Machine Learning With Python

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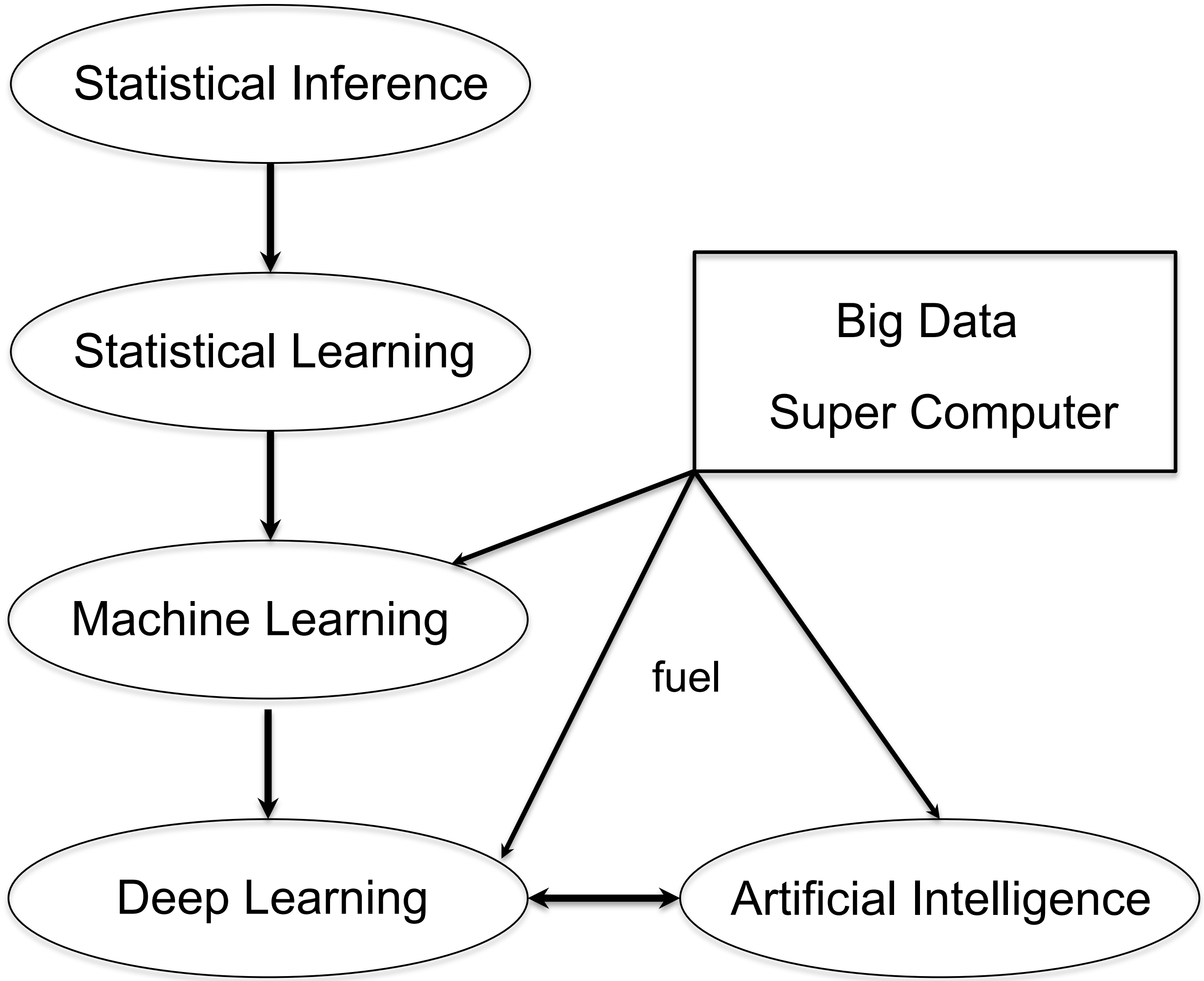
Outline

- Introduction to Machine Learning (ML)
- Introduction to Neural Network (NN)
- Introduction to Deep Learning NN
- Introduction to TensorFlow
- A little about GPUs

Motivation



Statistical Inference
Statistical Learning
Machine Learning
Deep Learning
Big Data
Super Computer
fuel
Artificial Intelligence

Machine Learning (p1)

- Supervised VS Unsupervised learning
- Regression VS Classification
- Linear VS Nonlinear Regression
- Binary VS Multivariate Classification.
- Clustering (e.g., K-Means)
- Support Vector Machine (SVM)
- Neural Network, Deep Neural Network

Machine Learning (p2)

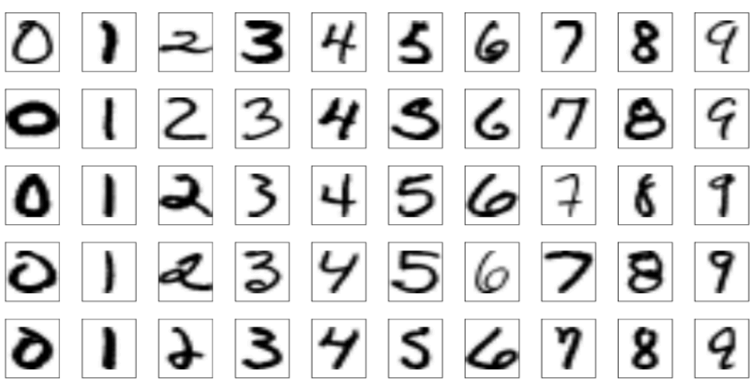
- Regression:

  Predict the price of a house.

- Binary classification y = [0,1]:

  Online advertisement. (will this customer hit this AD?)

- Multivariate classification
  - Digit recognition y = [0,1,2,3,4,5,6,7,8,9]
  - Image recognition (is this a cat?)



Machine Learning (p3)

- Structured data:
  - Data like tables with records,
  - say, predicting house price, loan approvals.
- Unstructured data:
  - Images, Audios.
  - human's natural perceptions often do a great job with accuracy close to Bayes error.
- ML has beaten human beings on many structured data
  - Amazon's recommended list of books
- Deep learning is doing the same thing for unstructured data.
  - Autonomous driving
  - Natural language processing (NLP)

Machine Learning (p4)

- Deep learning is a subset of machine learning.
- The statistics is essentially the same, e.g.,

  loss/cost function (minimize the cost)

  training/dev/test set

  bias-variance tradeoff

  model tuning/regularizing (hyper-parameters)
- Details differ, and there are new concepts, e.g.,

  activation function (sigmoid, ReLU)

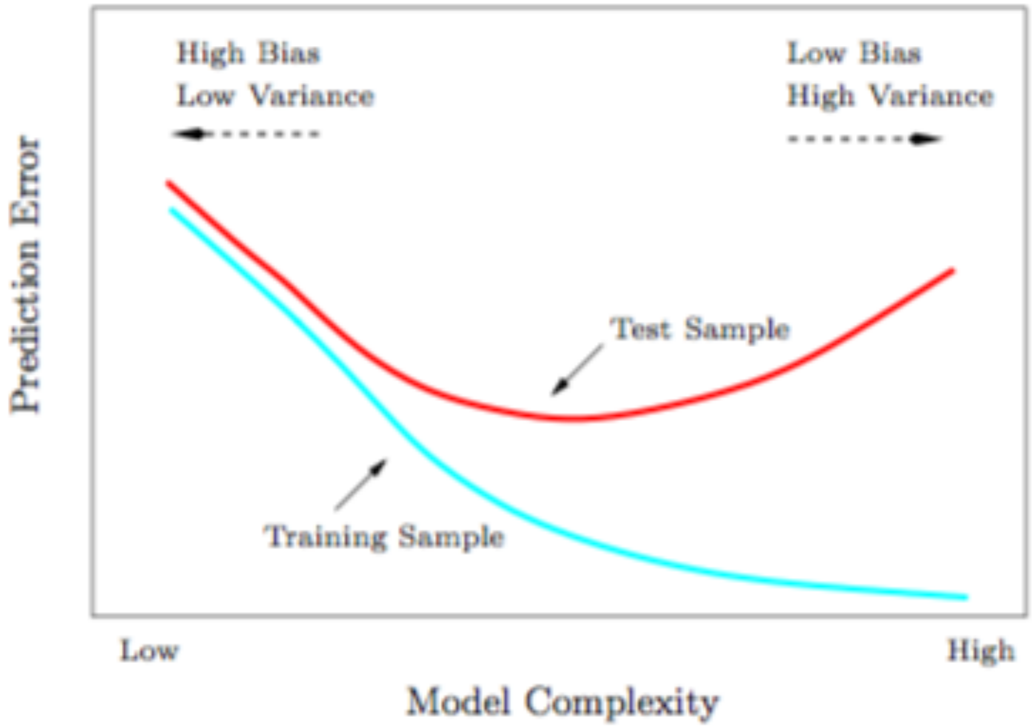
  gradient descent (momentum, RMSprop, AdamOptimizer)

  forward/backward propagation(vanishing/exploding gradient)

  dropout, batch normalization.

Machine Learning (p5)

- Am I under/over-fitting my data (Bias-Variance tradeoff)?



(source: Hastie, Tibshirani, & Friedman, text book E.S.L)

Machine Learning (p6)

- Training/Dev/Test splitting of data

(Traditional Machine Learning)

Train ~60% Dev ~20% Test ~20%

(Deep Learning)

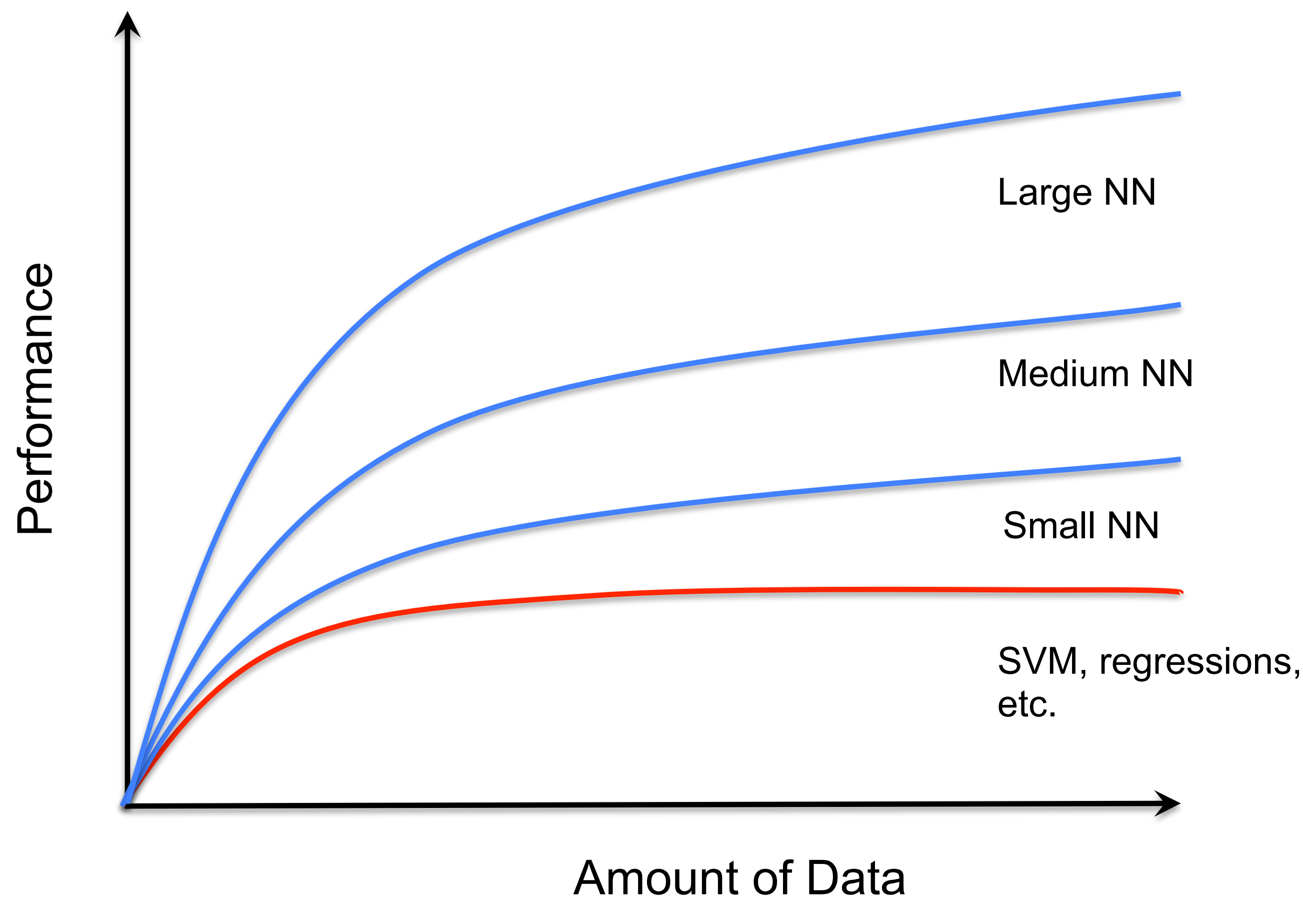
Train ~98% Dev ~1% Test ~1%

(Deep Learning with Mis-Matched Data)

Train ~78% Train-Dev 20% Dev 1% Test 1%

What Drives Deep Learning? (p1)

- Scale-Performance Relationship



What Drives Deep Learning? (p2)

- **The amount of data available**
- **The amount of computation**

  The width and depth of the network
- **Progress in algorithm design**

  Activation function (from sigmoid to ReLU)

  from SNN, to CNN, RNN, etc.
- **The computing power of modern hardware**
  - E.g., Graphics Processing Units (GPUs)

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- Introduction to Deep Learning NN
- Introduction to TensorFlow
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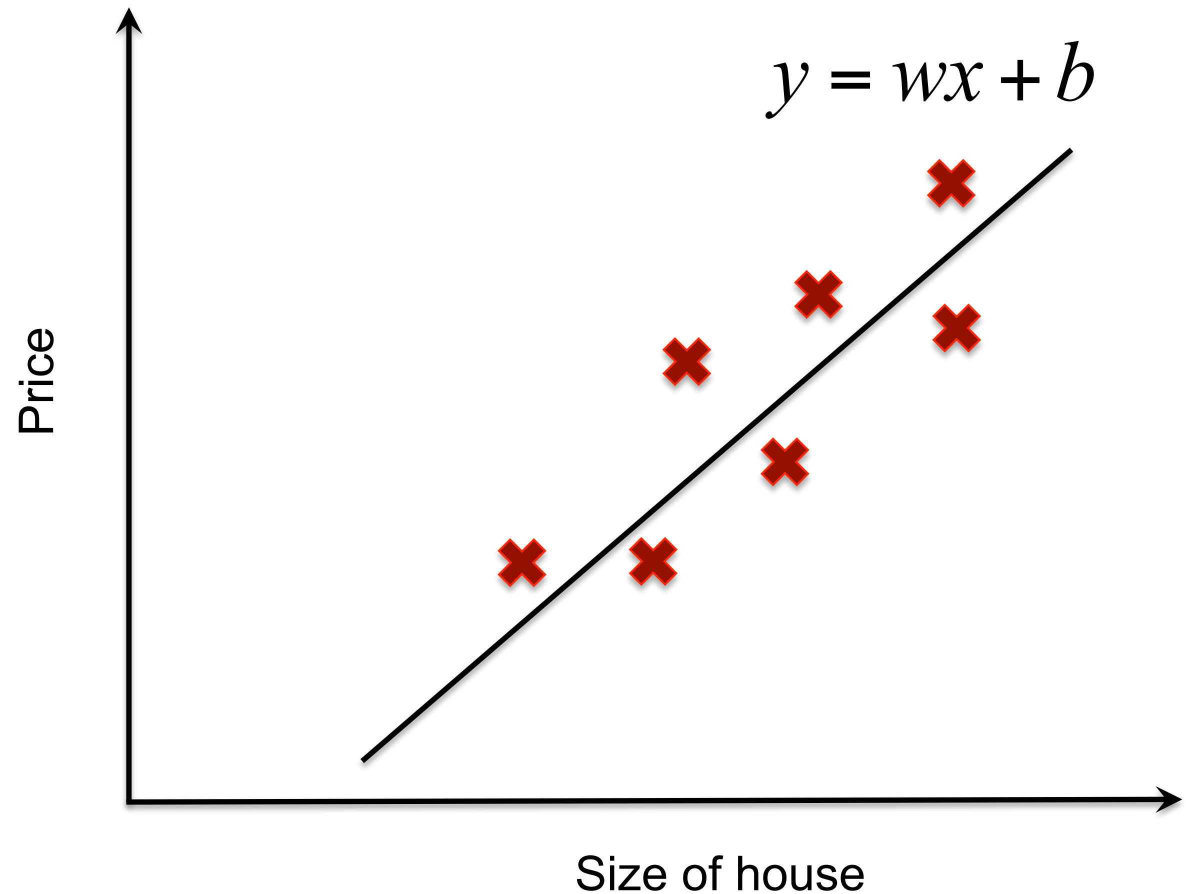
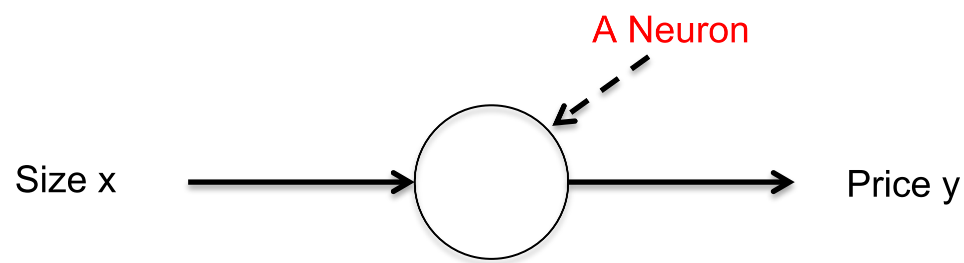
From Regression to Neural Network (p1)



Standard linear regression

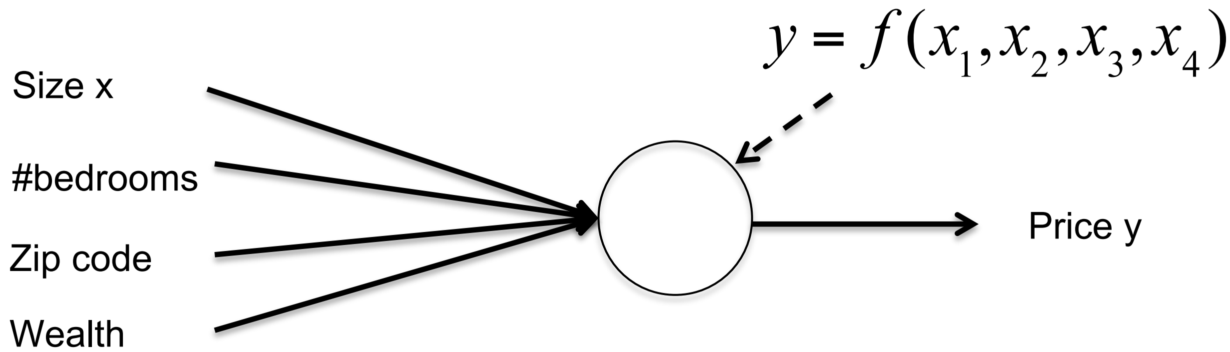
From Regression to Neural Network (p2)

- A deep learner's abstraction of the linear regression:

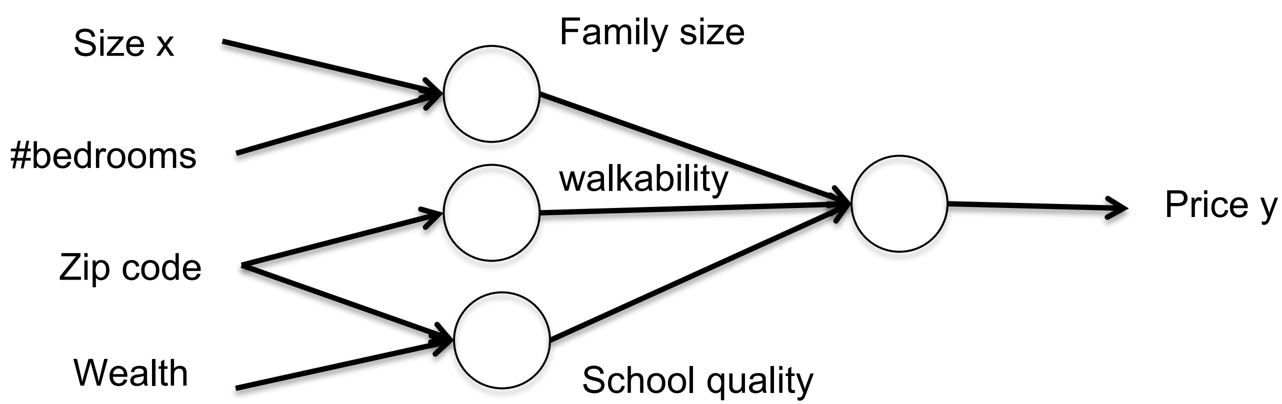


- Q1. So can I consider my simple linear regression as a neural network?
- Answer: Yes, sort of.
- It is a single-layer network, with **activation function** $g(x) = x$
- Such simplistic activation function is almost never used.

From Regression to Neural Network (p3)

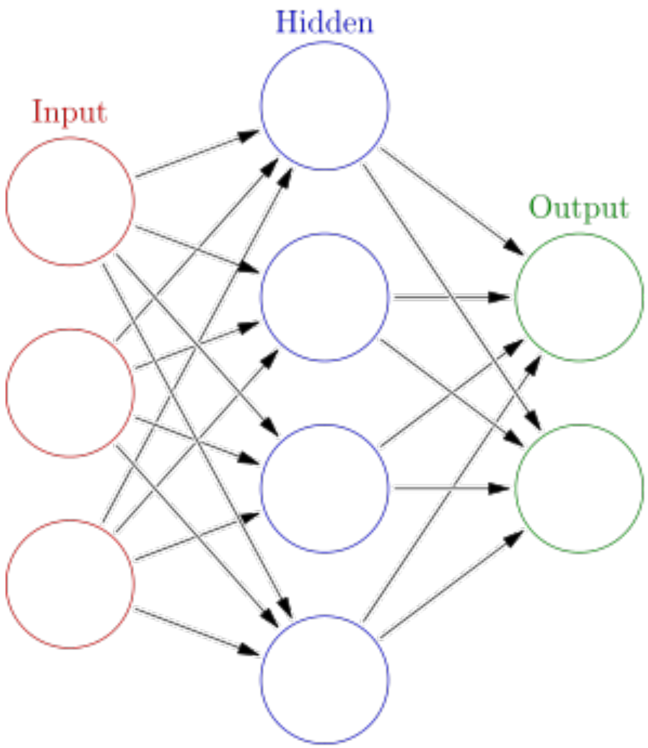


Still regression!



Neural network with one hidden layer

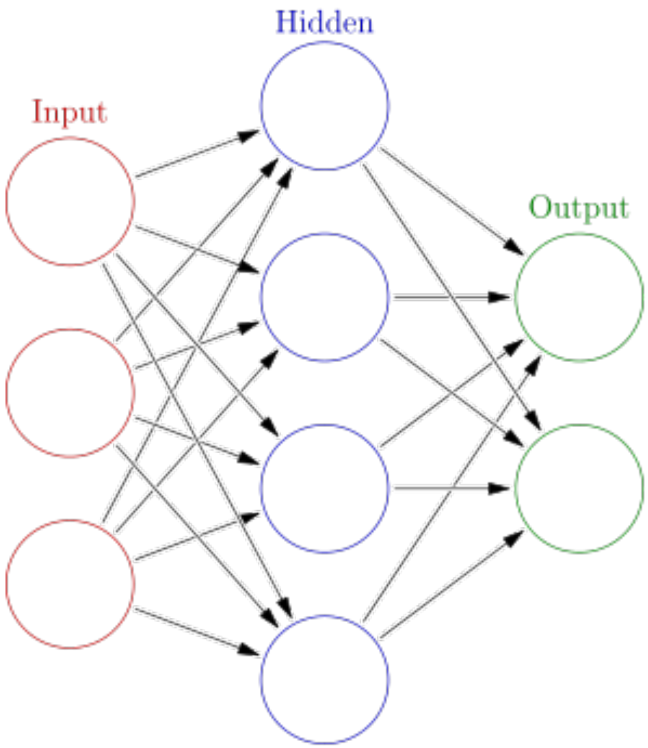
What is a neural network? (p1)



(Picture from Wikipedia)

- Q1. How many layers are there?
- Q2. How many hidden units?
- Q2. Is it a deep neural network?
- Q3. What does the arrow mean?

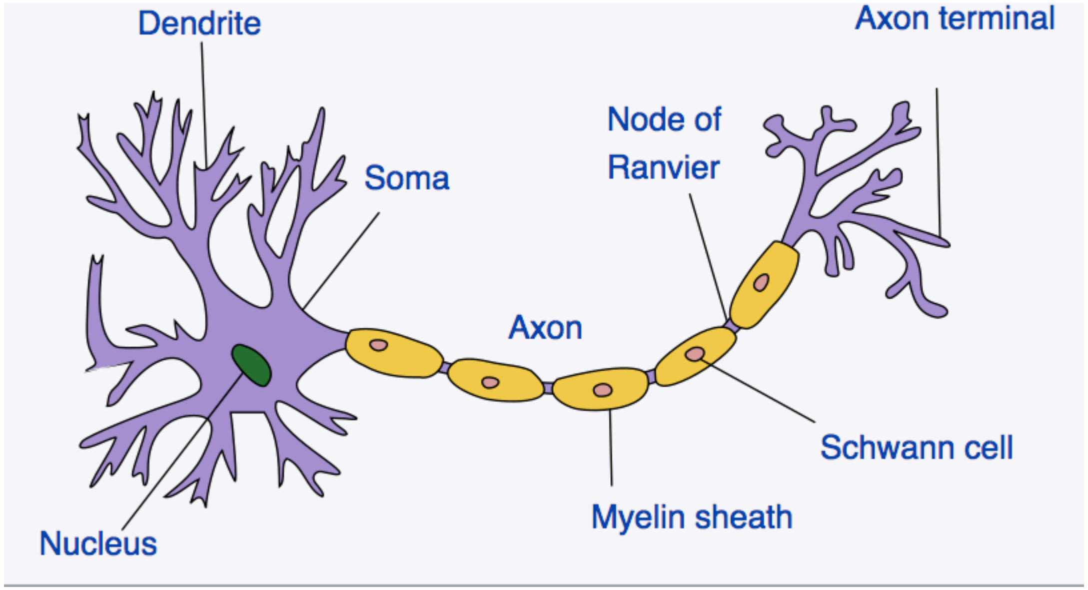
What is a neural network? (p2)



(Picture from Wikipedia)

- Q1. How many layers are there?
- A1: 2 (instead of 3).
- Q2. How many hidden units?
- A2: 4.
- Q3. Is it a deep neural network?
- A4: no! (>=2 hidden layers)
- Q4. What does the arrow mean?
- A4: flow of data (tensorflow)

What is a neuron? (p1)

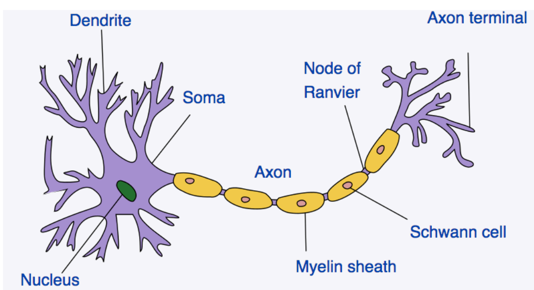


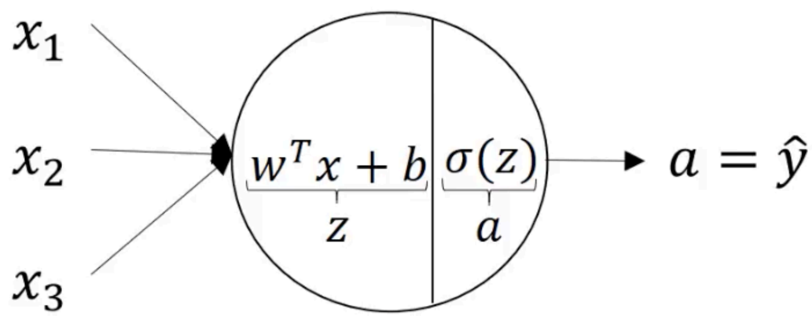
(Picture from Wikipedia)

What is a neuron? (p2)

A neuron does simple and specific task: an **affine transformation** composed with an **activation function**.

(Pay attention to the naming of each variables: z, w, a, b, etc.)





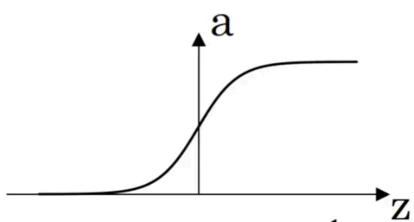
$$z = w^T x + b$$

$$a = \sigma(z)$$

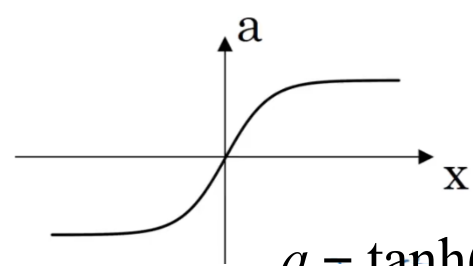
(Picture from Andrew Ng)

Activation function

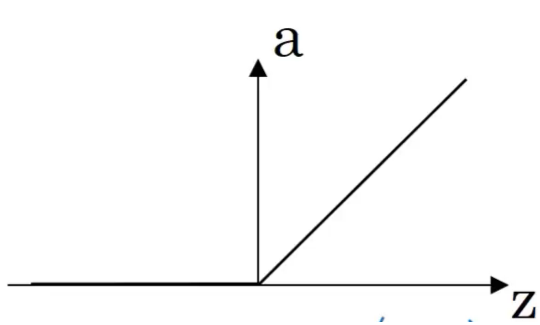
- Activation function adds non-linearity to your network.
- Popular activation functions include, sigmoid, tanh, ReLU
- Different layers of can use different activation function.



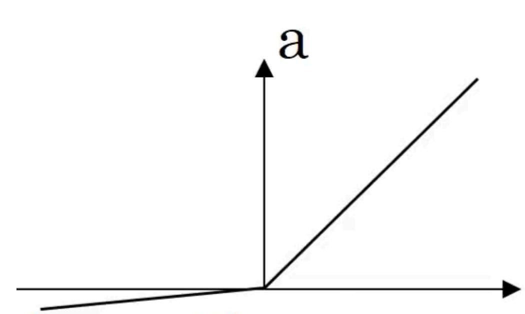
sigmoid: $a = \dfrac{1}{1 + e^{-z}}$



$a = \tanh(z)$



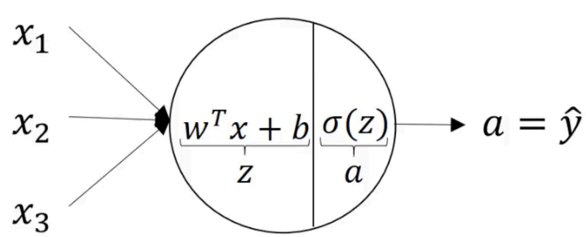
ReLU



Leaky ReLU

Logistic Regression VS Neural Network

- The sigmoid activation function was also used in logistic regression in traditional statistical learning.
- Logistic regression is simple Neural Network with sigmoid activation function.



$$a = \hat{y} = \frac{1}{1 + e^{-(w^T x + b)}}$$

$$z = w^T x + b$$

$$a = \sigma(z)$$

Loss Function and Cost Function

- The **Loss function** $L(\hat{y}_i, y_i)$ tells how well your model fits a data point (here i labels the data point).
- **Cost Function J** is the **average** of the loss function over the sample.
- Binary Classification as an example

$$L(\hat{y}_i, y_i) = -[y_i \log \hat{y}_i + (1 - y_i)\log(1 - \hat{y}_i)]$$

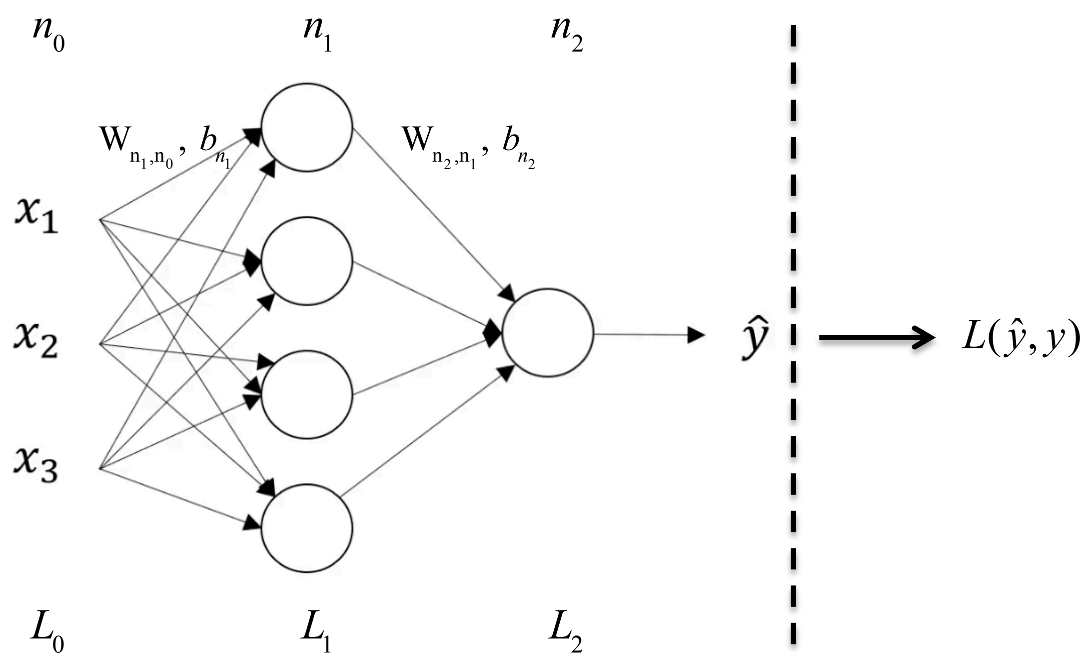
$$J = \frac{1}{m}\sum_{i=1}^{m} L(\hat{y}_i, y_i)$$

- Chi-square for regression analysis as another…

$$J = \frac{1}{m}\sum_{i=1}^{m} (\hat{y}_i - y_i)^2$$

Loss Function and Cost Function (p2)

- Why we need the **Loss function, or the cost function**?
- Answer: we need them to determine the model parameters
- To train the NN we optimize the cost via gradient descent.

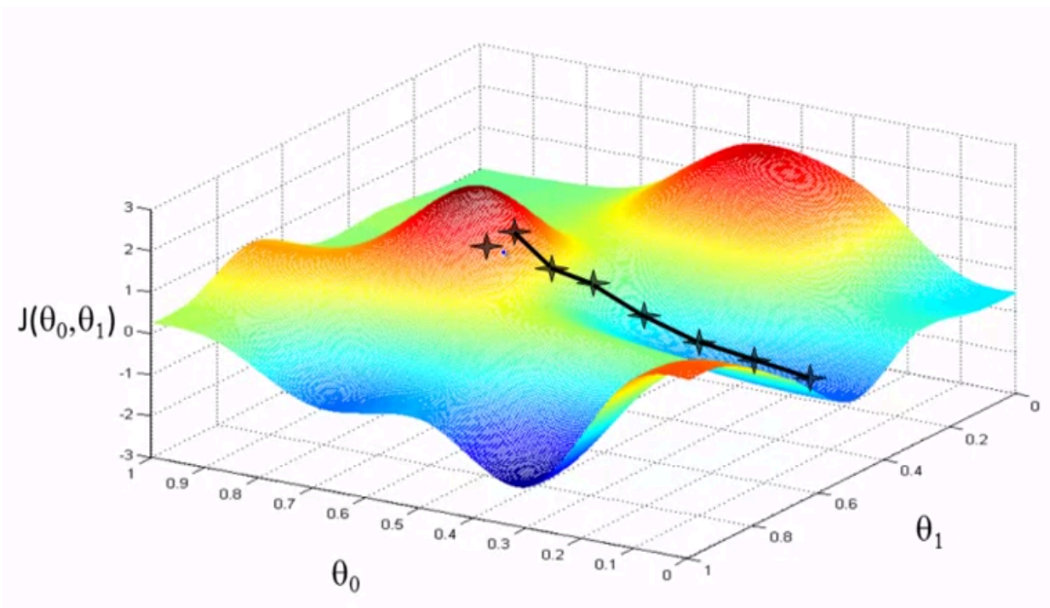


Inference Graph and Train Graph

TensorFlow

Gradient Descent

- Given labeled data (x_i, y_i), find the parameters (W_{jk}, b_j) by minimizing the cost function J.
- Method: gradient descent



$$\theta_j := \theta_j - \alpha \frac{\partial J}{\partial \theta_j}$$

(α is the learning rate)

(From Andrew Ng's Lecture Notes)

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- **Introduction to Deep Neural Network**
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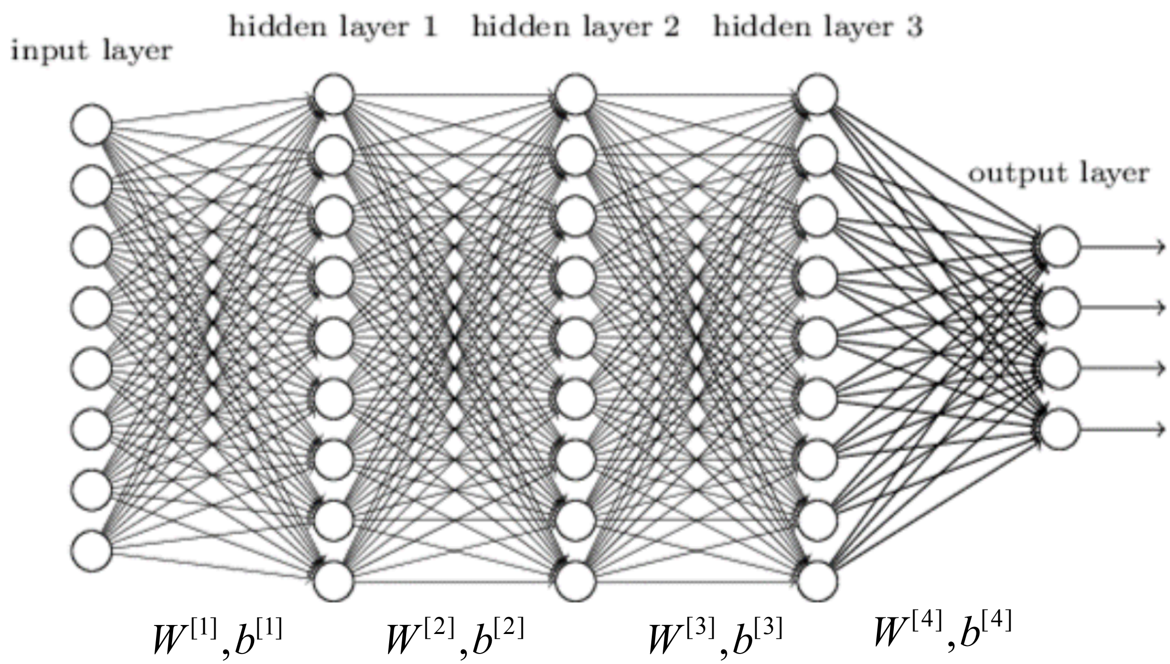
- A little about GPUs

Deep Neural Network

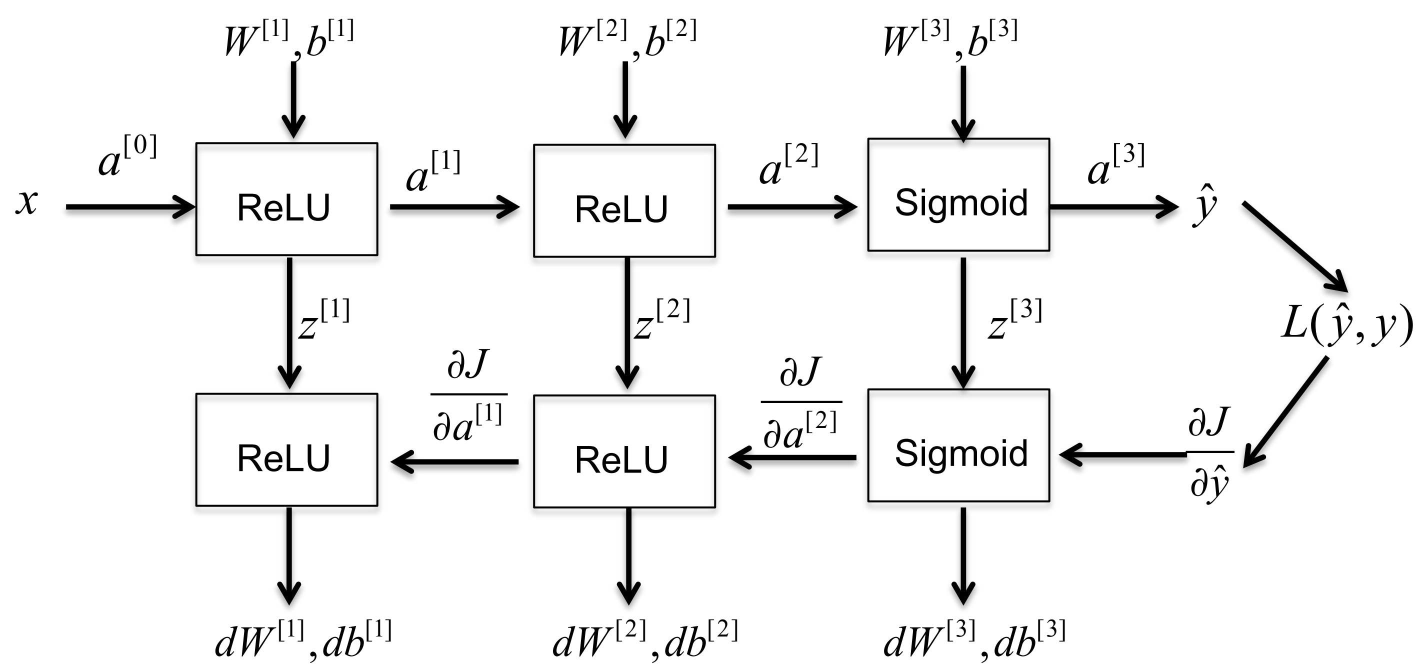
- A neural network with at least 2 hidden layers
- The hidden layers can be very wide (millions of hidden units)
- The width (# of units) varies from layer to layer.



A 4-layer deep neural network

Forward and Backward Propagation

- Forward propagation: given labeled data (x_i, y_i), and parameters (W, b) compute the cost function *J*.
- Backward propagation: compute the derivatives of *cost function* w.r.t the model parameters. Update the model parameters (W, b).



Compute the Derivatives

- Using binary classification an example

$$L(\hat{y}_i, y_i) = -[y_i \log \hat{y}_i + (1 - y_i)\log(1 - \hat{y}_i)]$$

$$\Rightarrow \frac{\partial L}{\partial \hat{y}} = -\frac{y_i}{\hat{y}_i} + \frac{1 - y_i}{1 - \hat{y}_i}$$

- Assuming sigmoid activation function

$$\hat{y} = a = g(z) = \frac{1}{1 + e^{-z}} \Rightarrow \frac{\partial a}{\partial z} = a(1 - a)$$

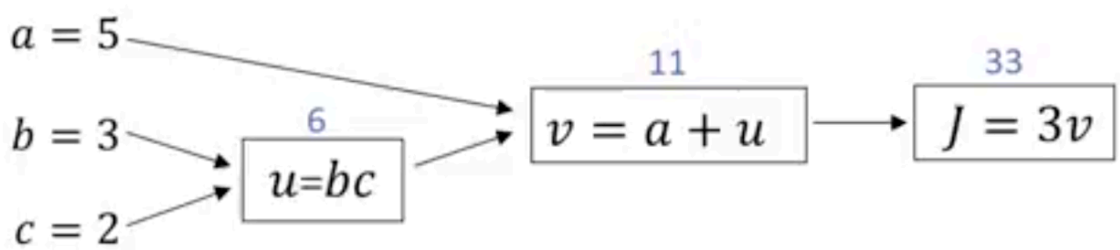
- Derivatives for the affine/linear transformation is easy

$$\vec{z} = W\vec{x} + \vec{b} \Rightarrow \frac{\partial z_i}{\partial W_{ij}} = x_j, \frac{\partial z_i}{\partial b_j} = \delta_{ij}$$

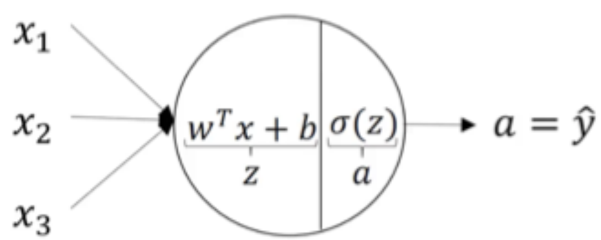
- Now using chain rule to concatenate the above together.

Computation Graph (Divide & Conquer)

- The computation graph for $J = 3*(a + b*c)$



- This really helps when you think about forward/backward propagation.



- Understand/Stick with a good notation is also critical.

Parameters VS Hyper-parameters

- Parameters: (W, b) for each layer of the NN.

  (W, b) can be learned by training the NN using the training data set.

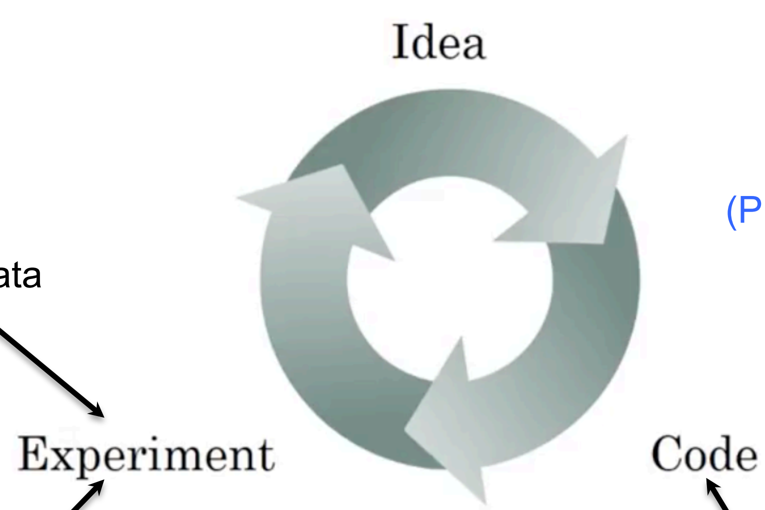
- Hyper-parameters include:

  1. # layers for the NN;
  2. # units for each layer;
  3. # learning rate α.
  4. the choice of activation function.
  5. batch data size.
  6. # iteration for convergence.

- Deep learning tends to have many more hyper-parameters than normal ML methods.
- Hyper-parameters are determined via the dev data set.

Parameters VS Hyperparameters (p2)

- Choosing between other machine learning methods and deep leaning can be empirical.
- Large number of hyper-parameters make deep learning very empirical.



(Pic from Andrew Ng)

Collect Data

Hardware (GPU,CPU)

FSU/RCC

Software packages
(Sklearn, Torch, Caffe, Keras, Tensorflow)

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Introduction to TensorFlow (p1)

- A framework (library/package) for deep learning.
- Open source (originally by Google Brain Team).
- Python/C++ frontend, and C++ backend.
- Support hardware accelerators GPU.
- Current stable release v1.3

How does TensorFlow work?

- User defines the architecture of the NN (inference graph).
- User defines the loss/cost function (train graph).
- User provides the data (train/dev/test).
- User chooses the optimizer to try.
- User picks hyper-parameters (mini-batch size, learning rate).
- Tensorflow does the rest automatically for you.

  forward propagation to compute the loss function;

  backward propagation to compute the derivatives;

  many optimization algorithms are included

  (e.g., tf.train.GradientDescentOptimizer(),

  tf.train.AdamOptimizer(…))

A Toy Example (ex01)

- Goal: train a toy Neural network with loss function

$$L(w) = w^2 - 12w + 36$$

- Here w is the only parameter to learn.
- The training output should be very close to 6.
- Sorry (no input at all, but will add later on).

A Toy Example (ex01)

In [1]:
```
import tensorflow as tf
import numpy as np
```

In [2]:
```
# cost function J = w**2 - 12*w + 36
# optimized w should be  6.

w      = tf.Variable(0, dtype=tf.float32)
J      = w**2 - 12*w + 36    # operator overloading
train  = tf.train.GradientDescentOptimizer(0.01).minimize(J)
```

In [3]:
```
# you must always create a Session, and initialize your variables
init = tf.global_variables_initializer()
session = tf.Session()
session.run(init)
```

In [4]:
```
# before training, w = 0.0
print(session.run(w))

# train with 1000 iteration
for i in range(1000):
    session.run(train)

# now the w should be very close to 5 now
print(session.run(w))
```

```
0.0
5.99999
```

Toy Example Improved (ex01b)

- Loss function $L = x_0 w^2 - x_1 w + x_2$

In [2]:
```
# data x is defined as placeholder
# variables is trainable, placeholders are not!
x      = tf.placeholder(tf.float32, [3,1])

w      = tf.Variable(0, dtype=tf.float32)
J      = x[0] * w**2 + x[1] * w + x[2]   # operator overloading
train  = tf.train.GradientDescentOptimizer(0.01).minimize(J)
```

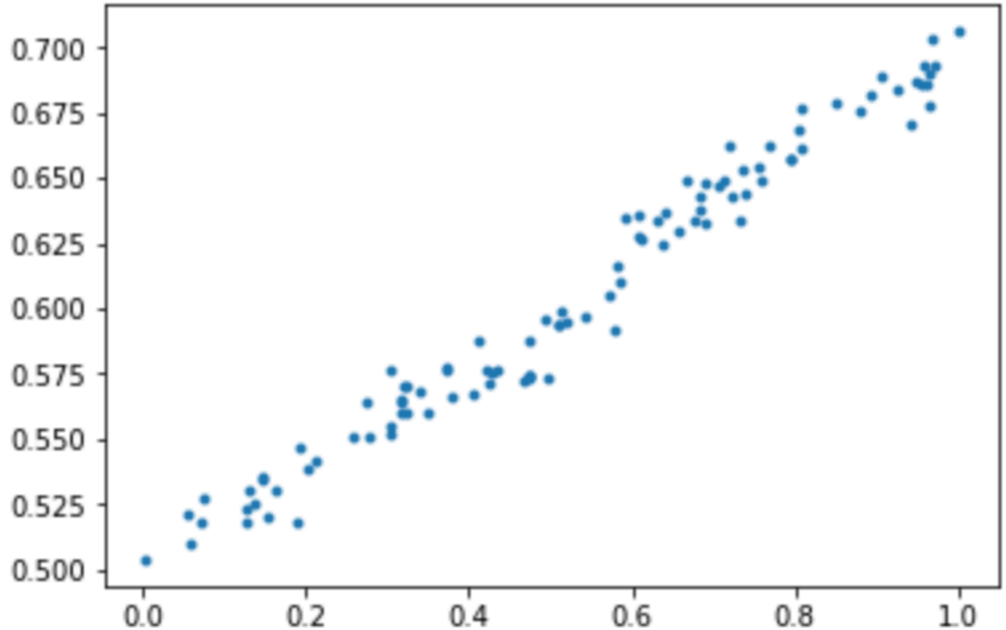
In [3]:
```
# you must always create a Session, and initialize your variables
init = tf.global_variables_initializer()
session = tf.Session()
session.run(init)
```

In [4]:
```
# this will be my data "x"
coeffs = np.array([[1], [-12], [36]])

# train with 1000 iteration
for i in range(1000):
    session.run(train, feed_dict={x:coeffs} )

# now the w should be very close to 5 now
print(session.run(w))
```

```
5.99999
```

Example-02: Linear Regression

- Mysterious equation: $y = 0.2x + 0.5 + \varepsilon$
- Model: $y = wx + b$
- Goal: given enough (x_i, y_i) pairs, find out (w,b).



Example-02: Linear Regression (p2)

- Generate the data: $y = 0.2x + 0.5 + \varepsilon$

```
In [1]: import tensorflow as tf
        import numpy as np
        import pylab as pl
        %matplotlib inline
```

```
In [2]: # y = 0.2*x + 0.5 + epsilon
        x_data  = np.random.rand(100,1)
        epsilon = 0.01*np.random.randn(100,1)
        y_data  = 0.2*x_data + 0.5 + epsilon
        pl.plot(x_data, y_data,'.')
```

Example-02: Linear Regression (p3)

- Define the model and the loss function, train it:

In [4]:
```
# syntax: tf.Variable(<initial-value>, name=<optional-name>)
w = tf.Variable(1, name='weight', dtype=tf.float32)
b = tf.Variable(0, name='bias',   dtype=tf.float32)
y = w*x_data + b      # note the overloading and broadcasting
# loss function J
J     =  tf.reduce_mean((y - y_data)**2)
train =  tf.train.GradientDescentOptimizer(0.25).minimize(J)
```

In [5]:
```
# train the model
session = tf.Session()
init    = tf.global_variables_initializer()
session.run(init)
y_init  = session.run(y)  # y prediction with untrained w, b
for i in range(5000):
    session.run(train)
print(session.run([w,b]))
```

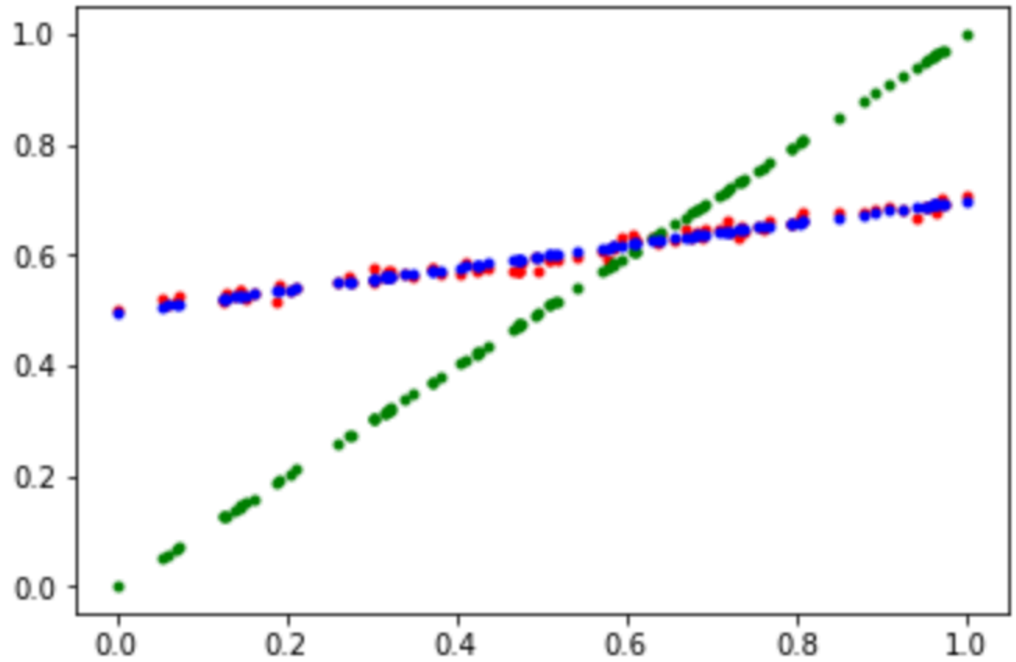
```
[0.2023287, 0.49739757]
```

Example-02: Linear Regression (p4)

- Visualize the training out:

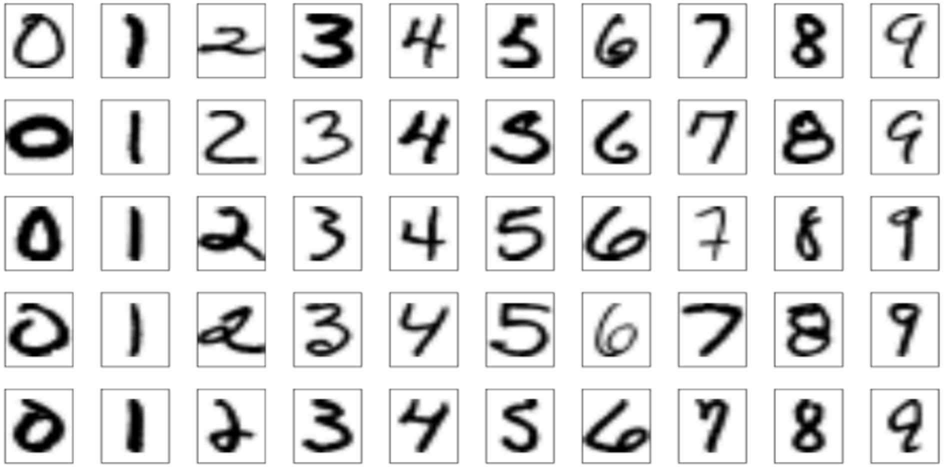
```
In [6]: pl.plot(x_data, y_data,          '.', color='r')
        pl.plot(x_data, y_init,          '.', color='g')
        pl.plot(x_data, session.run(y), '.', color='b')
```

```
Out[6]: [<matplotlib.lines.Line2D at 0x1149e7908>]
```



Example-03: digit recognition (p1)

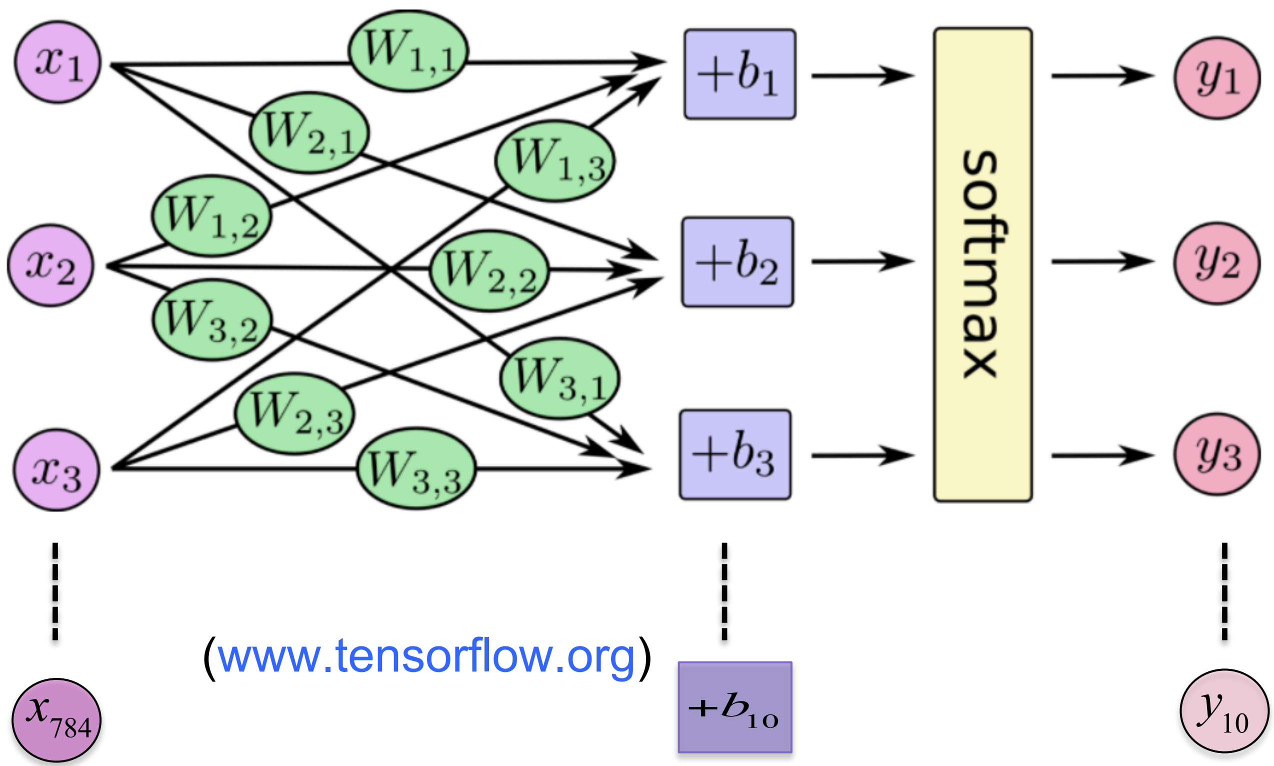
- Goal: given enough images and labels, find the weights, biases to identify digits.
- Dataset: MNIST dataset: http://yann.lecun.com/exdb/mnist/
- Ref: https://www.tensorflow.org/get_started/mnist/beginners
- Image size: 28*28=784, so x[784, m], y[10, m]



Example-03: digit recognition (p2)

- Model: simple 1-layer neural network.
- Activation function:

$$\text{softmax}(x)_i = \frac{\exp(x_i)}{\sum_j \exp(x_j)}$$



(www.tensorflow.org)

Example-03: digit recognition (p3)

- Cross entropy loss function

$$L(y^{(i)}, \hat{y}^{(i)}) = -\sum_{j=1}^{10} y_j^{(i)} \log \hat{y}_j^{(i)}$$

- Cost function

$$J = \frac{1}{m} \sum_{i=1}^{m} L(y^{(i)}, \hat{y}^{(i)})$$

- One-hot vector

0	1	2	3	4	5	6	7	8	9
0	0	0	0	0	0	1	0	0	0

Example-03: digit recognition (p4)

- Import the data, and define the model

```
import tensorflow as tf
from tensorflow.examples.tutorials.mnist import input_data

def myfunc():

  data_dir="/Users/binchen/Desktop/RCC/MachineLearn/tensorflow/examples
  mnist   = input_data.read_data_sets(data_dir, one_hot=True)

  # Create the model
  x = tf.placeholder(tf.float32, [None, 784])
  W = tf.Variable(tf.zeros([784, 10]))
  b = tf.Variable(tf.zeros([10]))
  y = tf.matmul(x, W) + b
  y_ = tf.placeholder(tf.float32, [None, 10])
```

Example-03: digit recognition (p5)

- Define the loss function (cross_entropy), and train the model

```
cross_entropy = tf.reduce_mean(
    tf.nn.softmax_cross_entropy_with_logits(labels=y_, logits=y))
train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)

init = tf.global_variables_initializer()
sess = tf.Session()
sess.run(init)

# train the model
for _ in range(1000):
  batch_xs, batch_ys = mnist.train.next_batch(100)
  sess.run(train_step, feed_dict={x: batch_xs, y_: batch_ys})

# Test trained model
correct_prediction = tf.equal(tf.argmax(y, 1), tf.argmax(y_, 1))
accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))
print("\nThe accuracy on test data is ",
      sess.run(accuracy, feed_dict={x: mnist.test.images,
                                    y_: mnist.test.labels}))
```

Example-03: digit recognition (p5)

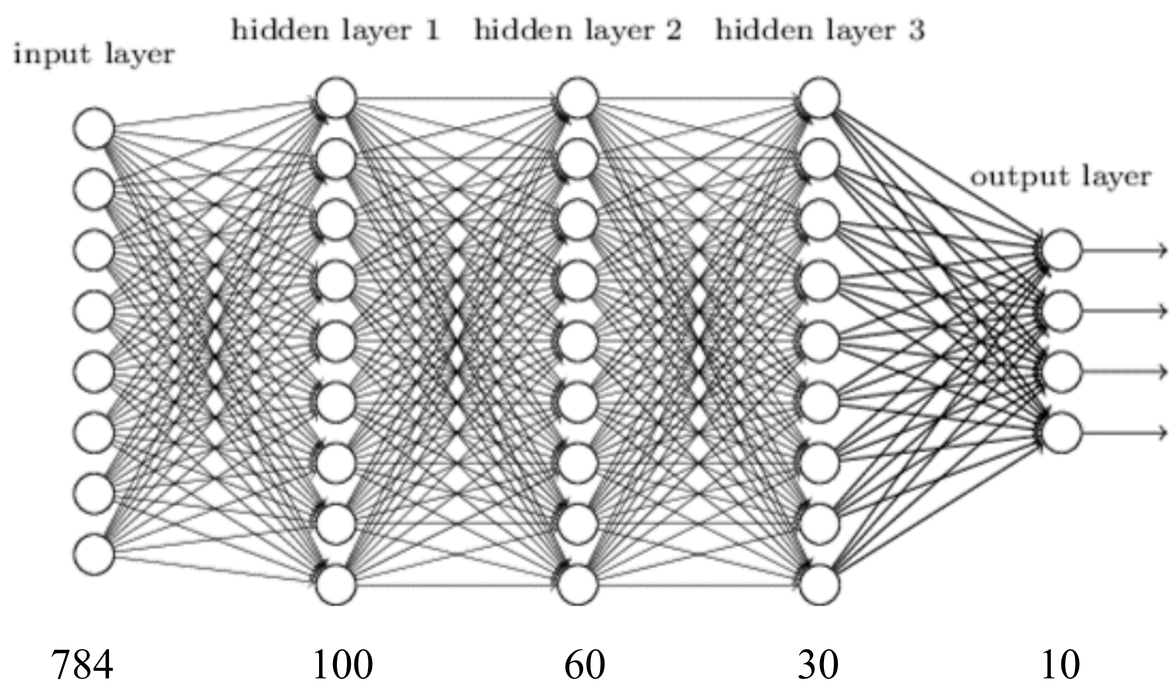
- Accuracy on test data: ~91%

```
myfunc()
```

```
Extracting /Users/binchen/Desktop/RCC/MachineLearn/tensorflow/examples
/workshop/mnist/input_data/train-images-idx3-ubyte.gz
Extracting /Users/binchen/Desktop/RCC/MachineLearn/tensorflow/examples
/workshop/mnist/input_data/train-labels-idx1-ubyte.gz
Extracting /Users/binchen/Desktop/RCC/MachineLearn/tensorflow/examples
/workshop/mnist/input_data/t10k-images-idx3-ubyte.gz
Extracting /Users/binchen/Desktop/RCC/MachineLearn/tensorflow/examples
/workshop/mnist/input_data/t10k-labels-idx1-ubyte.gz

The accuracy on test data is  0.9171
```

Example-03 Improved (p1)

- Goal: MNIST, but with deep network, want higher accuracy
- 3 hidden layers with ReLU, output layer softmax



A 3 hidden layer deep neural network for MNIST

Example-03 Improved (p2)

- Goal: MNIST, but with deep network, want higher accuracy

```
# Create the model
x  = tf.placeholder(tf.float32,      [None, 784])

W1 = tf.Variable(tf.truncated_normal([784, 100], stddev=0.1))
b1 = tf.Variable(tf.zeros([100]))

W2 = tf.Variable(tf.truncated_normal([100, 60],  stddev=0.1))
b2 = tf.Variable(tf.zeros([60]))

W3 = tf.Variable(tf.truncated_normal([60, 30],   stddev=0.1))
b3 = tf.Variable(tf.zeros([30]))

W4 = tf.Variable(tf.truncated_normal([30, 10],   stddev=0.1))
b4 = tf.Variable(tf.zeros([10]))

y1 = tf.nn.relu(tf.matmul(x,  W1) + b1)
y2 = tf.nn.relu(tf.matmul(y1, W2) + b2)
y3 = tf.nn.relu(tf.matmul(y2, W3) + b3)
y  = tf.matmul(y3, W4) + b4
y_ = tf.placeholder(tf.float32, [None, 10])
```

Example-03 Improved (p3)

- The accuracy increases from ~91% to ~97%
- Note tensorflow automatically used all 4 cores of my laptop

```
tic_wall   = timeit.default_timer()
tic_cpu    = time.clock()
myfunc()
toc_wall   = timeit.default_timer()
toc_cpu    = time.clock()
print("the cpu  time is %9.5f seconds" % float(toc_cpu  - tic_cpu) )
print("the wall time is %9.5f seconds" % float(toc_wall - tic_wall))
```

```
Extracting /Users/binchen/Desktop/RCC/MachineLearn/tensorflow/example
s/workshop/mnist/input_data/train-images-idx3-ubyte.gz
Extracting /Users/binchen/Desktop/RCC/MachineLearn/tensorflow/example
s/workshop/mnist/input_data/train-labels-idx1-ubyte.gz
Extracting /Users/binchen/Desktop/RCC/MachineLearn/tensorflow/example
s/workshop/mnist/input_data/t10k-images-idx3-ubyte.gz
Extracting /Users/binchen/Desktop/RCC/MachineLearn/tensorflow/example
s/workshop/mnist/input_data/t10k-labels-idx1-ubyte.gz

The accuracy on test data is  0.9764
the cpu  time is  79.76172 seconds
the wall time is  22.18648 seconds
```

One Page about Python on HPC

- Python 2.7 and Python 3.5 are available on HPC nodes.
- Popular packages such as numpy, scipy, matplotlib are preinstalled.
- Anaconda python with ~200 packages including tensorflow is available at

  /panfs/storage.local/opt/python/anaconda/bin/python
- Users are encouraged to install packages to their own disk space via the python virtual environment:

  https://rcc.fsu.edu/software/python

One Page about GPUs on HPC

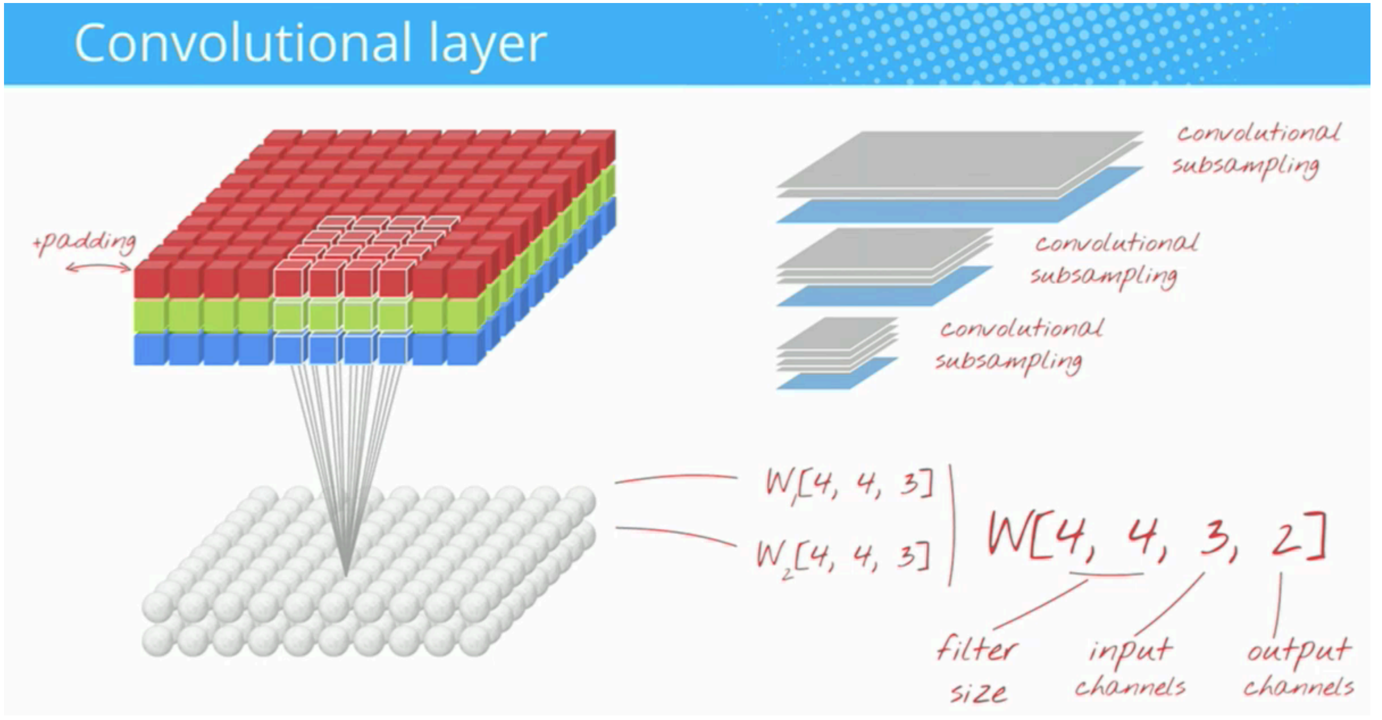
- Hardware upgrade from Tesla M2050 to GeForce1080 Ti.
- Compute capability from 2.0 to 6.1 (Fermi to Pascal)
- Cuda driver upgraded from 6.5 to 9.0
- Each compute node with GPUs have 4 GPU cards

  https://rcc.fsu.edu/software/cuda

```
#!/bin/bash

#SBATCH -N 1
#SBATCH -n 1
#SBATCH -J "cuda-job"
#SBATCH -t 4:00:00
#SBATCH -p backfill
#SBATCH --gres=gpu:1
#SBATCH --mail-type=ALL

# load the cuda module to set up the environment
module load cuda

# the following line should provide the full path to the cuda compiler
which nvcc

# execute your cuda executable a.out
srun -n 1 ./a.out <input.dat >output.txt
```

A Little about Convolution

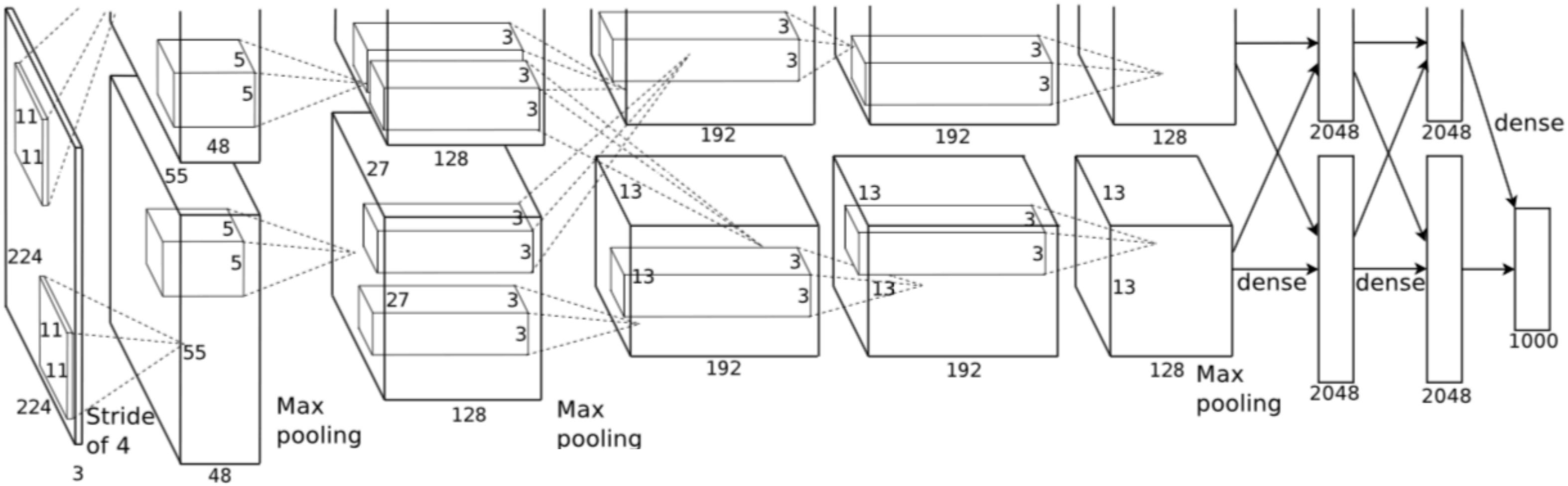
- From fully connected to partially connected.
- Convolution adds locality back.
- Convolution reduce the parameter size significantly

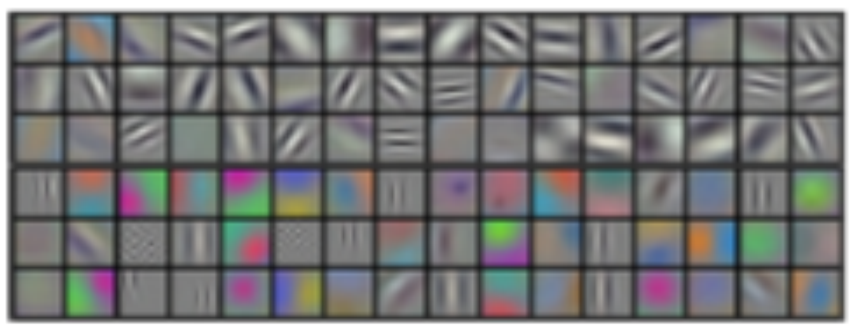


Picture from: Martin Gorner

A Little about Convolution (p2)

- Structure of the ILSVRC-2012 competition winner





(Alex Krizhevsky, Ilya Sutskever Geoffrey E. Hinton 2012 paper