# ML and PyTorch Basics

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### Piazza

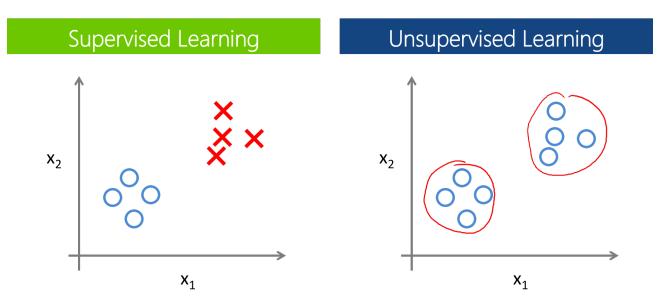
piazza.com/nyu/fall2019/csciga3033020

### Summary

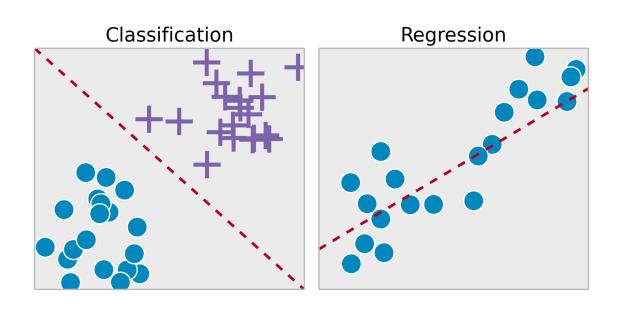
- Machine Learning definition
- Linear and Logistic Regression
- Feed forward, Loss function and Backpropagation
- Inference and Training
- PyTorch basics
  - tensors
  - graph
  - NN
  - training

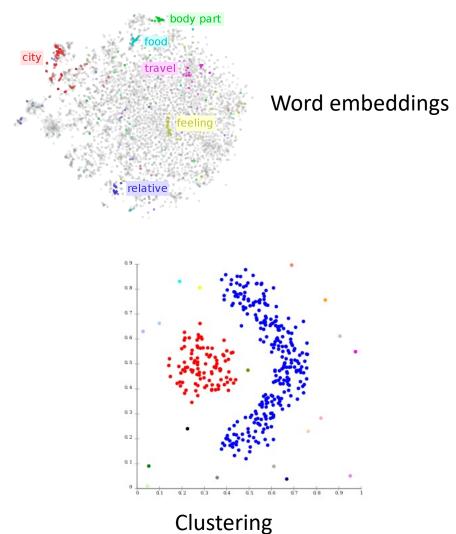
### Machine Learning

- Machine Learning: algorithms that learn from the data to build a predictive analytical model
  - Supervised Learning: A labeled dataset (correct input and output) is available, so you
    can give it to the model to train it
  - Unsupervised Learning: A labeled dataset is not available (only input), the model has
    to learn from the data without knowing in advance what is the expected output

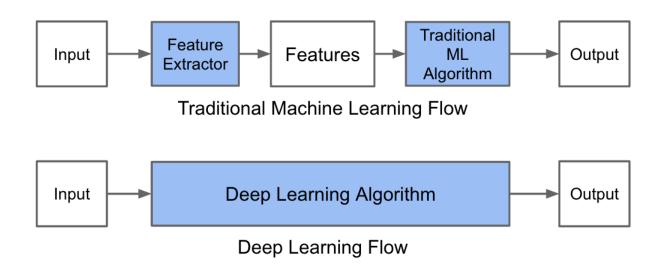


# Supervised vs Unsupervised Learning Examples





# Traditional Machine Learning vs. Deep Learning



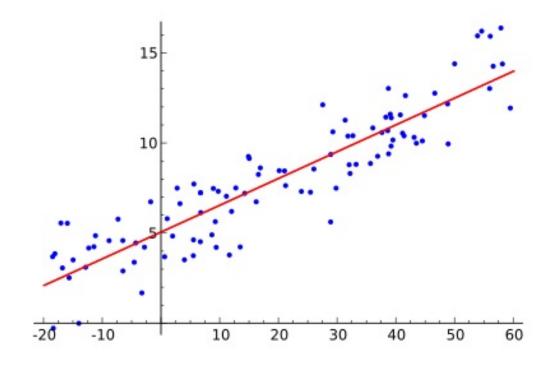
- In traditional Machine Learning an explicit feature extraction phase is needed
  - Feature engineering is difficult, time-consuming and requires domain expertise
- In Deep Learning its (typically) done by the algorithm

### Linear Regression

- Linear regression finds the best-fitting straight line (regression line)
  - The distance between the points to the regression line represent the errors
- Given training data  $\{(x_i, y_i): 1 \le i \le n\}$  i.i.d. from distribution D
- Find W, X and b such that:

$$\hat{Y} = f(x) = W^T X + b$$

- $\hat{Y}$  is the predicted value
- $W^T$  is the weights vector
- *X* is the features vector
- *b* is the bias



### Loss Function

- Loss function: maps output values (predictions) to losses
  - Minimize loss function => Optimizing parameters for fitting
- Examples of loss functions for the linear regression:
  - L1-norm: It is basically minimizing the sum of the absolute differences (S) between the target value  $(y_i)$  and the estimated values  $f(x_i)$ :

$$L = \sum_{i=1}^{n} |y_i - f(x_i)|$$

• L2-norm: It is basically minimizing the sum of the square of the differences (S) between the target value  $(y_i)$  and the estimated values  $f(x_i)$ :

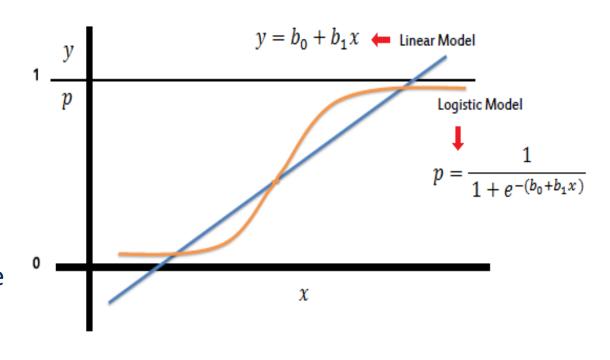
$$L = \sum_{i=1}^{n} (y_i - f(x_i))^2$$

### Logistic regression

• **Logistic Regression** is used to model the probability of a binary event: output is in [0,1]:

$$\widehat{Y} = f(z) = \frac{1}{1 + e^{-z}}$$
$$z = W^{T}X + b$$

- $\hat{Y}$  is the binary event probability (predicted value)
- ullet z is the scalar output of the linear combination
- $W^T$  is the vector of weights
- X is the vector of inputs (features)
- *b* is the bias scalar
- Linear regression output can assume all values while Logistic regression only [0,1]



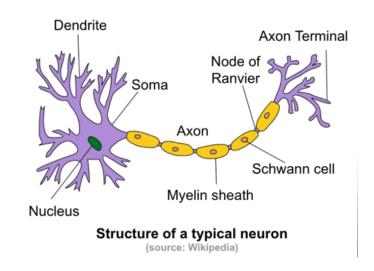
### Artificial Neuron

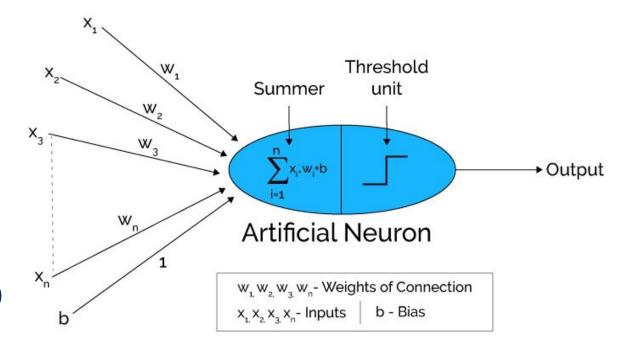
Artificial Neuron:

$$Z = W^T X + b$$

$$\hat{Y} = A(Z)$$

- $W^T$ : weights vector
- *X*: input features vector:
  - 1 sample has multiple features
- $\hat{Y}$ : prediction scalar
- b: bias scalar
- A(Z): activation function (threshold scalar)





### Neuron's Activation Functions

### Threshold (Activation) Functions:

• Sigmoid: 
$$A(Z) = \frac{1}{1+e^{-z}}$$

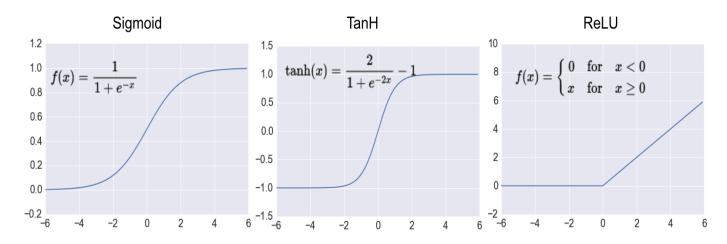
Used for binary classification (0,1)

• Tanh: 
$$A(Z) = \frac{2}{1 + e^{-2z}} - 1$$

Used for generic classification (-1,+1)

• RELU: 
$$A(Z) = \begin{cases} if \ Z < 0 \ then \ 0 \\ if \ Z \ge 0 \ then \ Z \end{cases}$$

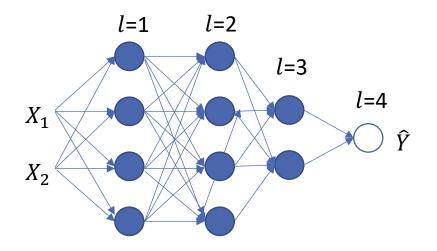
Faster than Sigmoid or Tanh



From: http://adilmoujahid.com/posts/2016/06/introduction-deep-learning-python-caffe/

### Neural Networks

- Able to model non-linear functions
- Each neuron computes its value based on linear combination of values of neurons that point into it
- Can add more layers of hidden units: deeper hidden unit response depends on earlier hidden layers



### Neural Networks Lifecycle

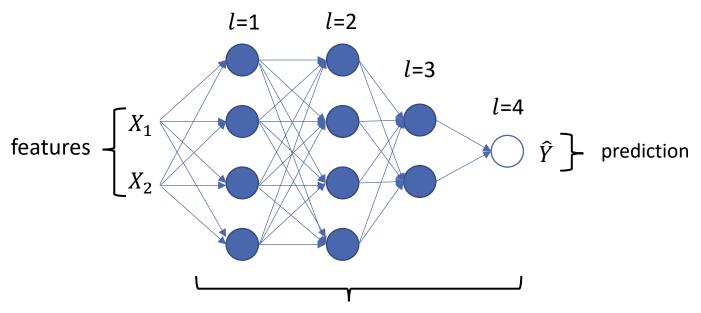
### 1. Definition phase:

- Define Number, Structure and Type of Layers

  Define other algorithmic and structural parameters (Hyperparameters)
- 2. Training phase: discover neuron's weights and biases
- 3. Inference phase: use model to make predictions (or classify)

### Neural Network Definition

Feed-Forward and Fully Connected NN:



Fully Connected Layers 1 to 4 (FC)

• Each output of the layer l is connected to all inputs of layer l+1

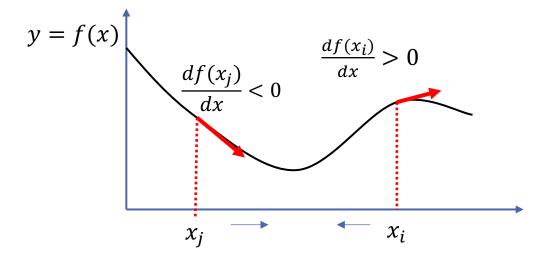
Two types of nodes:

$$Z^{[l]} = W^{[l]}A^{[l-1]} + b^{[l]}$$

$$A^{[l]} = RELU(Z^{[l]})$$

# Training - Gradient Descent

- Find  $x_k$  such that  $y_k = f(x_k)$  is a (local) minima
  - *f* is defined and differentiable
- Gradient Descent:
  - Start with random  $x_o$
  - Repeat:
    - $x_{n+1} < x_n \alpha \frac{df(x_n)}{dx}$
    - Until you don't see any improvement

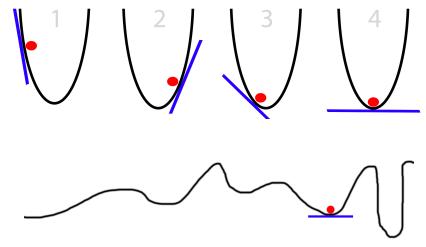


- $\alpha$  is the **Learning Rate**: determines how fast we descend the curve
  - $\alpha$  is usually very small: 0.01 or less

### Training - Gradient Descent

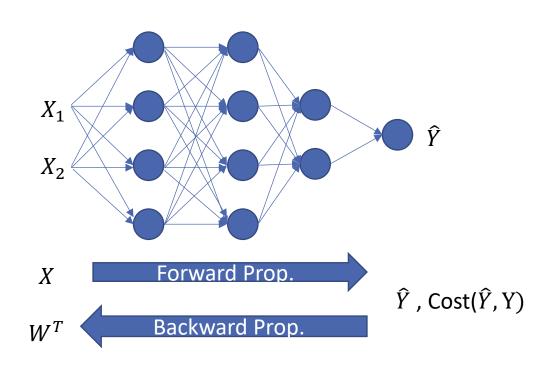
- Used to minimize the Cost Function (loss/error across all samples)
- Gradient descent is that it will more often than not get stuck into the first local minimum that it encounters
  - There is no guarantee that this local minimum it finds is the best (global) one (bottom figure)

# Algorithm 1 Gradient Descent Input: Differentiable function $f(\mathbf{x})$ where $f(\mathbf{x}): \mathbf{R^n} \to \mathbf{R}$ Start point $\mathbf{x_{old}}$ Output: The local minima $\mathbf{x^*}$ that minimize $\mathbf{f}(\mathbf{x})$ 1: while TRUE do 2: tmpDelta $\leftarrow \mathbf{x_{old}} - \alpha.(\nabla \mathbf{f}(\mathbf{x_{old}}))$ 3: if abs(tmpDelta $- \mathbf{x_{old}}) < \mathbf{CRITERIA}$ then 4: break 5: end if 6: $\mathbf{x_{old}} \leftarrow \mathbf{tmpDelta}$ 7: end while

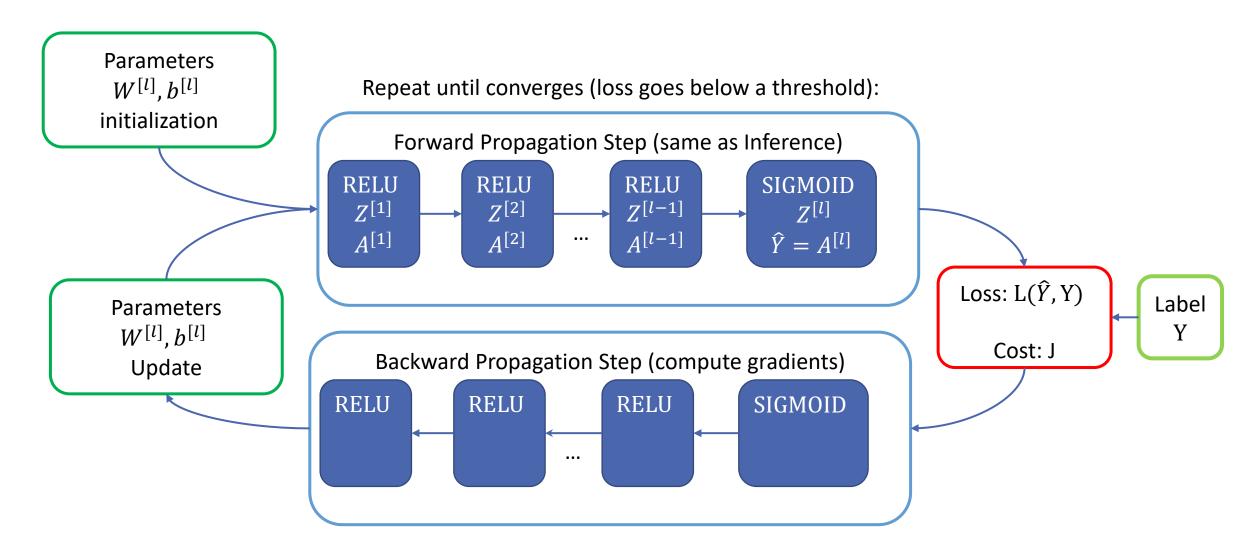


### Training - Gradient Descent

- Prerequisite: Network structure is already defined (hyperparameters)
  - Type and number of layers (FC or other types)
  - Number of neurons on each layer
  - Activation functions of each layer
- Batch Gradient Descent: use all samples
- Gradient Discover all weights and biases:
  - While (COST < threshold)</li>
    - Forward Propagation:
      - compute prediction
      - Same formulas as Inference
    - Backward Propagation
      - compute gradient
      - adjust weights

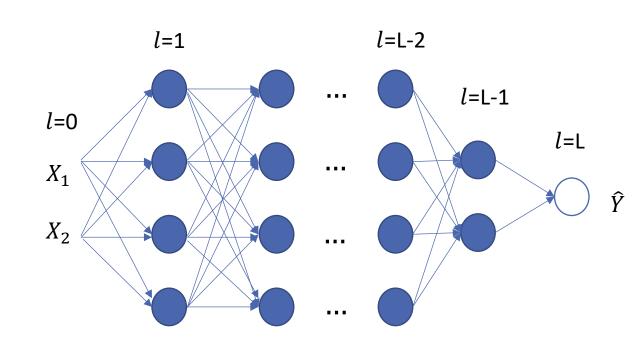


# Training - Gradient Descent Algorithm



# Forward Propagation (and Inference as well)

- *m* samples
- L layers
- $n^{[l]}$  is the number of neurons for layer l (where  $l \in [0, L]$ )
- $n^{[0]}$  is the number of features of each sample (layer 0)
- For each layer *l* compute:
  - $Z^{[l]} = W^{[l]}A^{[l-1]} + b^{[l]}$
  - $A^{[l]} = g^{[l]}(Z^{[l]})$
- Where
  - $A^{[0]} = X$
  - $g^{[L]}$  is a Sigmoid function
  - $g^{[l]}$  for l < L is a RELU function
- Matrices shapes
  - $W^{[l]}$ :  $(n^{[l]}, n^{[l-1]})$
  - $b^{[l]}:(n^{[l]},1)$
  - $A^{[l]}:(n^{[l]},m)$
  - $Z^{[l]}$ :  $(n^{[l]}, m)$



### Forward Propagation – Cost Function

Cost function (cross-entropy):

$$J = -\frac{1}{m} \sum_{i=1}^{m} (y^{(i)} \log(a^{[L](i)}) + (1 - y^{(i)}) \log(1 - a^{[L](i)}))$$

- $y^{(i)}$  is the target (label) value from the dataset of the *i*-th sample
- $a^{[L](i)}$  is the output of the forward propagation (prediction) of the *i*-th sample
- m is the number of samples used (dataset size)
- Cost function: a function of individual samples loss functions (J)

# Backward Propagation – Parameter Updates

For each layer, we want to update the parameters with the gradients

$$W^{[l]} \longleftarrow W^{[l]} - \alpha \frac{dJ}{dW^{[l]}}$$

$$b^{[l]} \longleftarrow b^{[l]} - \alpha \frac{dJ}{db^{[l]}}$$

- How do we compute  $\frac{dJ}{dW^{[l]}}$  and  $\frac{dJ}{db^{[l]}}$  ?
- Go backward from the cost function J: backward propagation

# Backward Propagation Example

- Initial Function f(x, y, z) = (x + y) \* z
- Computation Graph Functions:

$$\bullet \ q(x,y) = x + y$$

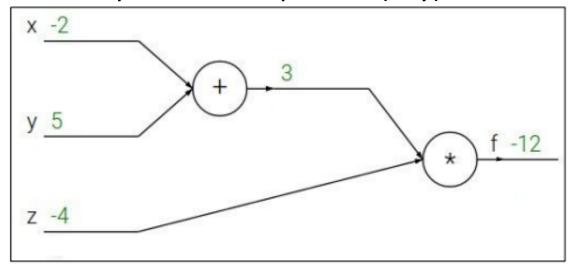
• 
$$f(q,z) = qz$$

- Inputs: x = -2, y = 5, z = -4
- Want to obtain:

• 
$$\frac{df}{dx}$$
,  $\frac{df}{dy}$ ,  $\frac{df}{dz}$ 

(Don't confuse **Computation Graph** with actual **Neural Network!**)

### Computation Graph for (x+y)\* z



From http://cs231n.stanford.edu/slides/2017/cs231n\_2017\_lecture4.pdf

# Backward Propagation Example

### Computation Graph Functions:

• 
$$q(x,y) = x + y$$

• 
$$f(q,z) = qz$$

• Basic gradients:

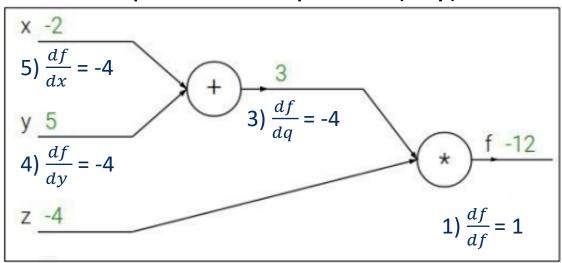
• 
$$\frac{dq(x,y)}{dx} = 1, \ \frac{dq(x,y)}{dy} = 1$$

• 
$$\frac{df(q,z)}{dq} = z$$
,  $\frac{df(q,z)}{dz} = q$ 

• Compute gradients with chain rule:

• 
$$\frac{df}{dz} = q = 3$$

### Computation Graph for (x+y)\* z



$$2) \frac{df}{dz} = 3$$

From http://cs231n.stanford.edu/slides/2017/cs231n 2017 lecture4.pdf

### Stochastic Gradient Descent with Mini-batch

- (Batch) Gradient descent: J is computed for all samples
  - J is computed as the mean of loss functions for all samples:

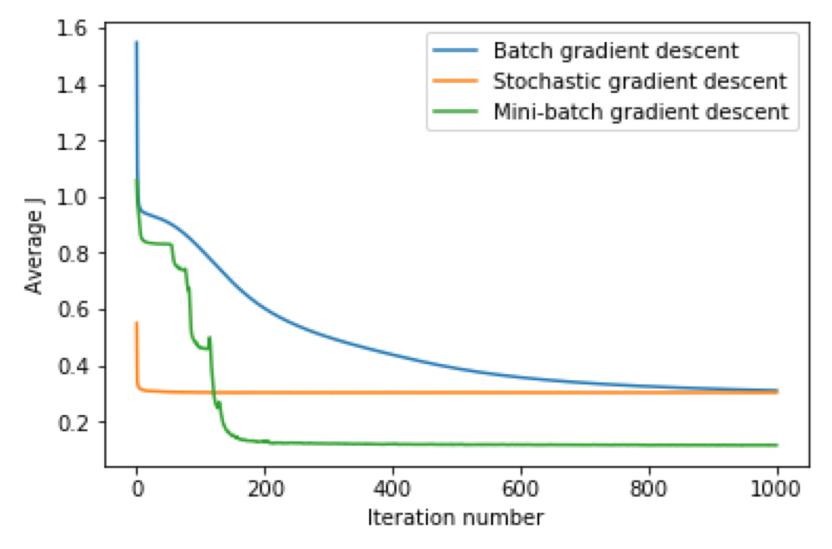
• 
$$J = -\frac{1}{m} \sum_{i=1}^{m} (y^{(i)} \log(a^{[L](i)}) + (1 - y^{(i)}) \log(1 - a^{[L](i)})$$

- Single update of weights with all samples at each iteration
- Very smooth => Local Minima
- Too much memory (all dataset)
- Stochastic Gradient Descent:
  - 1 Sample: J is computed with 1 sample and the weights updated
    - Too slow!
  - Mini-batch SGD (most used): J is computed with a batch (10-500) of samples

### SGD Mini batch size implications

- Step: update the model with 1 mini-batch
- Epoch: composed of all steps (complete training-set)
- Small mini-batch
  - More computation per Epoch
  - Converges faster
  - Can achieve a local minima (not general overfitting)
- Larger mini-batch
  - Converges slower
  - Can achieve a better minima

### Batch size comparison



From: http://adventuresinmachinelearning.com/stochastic-gradient-descent/

### PyTorch

[...] a Python based scientific computing package targeted at two sets of audiences:

- A replacement for numpy to use the power of GPUs
- a deep learning research platform that provides maximum flexibility and speed

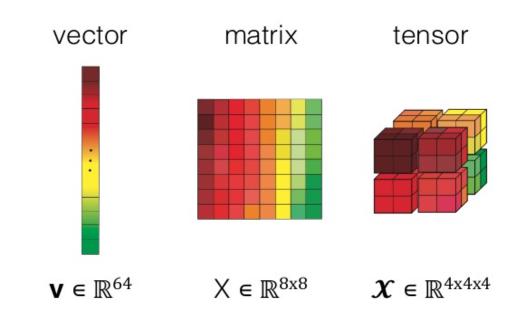
[This lesson uses material from <a href="http://pytorch.org/tutorials/">http://pytorch.org/tutorials/</a> throughout.]

- To install: <a href="https://github.com/pytorch/pytorch#installation">https://github.com/pytorch/pytorch#installation</a>
- For this course use the version 1.0

### Tensors

- Tensors are matrix-like data structures which are essential components in deep learning libraries and efficient computation.
- GPUs are especially effective at calculating operations between tensors

### tensor = multidimensional array



From: https://www.slideshare.net/BertonEarnshaw/a-brief-survey-of-tensors

- Tensor operations:
  - ones, zeros, add, dot, etc.
- PyTorch tensors can live on
  - CPU
  - GPU (speedup!)

### PyTorch Tensors

### • Import Torch:

```
from __future__ import print_function import torch
```

Construct a 2x3 matrix, uninitialized:

```
x = torch.Tensor(2, 3)

print(x)

0.00e+00 0.00e+00 1.15e-24

-1.58e+29 1.67e-37 2.97e-41

[torch.FloatTensor of size 2x3]
```

Use tensor in CUDA

```
device = torch.device("cuda")
y = torch.ones_like(x, device=device) # directly create a
tensor on GPU
x = x.to(device) # or just use .to("cuda")
```

Initialize zeros or ones tensors

```
x = torch.zeros(2,3)
x = torch.ones(2,3)
```

Convert a numpy array

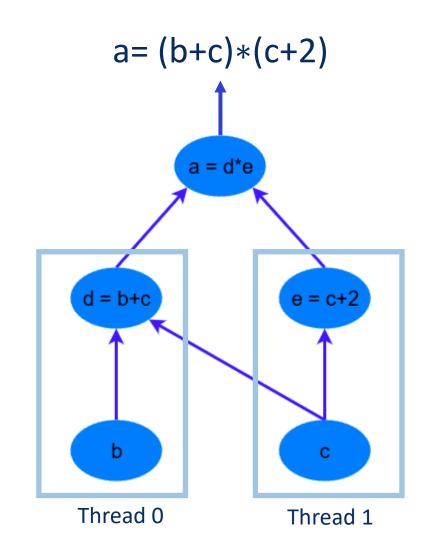
```
b = torch.from_numpy(a)
```

 the slice functionality is available like in numpy

```
x = torch.rand(2,3) \# Initialize a tensor randomly print x[:,1] \# second column 0.6297 0.1196 [torch.FloatTensor of size 2] print x[0,:] # first row 0.9749 0.6297 0.3045 [torch.FloatTensor of size 3]
```

# Computation Graphs

- A computational graph represents a function in a directed acyclic graph of its component functions
- Performance optimizations: Computation Graph exposes parallelism!
- In PyTorch the graph construction is **dynamic:** the graph is built at run-time
  - Easier debugging
  - Better for some algorithms (RNNs)
- In TensorFlow is graph construction is **static:** meaning the graph is "compiled" and then run
  - Compiler adds latency but can also apply optimizations



### Autograd in PyTorch

- Autograd builds the Computation Graph
   Dynamically
- The **Tensor** class is the main component of this autograd system in PyTorch (from PyTorch 0.4 version, the *Variable* class is deprecated)
- If you set its attribute .requires\_grad as True, it starts to track all operations on it
- The gradient for this tensor will be accumulated into .grad attribute
- Tensors allow automatic gradient computation when the .backward() function is called
- Based on the graph, <variable>.backward()
  computes the gradient and writes it in grad
  - Example: **b.backward()** computes  $\frac{d(y)}{dx}$

### PyTorch Tensors, Functions and Gradients

Create a tensor

```
x = torch.tensor(torch.ones(2, 2) * 2,
requires_grad=True)
```

Do a simple math equation:

$$z = 2 * (x * x) + 5 * x$$

 To get the gradient of this operation with respect to x i.e. dz/dx we can analytically calculate this.

- If all elements of x are 2, then we should expect the gradient dz/dx to be a (2, 2) shaped tensor with 13-values.
- However, first we have to run the .backwards() operation to compute these gradients.
- To compute gradients, we need to compute them with respect to something.
- In this case, we can supply a (2,2) tensor of 1-values to be what we compute the gradients against so the calculation simply becomes d/dx:

# PyTorch Neural Network

- torch.nn.module is used to define a neural network
- Example: NN with 3 fully connected layers
  - Using RELU activation for 1<sup>st</sup> and 2<sup>nd</sup> layer
  - Input to 1<sup>st</sup> FC layer: 256 features
  - Input to 2<sup>nd</sup> FC layer: 120 values
  - Input to 3<sup>rd</sup> FC layer: 10 values
- Define only forward prop.: backward prop is automatically derived from it

```
import torch
import torch.nn as nn
import torch.nn.functional as F
#Inherit from class nn.Module
class Net(nn.Module):
  def __init__(self):
    super(Net, self).__init__()
    #y = Wx + b
    self.fc1 = nn.Linear(256, 120)
    self.fc2 = nn.Linear(120, 84)
    self.fc3 = nn.Linear(84, 10)
  def forward(self, x):
    x = F.relu(self.fc1(x))
    x = F.relu(self.fc2(x))
    x = self.fc3(x)
    return x
```

### PyTorch Loss Function

- Loss function:
  - How "far" from the target is the output of forward propagation (prediction)
- NN provides various loss functions with syntax:
  - loss = <loss-function>(output, target)
  - loss, output and target are Tensors

```
#net is the network previously defined
#input is the input data of the network
net = Net()
input = torch.randn(256) # a dummy input
output = net(input)
#criterion is a Mean-Squared Error loss function
criterion = nn.MSELoss()
```

```
target = torch.arange(1, 11) # a dummy target
#target comes from the labelled dataset
loss = criterion(output, target)
```

print(loss)

### PyTorch Backpropagation and weights update

- First reset gradients of the network
- Compute backward prop.
  - It uses *autograd* insides
- Update the weights with STG: weight = weight learning\_rate \* gradient
- Different optimization algorithms are in torch.optim

```
# Zeroes the gradient buffer of all parameters
net.zero_grad()

#Backpropagation step
loss.backward()

#Stocastic Gradient Descent weights update
learning_rate = 0.01
for f in net.parameters():
    f.data.sub_(f.grad.data * learning_rate)
```

# PyTorch Examples

# Autograd Example (1)

### From:

http://pytorch.org/tutorials/begin ner/pytorch\_with\_examples.html

### Import torch

```
dtype = torch.float
device = torch.device("cpu") # Use the CPU as device
# Alternatively, use device = torch.device("cuda:0") to run on GPU
```

```
# N is batch size; D_in is input dimension;
# H is hidden dimension; D_out is output dimension.
N, D_in, H, D_out = 64, 1000, 100, 10
```

# Create random Tensors to hold input and outputs.

# Setting requires\_grad=False indicates that we do not need to compute gradients # with respect to these Tensors during the backward pass.

x = torch.randn(N, D\_in, device=device, dtype=dtype)
y = torch.randn(N, D\_out, device=device, dtype=dtype)

# Create random Tensors for weights.

# Setting requires\_grad=True indicates that we want to compute gradients with # respect to these Tensors during the backward pass.

w1 = torch.randn(D\_in, H, device=device, dtype=dtype, requires\_grad=True) w2 = torch.randn(H, D\_out, device=device, dtype=dtype, requires\_grad=True)

# Autograd Example (2)

```
learning_rate = 1e-6
for t in range(500):
  # Forward pass: compute predicted y using operations on Variables;
  # mm: matrix multiply; clamp: clamp in [min;max]
  y pred = x.mm(w1).clamp(min=0).mm(w2)
  # Compute and print loss. Now loss is a Tensor of shape (1,)
  # loss.item() is a scalar value holding the loss.
  loss = (y pred - y).pow(2).sum()
  print(t, loss.item())
  # Use autograd to compute the backward pass.
  loss.backward()
  # Update weights using gradient descent; w1.data and w2.data are Tensors,
  # w1.grad and w2.grad are Variables and w1.grad.data and w2.grad.data are Tensors.
  with torch.no_grad():
    w1 -= learning rate * w1.grad
    w2 -= learning_rate * w2.grad
    # Manually zero the gradients after updating weights
    w1.grad.zero ()
    w2.grad.zero_()
```

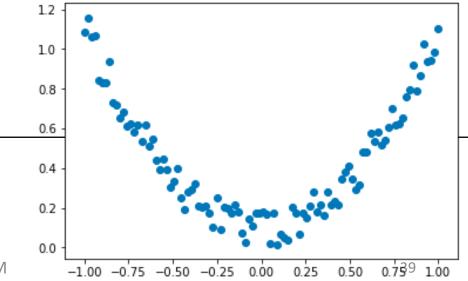
From: http://pytorch.org/tutorials/ beginner/pytorch\_with\_exa mples.html

# Linear Regression Example (1)

```
import torch
import torch.nn.functional as F
import matplotlib.pyplot as plt
```

```
x = torch.unsqueeze(torch.linspace(-1, 1, 100), dim=1) # x data (tensor), shape=(100, 1)
#unsqueeze: reshape tensor
#linspace: return a one-dimensional vector of 100 points between -1 and 1
y = x.pow(2) + 0.2*torch.rand(x.size()) # noisy y data (tensor), shape=(100, 1)
```

plt.scatter(x.numpy(), y.numpy())
plt.show()



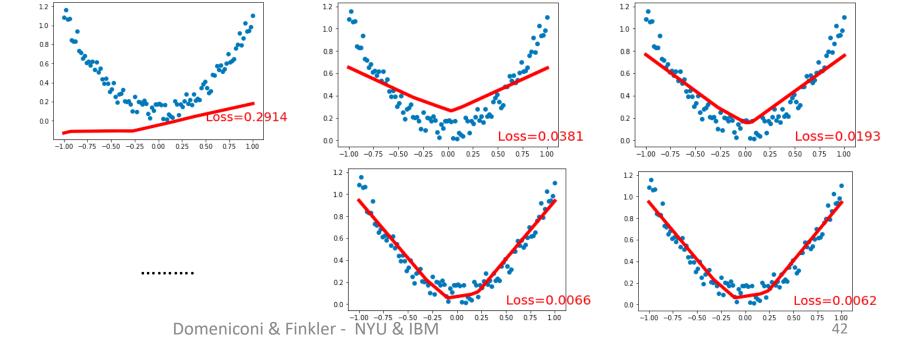
# Linear Regression Example (2)

```
class Net(torch.nn.Module):
    def __init__(self, n_feature, n_hidden, n_output):
         super(Net, self).__init__()
         self.hidden = torch.nn.Linear(n_feature, n_hidden) # hidden layer
         self.predict = torch.nn.Linear(n_hidden, n_output) # output layer
    # For the forward() method, we supply the input data x as the primary argument.
    # The we pass through the two layers of our simple network
    def forward(self, x):
         x = F.relu(self.hidden(x))
                                      # activation function for hidden layer
         x = self.predict(x)
                                      # linear output
         return x
```

# Linear Regression Example (3)

```
# create the network
net = Net(n_feature=1, n_hidden=10, n_output=1) # define the network
print(net) # net architecture
# create a stochastic gradient descent optimizer
# the method net.parameters() (from the base nn.Module class that we inherit in the Net
class), contains all the parameters of our network
optimizer = torch.optim.SGD(net.parameters(), Ir=0.2)
# define the loss, we use the regression mean squared loss
loss func = torch.nn.MSELoss()
plt.ion() # something about plotting
for t in range(200):
  prediction = net(x) # input x and predict based on x
  loss = loss_func(prediction, y) # must be (1. nn output, 2. target)
  # With optimizer.zero_grad() we resets all the gradients in the model
  # so that it is ready to go for the next back propagation pass.
  optimizer.zero_grad() # clear gradients for next train
  loss.backward()
                      # backpropagation, compute gradients
  # runs a back-propagation operation from the loss Tensor backwards
  # through the network and execute a gradient descent step based on
  # the gradients calculated during the .backward() operation.
  optimizer.step()
                      # apply gradients
```

# Linear Regression Example (4)



# NN Example (1)

```
import torch
# N is batch size; D in is input dimension;
# H is hidden dimension; D_out is output dimension.
N, D_in, H, D_out = 64, 1000, 100, 10
# Create random Tensors to hold inputs and outputs
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
# Use the nn package to define our model as a sequence of layers. nn.Sequential
# is a Module which contains other Modules, and applies them in sequence to
# produce its output. Each Linear Module computes output from input using a
# linear function, and holds internal Tensors for its weight and bias.
model = torch.nn.Sequential(
  torch.nn.Linear(D_in, H),
  torch.nn.ReLU(),
  torch.nn.Linear(H, D_out),
```

# The nn package also contains definitions of popular loss functions; in this

# case we will use Mean Squared Error (MSE) as our loss function.

### From:

http://pytorch.org/tutorials/begin ner/pytorch\_with\_examples.html

loss\_fn = torch.nn.MSELoss(reduction='sum')

**HPML** 

# NN Example (2)

### From:

http://pytorch.org/tutorials/begin ner/pytorch\_with\_examples.html

HPML

```
learning_rate = 1e-4
for t in range(500):
  # Forward pass: compute predicted y by passing x to the model. Module objects
  # override the call operator so you can call them like functions. When
  # doing so you pass a Tensor of input data to the Module and it produces
  # a Tensor of output data.
  y pred = model(x)
  # Compute and print loss. We pass Tensors containing the predicted and true
  # values of y, and the loss function returns a Tensor containing the loss.
  loss = loss fn(y pred, y)
  print(t, loss.item())
  # Zero the gradients before running the backward pass.
  model.zero_grad()
  # Backward pass: compute gradient of the loss with respect to all the learnable
  # parameters of the model. Internally, the parameters of each Module are stored
  # in Tensors with requires_grad=True, so this call will compute gradients for
  # all learnable parameters in the model.
  loss.backward()
  # Update the weights using gradient descent. Each parameter is a Tensor, so
  # we can access its gradients like we did before.
  with torch.no_grad():
```

for param in model.parameters():

param -= learning\_rate \* param.grad

### Lesson Key Points

- ML Basics:
  - Linear Regression, Logistic Regression, Gradient Descent
  - Neural Networks (Inference/Training, STG, Batch Size)
- PyTorch:
  - Tensors, Variables, Autograd
  - Examples: Autograd, Linear Regression, NN

### Al services in real life

- Speech recognition
  - https://www.ibm.com/watson/services/speech-to-text/
- Natural language classifier
  - https://www.ibm.com/watson/services/natural-language-classifier/