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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 MinoTauro Cluster

- MinoTauro is a heterogeneous cluster where the main computational power is provided by NVIDIA GPUS.
  - 61 Bull B505 blades (88.60 TFLOP/s peak performance)
  - 39 bullx R421-E4 servers (250.94 TFLOP/s)

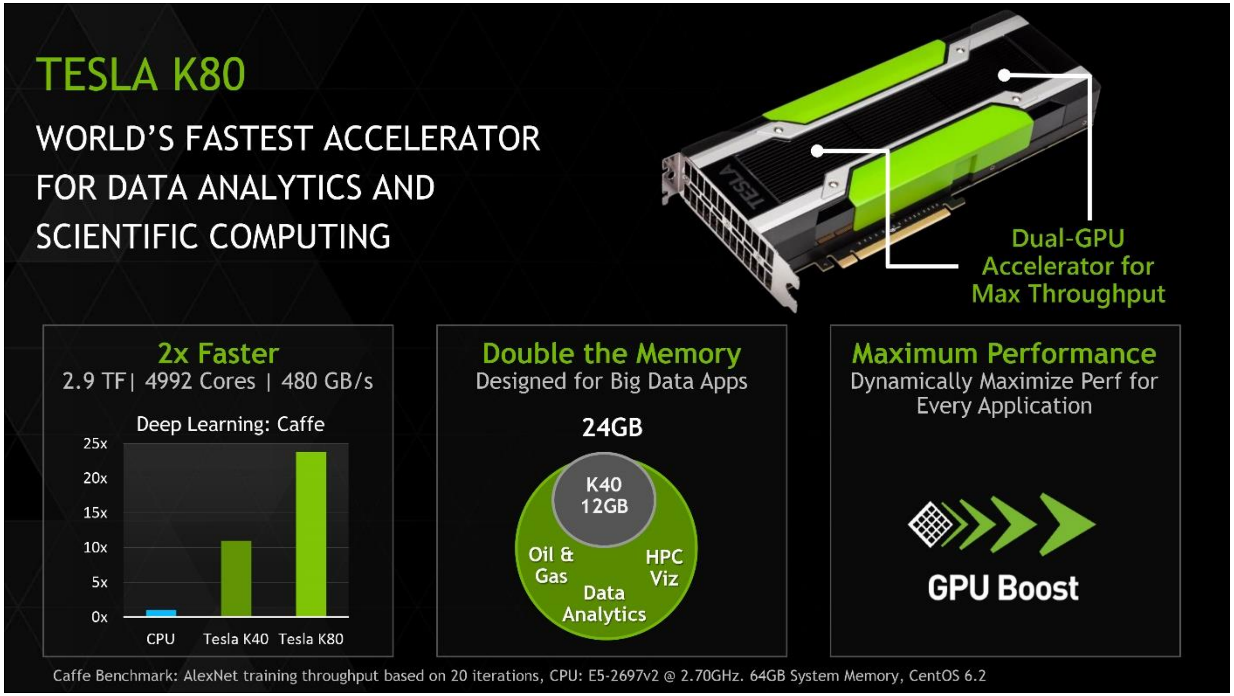
Image of the mythological Minotaur taken from a wine drinking cup found in the greek region of Attica.

MinoTauro

- MinoTauro is a heterogeneous cluster where the main computational power is provided by NVIDIA GPUS.
  - 61 Bull B505 blades (88.60 TFLOP/s peak performance)
  - 39 bullx R421-E4 servers (250.94 TFLOP/s)
    - 2 Intel Xeon E5-2630 v3 (Haswell) 8-core processors, (each core at 2.4 GHz, and with 20 MB L3 cache)
    - 2 K80 NVIDIA GPU Cards
    - 128 GB of Main memory, distributed in 8 DIMMs of 16 GB – DDR4
    - Peak Performance: 226.98 TFLOP/s (K80) + 23.96 TFLOP/s (Haswell) = 250.94 TFLOP/s
    - 120 GB SSD (Solid State Disk) as local storage
    - 1 PCIe 3.0 x8 8GT/s, Mellanox ConnectX®-3FDR 56 Gbit
    - 4 Gigabit Ethernet ports.

NVIDIA K80 (2014)

- Tesla K80 is rated for a maximum double precision (FP64) throughput of 2.9 TFLOPS, or a single precision (FP32) throughput of 8.7 TFLOPS.
- Each Tesla K80 single card contains two GPU's GK210.



From anandtech.com (2014)

Setting Up the Environment

- ssh to Minotauro
- Pick up the files of this lab and put them in a folder
  - Remove the txt prefix and untar the file.
- Type “ . module.sh ”
  - module load K80 cuda/8.0 mkl/2017.1 CUDNN/5.1.10-cuda_8.0 intel-opencl/2016 python/3.6.0+_ML
    - This command loads libraries required to run experiments on the K80 GPU’s
  - mnsh -g –k
    - To allocate an interactive session in the debug partition
    - -g to reserve a gpu
    - -k to access the new k80 GPU’s
- Use “mnsubmit launcher.sh” to submit jobs to Minotauro’s queues.

Setting Up the Environment

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```
#!/bin/bash
# @ job_name= multiGPUproof
# @ initialdir= .
# @ output= multigpu-%j.out
# @ error= %j.err
# @ total_tasks= 1
# @ gpus_per_node= 4
# @ cpus_per_task= 1
# @ features= k80
# @ wall_clock_limit= 00:00:30

##SBATCH --reservation=PATC_DL2

#::Code for running in MT with Python 2.7.12
module purge
module load merovingian
module load K80 cuda/8.0 mkl/2017.1 CUDNN/5.1.10-cuda_8.0 intel-opencl/2016 python/3.6.0+_ML
python multilayer.py
#python /gpfs/home//nct01/nct01022/multiGPUproof.py

~
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                                                                    10,1          All
```

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TensorFlow Basics

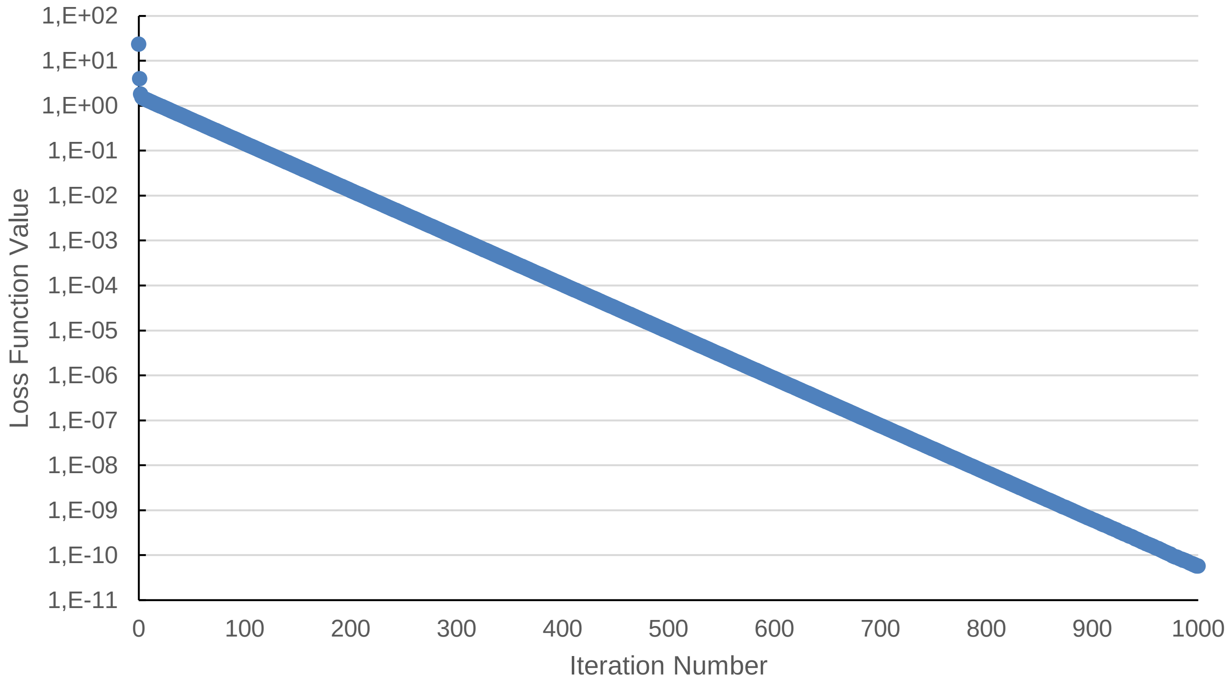
- The central unit of data in TensorFlow (TF) is the **tensor**
- A tensor consists of a set of primitive values shaped into an array of any number of dimensions
- A tensor's **rank** is its number of dimensions.

```
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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```python
#!/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))
```

1,1 Top

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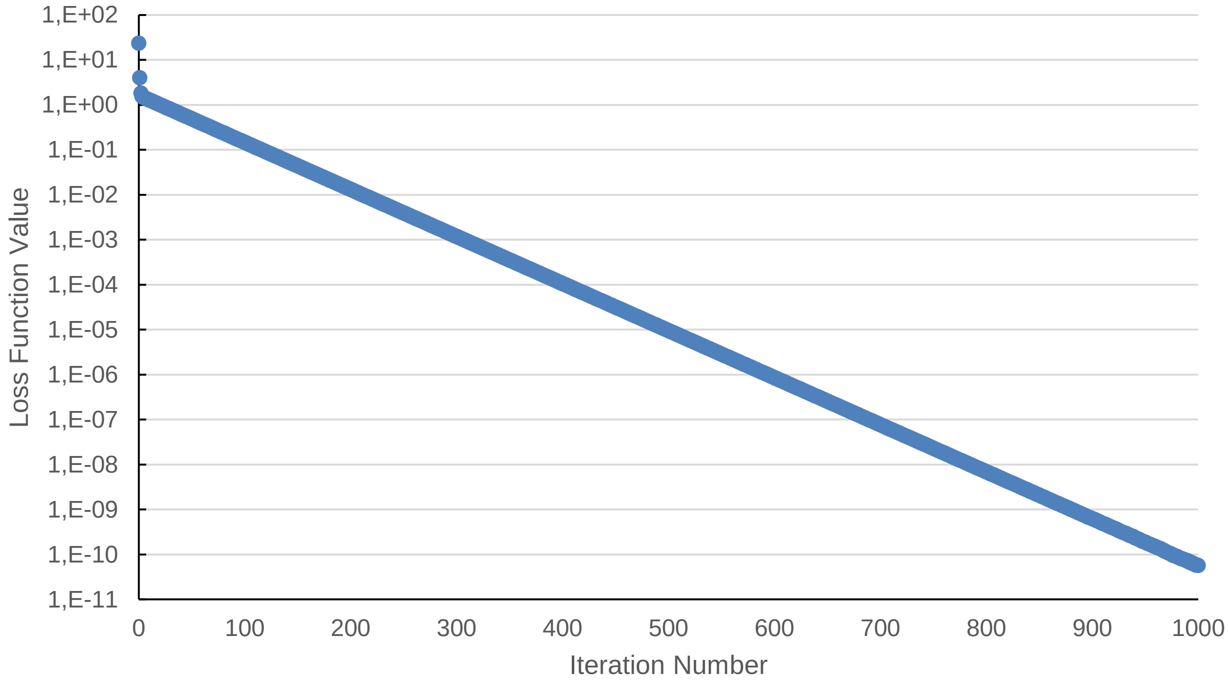
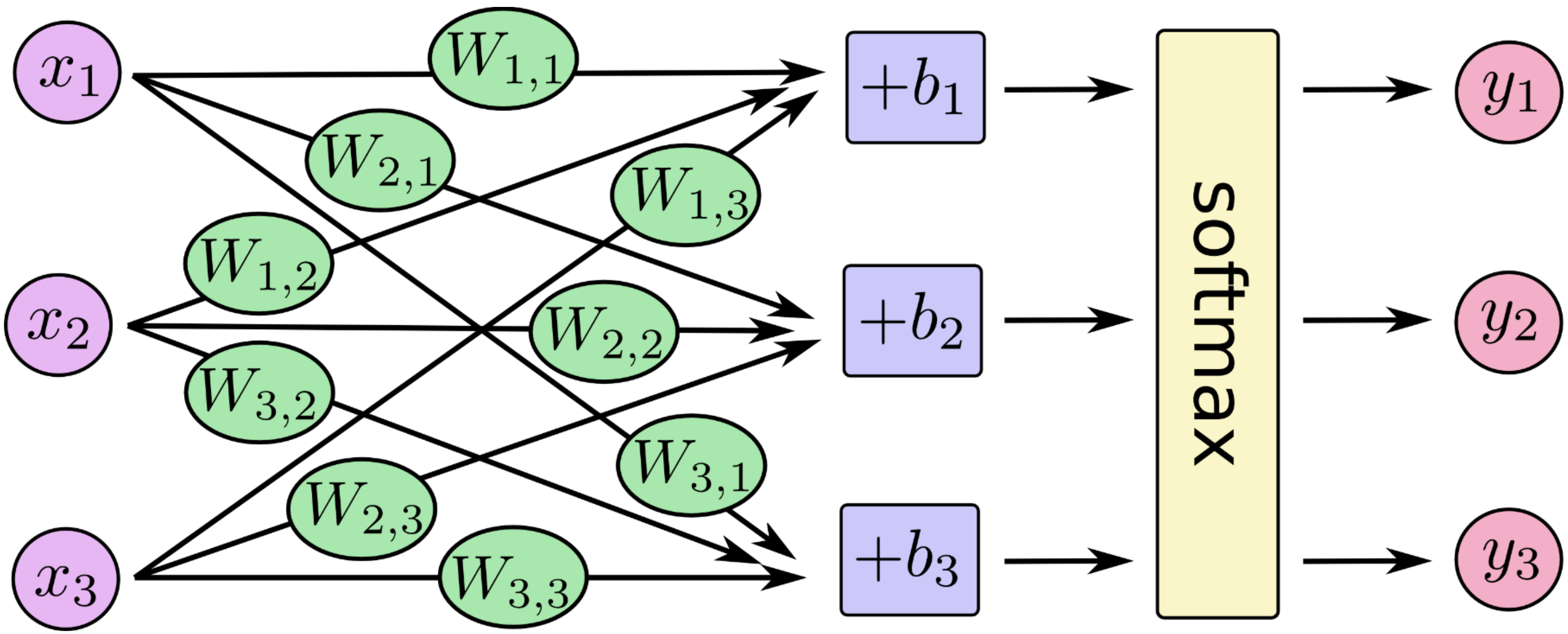
First TensorFlow example: Optimization Problem

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



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

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- The provided implementation obtains a 90.79% accuracy

Second TensorFlow Example: Single Layer Network

```python
#!/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
```

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 solvers and progress 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
  - HINT: It is possible to reach accuracies below 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 a Minotauro node.
  - Provide training execution time using 1, 2 and 4 GPU's.

Third TensorFlow Example: Multiple Layer Network

```
#!/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])
```

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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```
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 7/06/2019

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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