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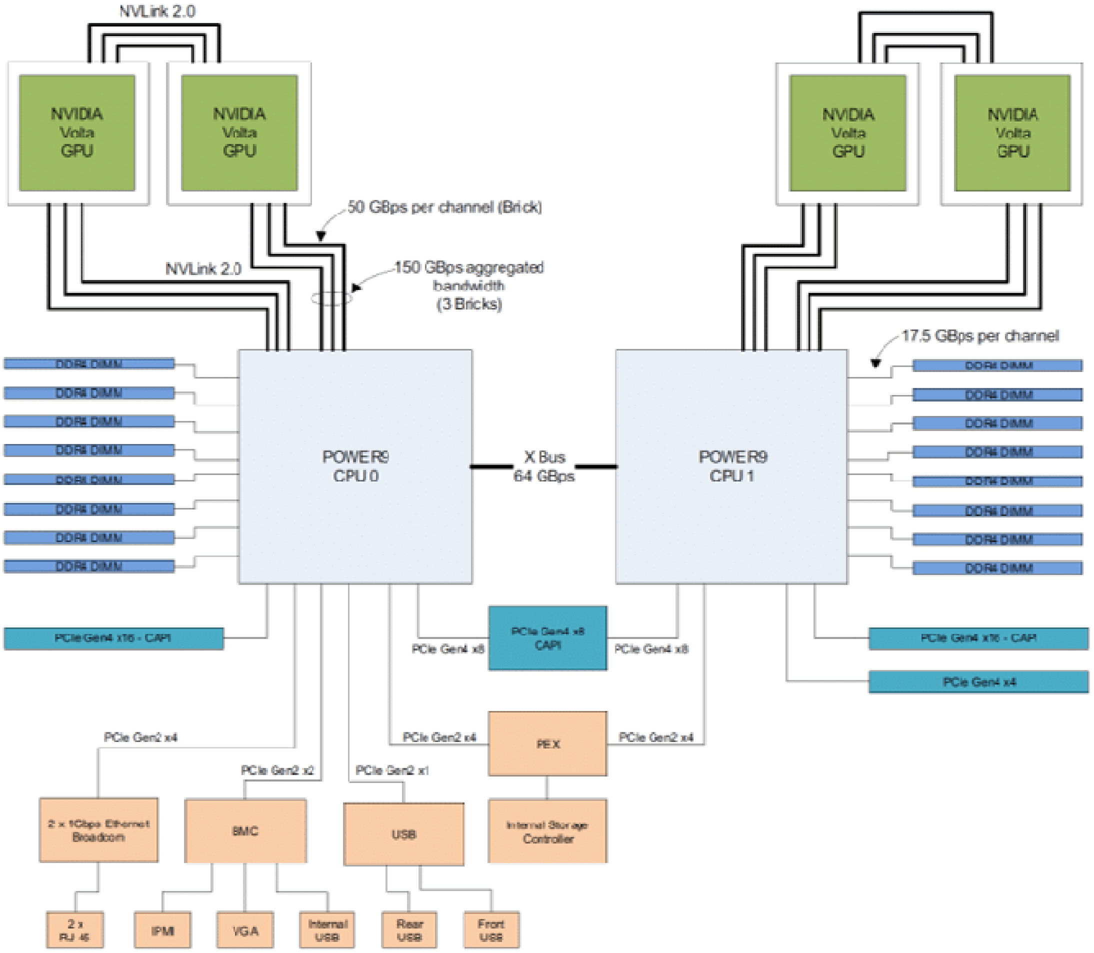
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Guided Laboratory on High Performance Computing Aspects of Deep Learning

Marc Casas (marc.casas@bsc.es)

The Power9 Cluster

- It is a heterogeneous CPU-GPU cluster.
- Its main computational power is provided by NVIDIA GPUS.
  - 2 x IBM Power9 8335-GTH @ 2.4GHz
    - 3.0GHz on turbo,
    - 20 cores and 4 threads/core, total 160 threads per node.
  - 512GB of main memory distributed in 16 dimms x 32GB @ 2666MHz
  - 4 x GPU NVIDIA V100 (Volta) with 16GB HBM2.



Setting Up the Environment

- ssh to Power9: “ssh plogin1.bsc.es”

- Pick up the files of this lab and put them in a folder
  - Decompress and untar the file.

- Use “sbatch script2launch.sh” to submit jobs to the queues.

Setting Up the Environment

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```
#SBATCH --job-name=" multiGPUproof"
#SBATCH --qos=debug
#SBATCH --workdir=.
#SBATCH --output=multiGPU_%j.out
#SBATCH --error=multiGPU_%j.err
#SBATCH --cpus-per-task=40
#SBATCH --gres gpu:1
#SBATCH --time=00:02:00

module purge; module load ffmpeg/4.0.2 gcc/6.4.0 cuda/9.1 cudnn/7.1.3 openmpi/3.0.0 atlas/3.10.3 scalapack/2.0.2 fftw/3.3.7 szip/2.1.1 opencv/3.4.1 python/3.6.5_ML

python gradient_descent.py
#python singlelayer.py
#python multilayer.py
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```

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TensorFlow Basics

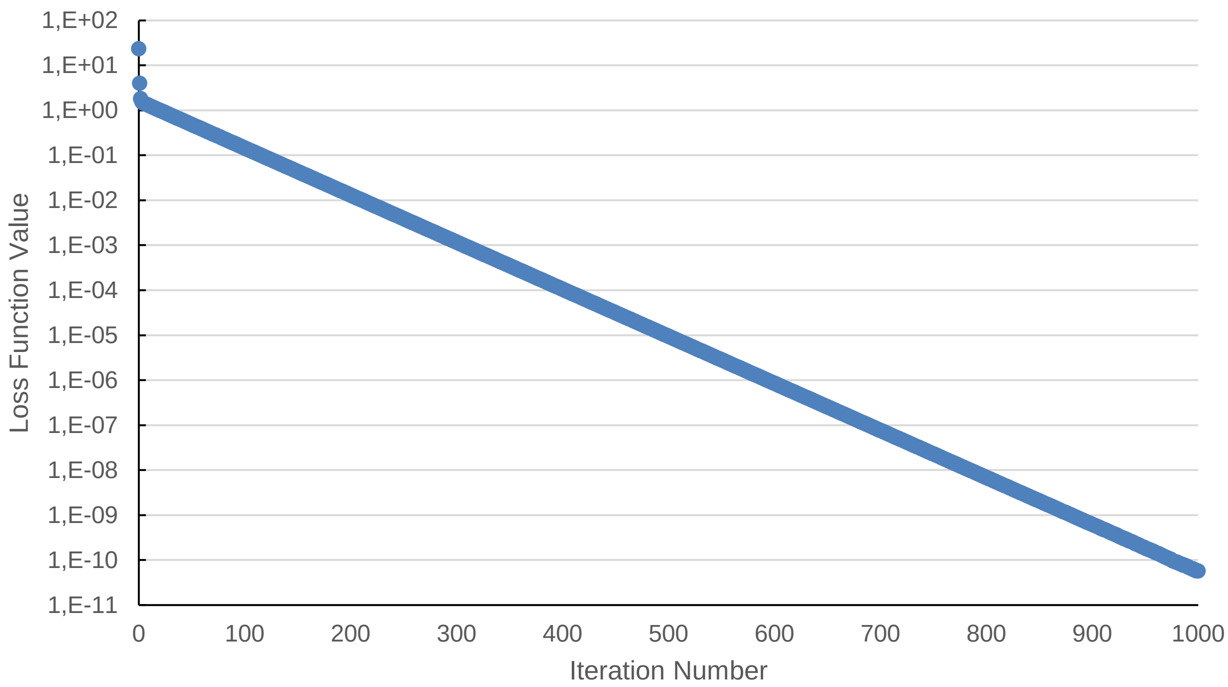
- The central unit of data in TensorFlow (TF) is the **tensor**
- A tensor consists of a set of primitive values shaped into an array of any number of dimensions
- A tensor's **rank** is its number of dimensions.

```
3 # a rank 0 tensor; a scalar with shape []
[1., 2., 3.] # a rank 1 tensor; a vector with shape [3]
[[1., 2., 3.], [4., 5., 6.]] # a rank 2 tensor; a matrix with shape [2, 3]
[[[1., 2., 3.]], [[7., 8., 9.]]] # a rank 3 tensor with shape [2, 1, 3]
```

- TF codes are composed of operations on tensors
- The sequences can be conceived as a computational graph
- TF codes carry out two discrete operations:
  - Building the computational graph
  - Running the computational graph

First TensorFlow example: Optimization Problem

- Goal:
  - Find the linear model $y = Wx + b$ that better fits a set of points
- Optimization Method:
  - GradientDescentOptimizer with a 0.01 step
- Result:



First TensorFlow example: Optimization Problem

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```
#!/usr/bin/env python
import tensorflow as tf


# Model parameters
W = tf.Variable([.3], dtype=tf.float32)
b = tf.Variable([-.3], dtype=tf.float32)
# Model input and output
x = tf.placeholder(tf.float32)
linear_model = W * x + b
y = tf.placeholder(tf.float32)

# loss
loss = tf.reduce_sum(tf.square(linear_model - y)) # sum of the squares
# optimizer
optimizer = tf.train.GradientDescentOptimizer(0.01)
train = optimizer.minimize(loss)

# training data
x_train = [1, 2, 3, 4]
y_train = [0, -1, -2, -3]
# training loop
init = tf.global_variables_initializer()
sess = tf.Session()
sess.run(init) # reset values to wrong

curr_W, curr_b, curr_loss = sess.run([W, b, loss], {x: x_train, y: y_train})
print("W: %s b: %s loss: %s"%(curr_W, curr_b, curr_loss))


for i in range(1000):
  sess.run(train, {x: x_train, y: y_train})
  curr_W, curr_b, curr_loss = sess.run([W, b, loss], {x: x_train, y: y_train})
  print("W: %s b: %s loss: %s"%(curr_W, curr_b, curr_loss))
```

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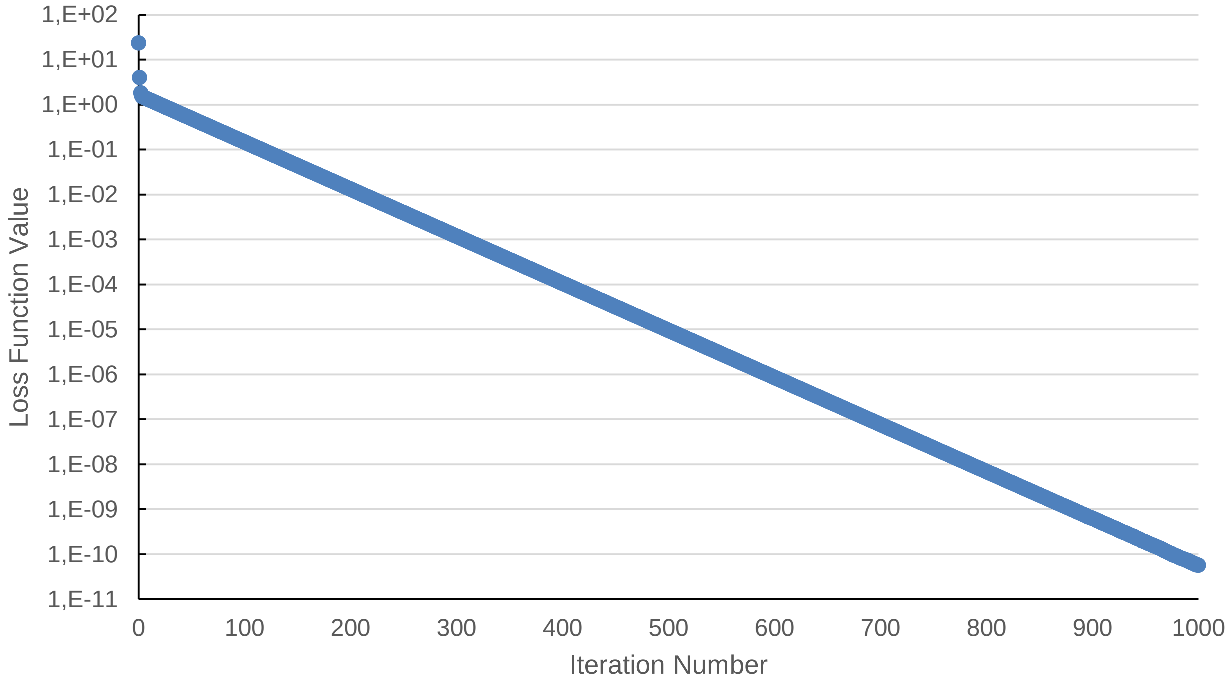
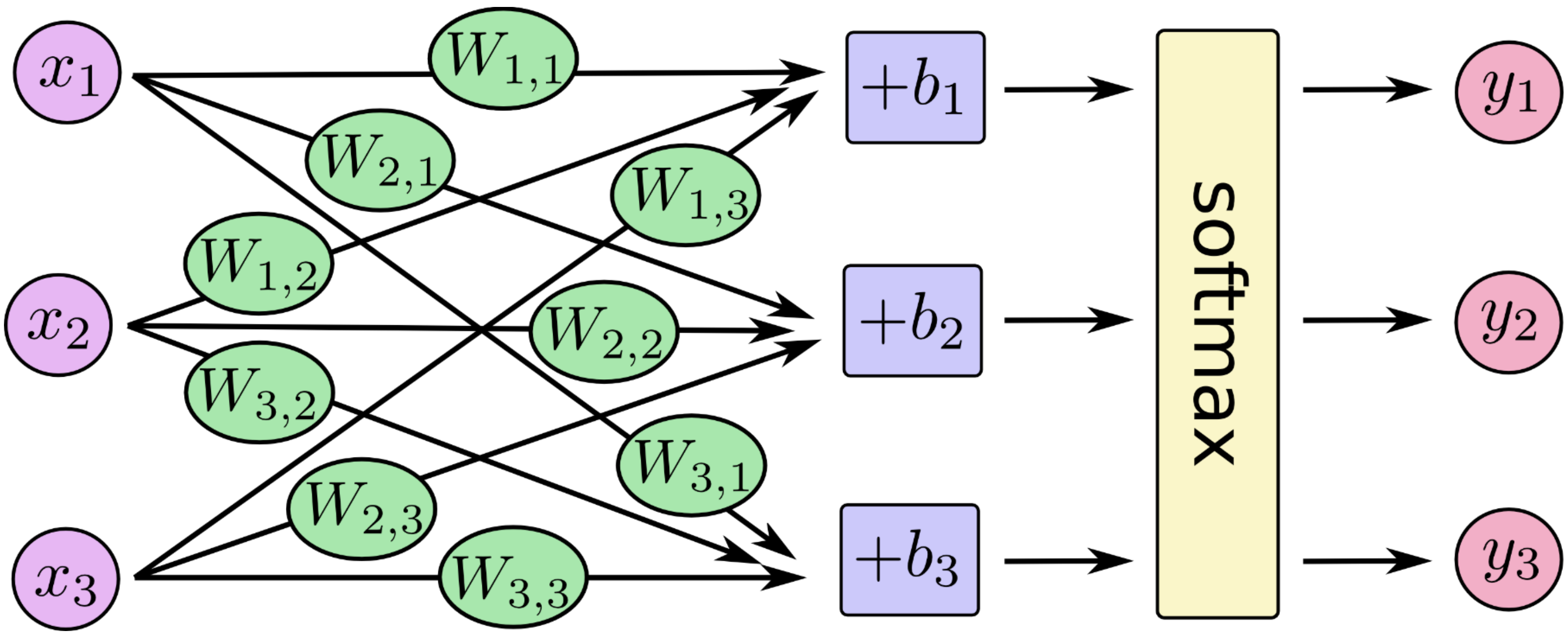
First TensorFlow example: Optimization Problem

- Exercise 1:
  – Try GradientDescentOptimizer with different learning rates
  – Check out other descent methods (look for options online)
  – Represent these extra experiments plus the Gradient Descent with 0.01 learning rate



Second TensorFlow Example: Single Layer Network

- Data Set: MNIST, which is composed of 28x28 pixel images representing a number between 0 and 9. These 28x28 pixel images can be represented by 784 floating point values
- In this example, we implement a very simple single-layer experiment



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- Data Set: MNIST, which is composed of 28x28 pixel images representing a number between 0 and 9. These 28x28 pixel images can be represented by 784 floating point values
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$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \text{softmax}\left(\begin{bmatrix} W_{1,1} & W_{1,2} & W_{1,3} \\ W_{2,1} & W_{2,2} & W_{2,3} \\ W_{3,1} & W_{3,2} & W_{3,3} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)$$

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- The provided implementation obtains a 90.79% accuracy

Second TensorFlow Example: Single Layer Network

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```
#!/usr/bin/env python
import tensorflow as tf
import read_inputs
import numpy as N

#read data from file
data_input = read_inputs.load_data_mnist('MNIST_data/mnist.pkl.gz')
#FYI data = [(train_set_x, train_set_y), (valid_set_x, valid_set_y), (test_set_x, test_set_y)]
data = data_input[0]
#print ( N.shape(data[0][0])[0] )
#print ( N.shape(data[0][1])[0] )

#data layout changes since output should an array of 10 with probabilities
real_output = N.zeros( (N.shape(data[0][1])[0] , 10), dtype=N.float )
for i in range ( N.shape(data[0][1])[0] ):
  real_output[i][data[0][1][i]] = 1.0

#data layout changes since output should an array of 10 with probabilities
real_check = N.zeros( (N.shape(data[2][1])[0] , 10), dtype=N.float )
for i in range ( N.shape(data[2][1])[0] ):
  real_check[i][data[2][1][i]] = 1.0



#set up the computation. Definition of the variables.
x = tf.placeholder(tf.float32, [None, 784])
W = tf.Variable(tf.zeros([784, 10]))
b = tf.Variable(tf.zeros([10]))
y = tf.nn.softmax(tf.matmul(x, W) + b)
y_ = tf.placeholder(tf.float32, [None, 10])

cross_entropy = tf.reduce_mean(-tf.reduce_sum(y_ * tf.log(y), reduction_indices=[1]))

train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)

sess = tf.InteractiveSession()
tf.global_variables_initializer().run()

#TRAINING PHASE
print("TRAINING")

for i in range(500):
  batch_xs = data[0][0][100*i:100*i+100]
  batch_ys = real_output[100*i:100*i+100]
  sess.run(train_step, feed_dict={x: batch_xs, y_: batch_ys})

#CHECKING THE ERROR
print("ERROR CHECK")

correct_prediction = tf.equal(tf.argmax(y, 1), tf.argmax(y_, 1))
accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))
print(sess.run(accuracy, feed_dict={x: data[2][0], y_: real_check}))

"singlelayer.py" 54L, 1748C                                    1,1           Top
```

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Second TensorFlow Example: Single Layer Network

- Data Set: MNIST, which is composed of 28x28 pixel images representing a number between 0 and 9. These 28x28 pixel images can be represented by 784 floating point values
- In this example, we implement a very simple single-layer experiment

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \text{softmax}\left(\begin{bmatrix} W_{1,1} & W_{1,2} & W_{1,3} \\ W_{2,1} & W_{2,2} & W_{2,3} \\ W_{3,1} & W_{3,2} & W_{3,3} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)$$

- Exercise 2:
  - Plot convergence rates in a similar way as the previous exercise
  - Consider different optimizers and learning rates

Third TensorFlow Example: Multiple Layer Network

- Data Set: MNIST
- We consider a deep neural network with:
  – First convolutional layer: 32 features per each 5x5 patch
  – Second convolutional layer: 64 features for each 5x5 patch
  – Densely connected layer: Processes 64 7x7 images with 1024 neurons
  – Dropout rate: 50%
- Current version achieves 95.97% accuracy
- Exercise 3: Increase accuracy rate as much as possible.
  – HINT: It is possible to reach accuracies above 99% by just re-arranging the way batches are defined.
- Exercise 4: All 3 examples use a single GPU.
  – Reduce example 3 training time by using all the 4 GPU devices on either a node of the P9 cluster or some other multi-GPU system.
  – Provide training time using 1, 2 and 4 GPUs. Discuss implementation.

Third TensorFlow Example: Multiple Layer Network

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```
#!/usr/bin/env python
import tensorflow as tf
import read_inputs
import numpy as N

#read data from file
data_input = read_inputs.load_data_mnist('MNIST_data/mnist.pkl.gz')
#FYI data = [(train_set_x, train_set_y), (valid_set_x, valid_set_y), (test_set_x, test_set_y)]
data = data_input[0]
#print ( N.shape(data[0][0])[0] )
#print ( N.shape(data[0][1])[0] )

#data layout changes since output should an array of 10 with probabilities
real_output = N.zeros( (N.shape(data[0][1])[0] , 10), dtype=N.float )
for i in range ( N.shape(data[0][1])[0] ):
  real_output[i][data[0][1][i]] = 1.0

#data layout changes since output should an array of 10 with probabilities
real_check = N.zeros( (N.shape(data[2][1])[0] , 10), dtype=N.float )
for i in range ( N.shape(data[2][1])[0] ):
  real_check[i][data[2][1][i]] = 1.0

#set up the computation. Definition of the variables.
x = tf.placeholder(tf.float32, [None, 784])
W = tf.Variable(tf.zeros([784, 10]))
#b = tf.Variable(tf.zeros([10]))
#y = tf.nn.softmax(tf.matmul(x, W) + b)
y_ = tf.placeholder(tf.float32, [None, 10])

#declare weights and biases
def weight_variable(shape):
  initial = tf.truncated_normal(shape, stddev=0.1)
  return tf.Variable(initial)

def bias_variable(shape):
  initial = tf.constant(0.1, shape=shape)
  return tf.Variable(initial)


#convolution and pooling
def conv2d(x, W):
  return tf.nn.conv2d(x, W, strides=[1, 1, 1, 1], padding='SAME')

def max_pool_2x2(x):
  return tf.nn.max_pool(x, ksize=[1, 2, 2, 1],
                        strides=[1, 2, 2, 1], padding='SAME')

#First convolutional layer: 32 features per each 5x5 patch
W_conv1 = weight_variable([5, 5, 1, 32])
b_conv1 = bias_variable([32])

#Reshape x to a 4d tensor, with the second and third dimensions corresponding to image width an
d height.
#28x28 = 784
#The final dimension corresponding to the number of color channels.
x_image = tf.reshape(x, [-1, 28, 28, 1])
                                                                      1,1           Top
```

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Third TensorFlow Example: Multiple Layer Network

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```
x_image = tf.reshape(x, [-1, 28, 28, 1])

#We convolve x_image with the weight tensor, add the bias, apply the ReLU function, and finally
 max pool.
#The max_pool_2x2 method will reduce the image size to 14x14.

h_conv1 = tf.nn.relu(conv2d(x_image, W_conv1) + b_conv1)
h_pool1 = max_pool_2x2(h_conv1)

#Second convolutional layer: 64 features for each 5x5 patch.
W_conv2 = weight_variable([5, 5, 32, 64])
b_conv2 = bias_variable([64])

h_conv2 = tf.nn.relu(conv2d(h_pool1, W_conv2) + b_conv2)
h_pool2 = max_pool_2x2(h_conv2)

#Densely connected layer: Processes the 64 7x7 images with 1024 neurons
#Reshape the tensor from the pooling layer into a batch of vectors,
#multiply by a weight matrix, add a bias, and apply a ReLU.
W_fc1 = weight_variable([7 * 7 * 64, 1024])
b_fc1 = bias_variable([1024])

h_pool2_flat = tf.reshape(h_pool2, [-1, 7*7*64])
h_fc1 = tf.nn.relu(tf.matmul(h_pool2_flat, W_fc1) + b_fc1)

#drop_out
keep_prob = tf.placeholder(tf.float32)
h_fc1_drop = tf.nn.dropout(h_fc1, keep_prob)

#Readout Layer
W_fc2 = weight_variable([1024, 10])
b_fc2 = bias_variable([10])

y_conv = tf.matmul(h_fc1_drop, W_fc2) + b_fc2

#Crossentropy
cross_entropy = tf.reduce_mean(
    tf.nn.softmax_cross_entropy_with_logits(labels=y_, logits=y_conv))

train_step = tf.train.AdamOptimizer(1e-4).minimize(cross_entropy)

correct_prediction = tf.equal(tf.argmax(y_conv, 1), tf.argmax(y_, 1))

accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))

with tf.Session() as sess:
  sess.run(tf.global_variables_initializer())
  #TRAIN
  print("TRAINING")

  for i in range(1000):

    #until 1000 96,35%
    batch_ini = 50*i
    batch_end = 50*i+50
                                                                        76,1          75%
```

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Third TensorFlow Example: Multiple Layer Network

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```python
W_fc1 = weight_variable([7 * 7 * 64, 1024])
b_fc1 = bias_variable([1024])

h_pool2_flat = tf.reshape(h_pool2, [-1, 7*7*64])
h_fc1 = tf.nn.relu(tf.matmul(h_pool2_flat, W_fc1) + b_fc1)

#drop_out
keep_prob = tf.placeholder(tf.float32)
h_fc1_drop = tf.nn.dropout(h_fc1, keep_prob)

#Readout Layer
W_fc2 = weight_variable([1024, 10])
b_fc2 = bias_variable([10])

y_conv = tf.matmul(h_fc1_drop, W_fc2) + b_fc2

#Crossentropy
cross_entropy = tf.reduce_mean(
    tf.nn.softmax_cross_entropy_with_logits(labels=y_, logits=y_conv))

train_step = tf.train.AdamOptimizer(1e-4).minimize(cross_entropy)

correct_prediction = tf.equal(tf.argmax(y_conv, 1), tf.argmax(y_, 1))

accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))

with tf.Session() as sess:
  sess.run(tf.global_variables_initializer())
  #TRAIN
  print("TRAINING")

  for i in range(1000):

    #until 1000 96,35%
    batch_ini = 50*i
    batch_end = 50*i+50


    batch_xs = data[0][0][batch_ini:batch_end]
    batch_ys = real_output[batch_ini:batch_end]


    if i % 10 == 0:
      train_accuracy = accuracy.eval(feed_dict={
          x: batch_xs, y_: batch_ys, keep_prob: 1.0})
      print('step %d, training accuracy %g Batch [%d,%d]' % (i, train_accuracy, batch_ini, batc
h_end))

    train_step.run(feed_dict={x: batch_xs, y_: batch_ys, keep_prob: 0.5})

  #TEST
  print("TESTING")

  train_accuracy = accuracy.eval(feed_dict={x: data[2][0], y_: real_check, keep_prob: 1.0})
  print('test accuracy %g' %(train_accuracy))

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```

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Third TensorFlow Example: Multiple Layer Network

- The lab is due on 12/01/23.

- This practical exercise is individual.

Research Opportunities

- Are you interested in working in topics involving AI, HPC and computer architecture?
  - Contact marc.casas@bsc.es

- We have ongoing research projects with top-level IT multinational companies, as well as collaborations with US universities.

- Possibilities for
  - Master Projects
  - PhD
  - Others…


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