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

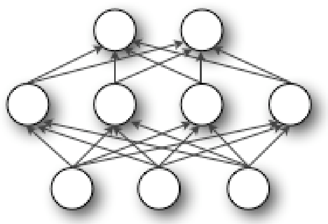
The code for this section is available for download here.

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 regression classifier where the input is first transformed using a learnt non-linear transformation Φ. This transformation projects 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.

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 is 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 $W^{(1)}_{\cdot i}$ 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 !

Going from logistic regression to MLP

This tutorial will focus on a single-hidden-layer MLP. We start off by implementing a class that will represent a 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, 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
```

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 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
```

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.

```
        lin_output = T.dot(input, self.W) + self.b
        self.output = (
            lin_output if activation is None
            else activation(lin_output)
        )
```

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 graph 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 softmax 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 HiddenLayer with a tanh activation function connected to the
        # LogisticRegression layer; the activation function can be replaced by
        # sigmoid or any other nonlinear function
        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 (sotred in params)
    # the resulting gradients will be stored in a list gparams
    gparams = [T.grad(cost, param) for param in classifier.params]

    # specify how to update the parameters of the model as a list of
    # (variable, update expression) pairs

    # given two lists of the same length, A = [a1, a2, a3, a4] and
    # B = [b1, b2, b3, b4], 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)]
    updates = [
        (param, param - learning_rate * gparam)
        for param, gparam in zip(classifier.params, gparams)
    ]

    # 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]
        }
    )
```

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 os
import sys
import timeit

import numpy

import theano
import theano.tensor as T


from logistic_sgd import LogisticRegression, load_data


# start-snippet-1
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
        # end-snippet-1

        # `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]


# start-snippet-2
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 softmax 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 HiddenLayer with a tanh activation function connected to the
        # LogisticRegression layer; the activation function can be replaced by
        # sigmoid or any other nonlinear function
        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
        )
        # end-snippet-2 start-snippet-3
        # 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
        # end-snippet-3

        # keep track of model input
        self.input = input


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
    )

    # start-snippet-4
    # 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
    )
    # end-snippet-4

    # 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]
        }
    )

    # start-snippet-5
    # compute the gradient of cost with respect to theta (sotred in params)
    # the resulting gradients will be stored in a list gparams
    gparams = [T.grad(cost, param) for param in classifier.params]

    # specify how to update the parameters of the model as a list of
    # (variable, update expression) pairs

    # given two lists of the same length, A = [a1, a2, a3, a4] and
    # B = [b1, b2, b3, b4], 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)]
```

```
    updates = [
        (param, param - learning_rate * gparam)
        for param, gparam in zip(classifier.params, gparams)
    ]

    # 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]
        }
    )
    # end-snippet-5

    ###############
    # 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_validation_loss = numpy.inf
    best_iter = 0
    test_score = 0.
    start_time = timeit.default_timer()

    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
```