tm1, *_: recurrence(v_t, u_tm1),
        sequences=v, outputs_info=[u0, None, None], non_sequences=params)
    v_sample, cost, monitor, updates_rbm = build_rbm(v, W, bv_t[:], bh_t[:],
                                                     k=15)
    updates_train.update(updates_rbm)

    # symbolic loop for sequence generation
    (v_t, u_t), updates_generate = theano.scan(
        lambda u_tm1, *_: recurrence(None, u_tm1),
        outputs_info=[None, u0], non_sequences=params, n_steps=200)

    return (v, v_sample, cost, monitor, params, updates_train, v_t,
            updates_generate)
```

12.2.3 Putting it all together

We now have all the necessary ingredients to start training our network on real symbolic sequences of polyphonic music.

```
class RnnRbm:
    '''Simple class to train an RNN-RBM from MIDI files and to generate sample
sequences.'''

    def __init__(self, n_hidden=150, n_hidden_recurrent=100, lr=0.001,
                 r=(21, 109), dt=0.3):
        '''Constructs and compiles Theano functions for training and sequence
generation.

n_hidden : integer
```

```
  Number of hidden units of the conditional RBMs.
n_hidden_recurrent : integer
  Number of hidden units of the RNN.
lr : float
  Learning rate
r : (integer, integer) tuple
  Specifies the pitch range of the piano-roll in MIDI note numbers, including
  r[0] but not r[1], such that r[1]-r[0] is the number of visible units of the
  RBM at a given time step. The default (21, 109) corresponds to the full range
  of piano (88 notes).
dt : float
  Sampling period when converting the MIDI files into piano-rolls, or
  equivalently the time difference between consecutive time steps.'''

        self.r = r
        self.dt = dt
        (v, v_sample, cost, monitor, params, updates_train, v_t,
         updates_generate) = build_rnnrbm(r[1] - r[0], n_hidden,
                                          n_hidden_recurrent)

        gradient = T.grad(cost, params, consider_constant=[v_sample])
        updates_train.update(((p, p - lr * g) for p, g in zip(params,
                                                              gradient)))
        self.train_function = theano.function([v], monitor,
                                              updates=updates_train)
        self.generate_function = theano.function([], v_t,
                                                 updates=updates_generate)

    def train(self, files, batch_size=100, num_epochs=200):
        '''Train the RNN-RBM via stochastic gradient descent (SGD) using MIDI
files converted to piano-rolls.

files : list of strings
  List of MIDI files that will be loaded as piano-rolls for training.
batch_size : integer
  Training sequences will be split into subsequences of at most this size
  before applying the SGD updates.
num_epochs : integer
  Number of epochs (pass over the training set) performed. The user can
  safely interrupt training with Ctrl+C at any time.'''

        assert len(files) > 0, 'Training set is empty!' \
                               ' (did you download the data files?)'
        dataset = [midiread(f, self.r,
                            self.dt).piano_roll.astype(theano.config.floatX)
                   for f in files]

        try:
            for epoch in xrange(num_epochs):
                numpy.random.shuffle(dataset)
                costs = []

                for s, sequence in enumerate(dataset):
```

```
                    for i in xrange(0, len(sequence), batch_size):
                        cost = self.train_function(sequence[i:i + batch_size])
                        costs.append(cost)

                print 'Epoch %i/%i' % (epoch + 1, num_epochs),
                print numpy.mean(costs)
                sys.stdout.flush()

        except KeyboardInterrupt:
            print 'Interrupted by user.'

    def generate(self, filename, show=True):
        '''Generate a sample sequence, plot the resulting piano-roll and save
it as a MIDI file.

filename : string
  A MIDI file will be created at this location.
show : boolean
  If True, a piano-roll of the generated sequence will be shown.'''

        piano_roll = self.generate_function()
        midiwrite(filename, piano_roll, self.r, self.dt)
        if show:
            extent = (0, self.dt * len(piano_roll)) + self.r
            pylab.figure()
            pylab.imshow(piano_roll.T, origin='lower', aspect='auto',
                         interpolation='nearest', cmap=pylab.cm.gray_r,
                         extent=extent)
            pylab.xlabel('time (s)')
            pylab.ylabel('MIDI note number')
            pylab.title('generated piano-roll')


if __name__ == '__main__':
    model = RnnRbm()
    model.train(glob.glob('../data/Nottingham/train/*.mid'))
    model.generate('sample1.mid')
    model.generate('sample2.mid')
    pylab.show()
```

12.3 Results

We ran the code on the Nottingham database for 200 epochs; training took approximately 24 hours.

The output was the following:

```
Epoch 1/200 -15.0308940028
Epoch 2/200 -10.4892606673
Epoch 3/200 -10.2394696138
Epoch 4/200 -10.1431669994
Epoch 5/200 -9.7005382843
```

```
Epoch 6/200 -8.5985647524
Epoch 7/200 -8.35115428534
Epoch 8/200 -8.26453580552
Epoch 9/200 -8.21208991542
Epoch 10/200 -8.16847274143

... truncated for brevity ...

Epoch 190/200 -4.74799179994
Epoch 191/200 -4.73488515216
Epoch 192/200 -4.7326138489
Epoch 193/200 -4.73841636884
Epoch 194/200 -4.70255511452
Epoch 195/200 -4.71872634914
Epoch 196/200 -4.7276415885
Epoch 197/200 -4.73497644728
Epoch 198/200 -inf
Epoch 199/200 -4.75554987143
Epoch 200/200 -4.72591935412
```

The figures below show the piano-rolls of two sample sequences and we provide the corresponding MIDI files:

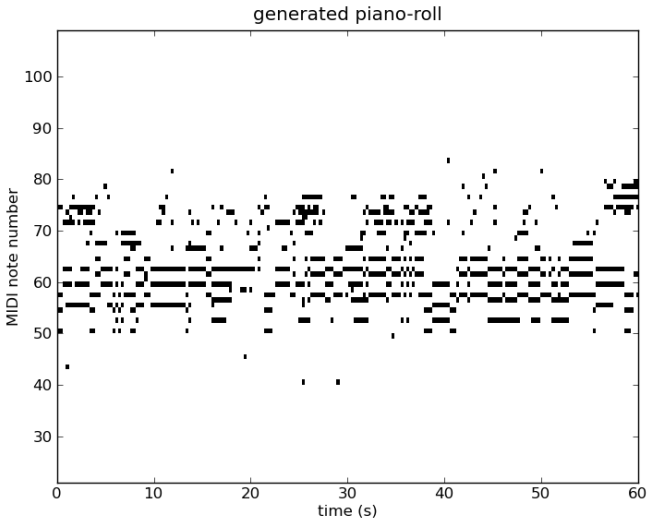


Figure 12.1: Listen to sample1.mid

12.4 How to improve this code

The code shown in this tutorial is a stripped-down version that can be improved in the following ways:

- Preprocessing: transposing the sequences in a common tonality (e.g. C major / minor) and normalizing the tempo in beats (quarternotes) per minute can have the most effect on the generative quality of the model.

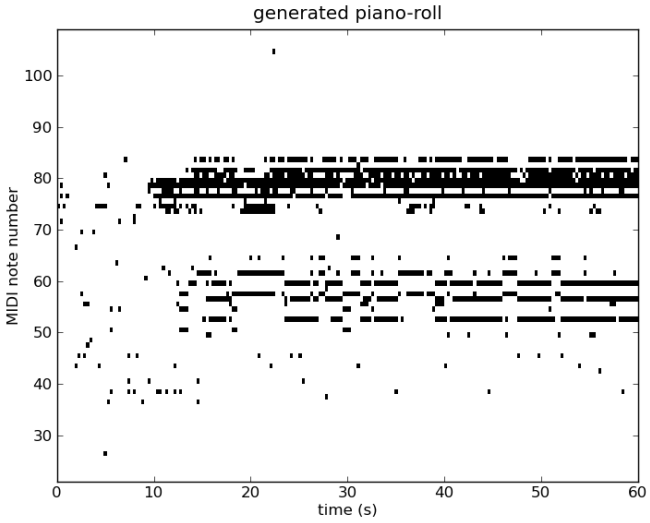


Figure 12.2: Listen to sample2.mid

- Pretraining techniques: initialize the W, b_v, b_h parameters with independent RBMs with fully shuffled frames (i.e. $W_{uh} = W_{uv} = W_{uu} = W_{vu} = 0$); initialize the $W_{uv}, W_{uu}, W_{vu}, b_u$ parameters of the RNN with the auxiliary cross-entropy objective via either SGD or, preferably, Hessian-free optimization [BoulangerLewandowski12].
- Optimization techniques: gradient clipping, Nesterov momentum and the use of NADE for conditional density estimation.
- Hyperparameter search: learning rate (separately for the RBM and RNN parts), learning rate schedules, batch size, number of hidden units (recurrent and RBM), momentum coefficient, momentum schedule, Gibbs chain length k and early stopping.
- Learn the initial condition $u^{(0)}$ as a model parameter.

A few samples generated with code including these features are available here: sequences.zip.

CHAPTER

THIRTEEN

MISCELLANEOUS

13.1 Plotting Samples and Filters

Note: The code for this section is available for download here.

To plot a sample, what we need to do is to take the visible units, which are a flattened image (there is no 2D structure to the visible units, just a 1D string of unit activations) and reshape it into a 2D image. The order in which the points from the 1D array go into the 2D image is given by the order in which the inital MNIST images where converted into a 1D array. Lucky for us this is just a call of the `numpy.reshape` function.

Plotting the weights is a bit more tricky. We have `n_hidden` hidden units, each of them corresponding to a column of the weight matrix. A column has the same shape as the visible, where the weight corresponding to the connection with visible unit j is at position j. Therefore, if we reshape every such column, using `numpy.reshape`, we get a filter image that tells us how this hidden unit is influenced by the input image.

We need a utility function that takes a minibatch, or the weight matrix, and converts each row (for the weight matrix we do a transpose) into a 2D image and then tile these images together. Once we converted the minibatch or the weights in this image of tiles, we can use PIL to plot and save. PIL is a standard python libarary to deal with images.

Tiling minibatches together is done for us by the `tile_raster_image` function which we provide here.

```
def scale_to_unit_interval(ndar, eps=1e-8):
  """ Scales all values in the ndarray ndar to be between 0 and 1 """
  ndar = ndar.copy()
  ndar -= ndar.min()
  ndar *= 1.0 / (ndar.max() + eps)
  return ndar


def tile_raster_images(X, img_shape, tile_shape, tile_spacing=(0, 0),
                       scale_rows_to_unit_interval=True,
                       output_pixel_vals=True):
  """
  Transform an array with one flattened image per row, into an array in
  which images are reshaped and layed out like tiles on a floor.

  This function is useful for visualizing datasets whose rows are images,
  and also columns of matrices for transforming those rows
```

```
    (such as the first layer of a neural net).

    :type X: a 2-D ndarray or a tuple of 4 channels, elements of which can
    be 2-D ndarrays or None;
    :param X: a 2-D array in which every row is a flattened image.

    :type img_shape: tuple; (height, width)
    :param img_shape: the original shape of each image

    :type tile_shape: tuple; (rows, cols)
    :param tile_shape: the number of images to tile (rows, cols)

    :param output_pixel_vals: if output should be pixel values (i.e. int8
    values) or floats

    :param scale_rows_to_unit_interval: if the values need to be scaled before
    being plotted to [0,1] or not


    :returns: array suitable for viewing as an image.
    (See:`PIL.Image.fromarray`.)
    :rtype: a 2-d array with same dtype as X.

    """

    assert len(img_shape) == 2
    assert len(tile_shape) == 2
    assert len(tile_spacing) == 2

    # The expression below can be re-written in a more C style as
    # follows :
    #
    # out_shape = [0,0]
    # out_shape[0] = (img_shape[0] + tile_spacing[0]) * tile_shape[0] -
    #                tile_spacing[0]
    # out_shape[1] = (img_shape[1] + tile_spacing[1]) * tile_shape[1] -
    #                tile_spacing[1]
    out_shape = [(ishp + tsp) * tshp - tsp for ishp, tshp, tsp
                        in zip(img_shape, tile_shape, tile_spacing)]

    if isinstance(X, tuple):
        assert len(X) == 4
        # Create an output numpy ndarray to store the image
        if output_pixel_vals:
            out_array = numpy.zeros((out_shape[0], out_shape[1], 4), dtype='uint8')
        else:
            out_array = numpy.zeros((out_shape[0], out_shape[1], 4), dtype=X.dtype)

        #colors default to 0, alpha defaults to 1 (opaque)
        if output_pixel_vals:
            channel_defaults = [0, 0, 0, 255]
        else:
            channel_defaults = [0., 0., 0., 1.]
```

```
        for i in xrange(4):
            if X[i] is None:
                # if channel is None, fill it with zeros of the correct
                # dtype
                out_array[:, :, i] = numpy.zeros(out_shape,
                        dtype='uint8' if output_pixel_vals else out_array.dtype
                        ) + channel_defaults[i]
            else:
                # use a recurrent call to compute the channel and store it
                # in the output
                out_array[:, :, i] = tile_raster_images(X[i], img_shape, tile_shape, tile_spa
        return out_array

    else:
        # if we are dealing with only one channel
        H, W = img_shape
        Hs, Ws = tile_spacing

        # generate a matrix to store the output
        out_array = numpy.zeros(out_shape, dtype='uint8' if output_pixel_vals else X.dtype)


        for tile_row in xrange(tile_shape[0]):
            for tile_col in xrange(tile_shape[1]):
                if tile_row * tile_shape[1] + tile_col < X.shape[0]:
                    if scale_rows_to_unit_interval:
                        # if we should scale values to be between 0 and 1
                        # do this by calling the `scale_to_unit_interval`
                        # function
                        this_img = scale_to_unit_interval(X[tile_row * tile_shape[1] + tile_c
                    else:
                        this_img = X[tile_row * tile_shape[1] + tile_col].reshape(img_shape)
                    # add the slice to the corresponding position in the
                    # output array
                    out_array[
                        tile_row * (H+Hs): tile_row * (H + Hs) + H,
                        tile_col * (W+Ws): tile_col * (W + Ws) + W
                        ] \
                        = this_img * (255 if output_pixel_vals else 1)
        return out_array
```

CHAPTER

FOURTEEN

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