ITCS 5356 Intro Machine Learning

Python Stack

Linear Algebra and Optimization in NumPy

Computation Graphs in PyTorch

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Python Programming Stack for Deep Learning

- Python = object-oriented, interpreted, scripting language.
  - imperative programming, with functional programming features.
- NumPy = package for powerful N-dimensional arrays:
  - sophisticated (broadcasting) functions.
  - useful linear algebra, Fourier transform, and random number capabilities.
- SciPy = package for numerical integration and optimization.
- Matplotlib = comprehensive 2D and 3D plotting library.

Python Programming Stack for Deep Learning

- PyTorch = a wrapper of NumPy that enables the use of GPUs and automatic differentiation:
  - **Tensors** similar to NumPy's ndarray, but can also be used on GPU.

- Jupyter Notebook = a web app for creating documents that contain live code, equations, visualizations and markdown text.

- Anaconda = an open-source distribution of Python and Python packages:
  - Package versions are managed through Conda.
  - Install all packages above using Anaconda / Conda install.

Anaconda Install

- **Anaconda**: Installation instructions for various platforms can be found at: https://docs.anaconda.com/anaconda/install/
  - For Mac and Linux users, the system PATH must be updated after installation so that 'conda' can be used from the command line.
    - Mac OS X:
      - For bash users: export PATH=~/anaconda3/bin:$PATH
      - For csh/tcsh users: setenv PATH ~/anaconda3/bin:$PATH
    - For Linux:
      - For bash users: export PATH=~/anaconda3/bin:$PATH
      - For csh/tcsh users: setenv PATH ~/anaconda3/bin:$PATH
  - It is recommend the above statement be put in the ~/.bashrc or ~/.cshrc file, so that it is executed every time a new terminal window is open.
  - To check that conda was installed, running "*conda list*" in the terminal should list all packages that come with Anaconda.

Installing Packages with Conda / Anaconda

- A number of tools and libraries that we will use can be configured from Anaconda:
  - Python 3, NumPy, SciPy, Matplotlib, Jupyter Notebook, Ipython, Pandas, Scikit-learn.
  - PyTorch can be installed from Anaconda, with ‘conda’ from the command line:
    - The actual command line depends on the platform as follows:
      - Using the GUI on pytorch.org, choose the appropriate OS, conda, Python 3.6, CUDA or CPU version.

import numpy as np

- np.array()
  - indexing, slices.
- ndarray.shape, .size, .ndim, .dtype, .T
- np.zeros(), np.ones(), np.arange(). np.eye()
  - *dtype* parameter.
  - tuple (shape) parameter.
- np.reshape(), np.ravel()
- np.amax(), np.maximum(), np.sum(), np.mean,() np.std()
  - *axis* parameter, also np.ndarray
- np.stack(), np.[hv]stack(), np.column_stack(), np.split()
- np.exp(), np.log(),
- https://docs.scipy.org/doc/numpy/user/quickstart.html

NumPy: Broadcasting

- Broadcasting describes how numpy treats arrays with different shapes during arithmetic operations.
- The smaller array is “broadcast” across the larger array so that they have compatible shapes, subject to broadcasting rules:
  - NumPy compares their shapes element-wise.
  - It starts with the trailing dimensions, and works its way forward.
  - Two dimensions are compatible when:
    - they are equal, or one of them is 1.
- https://docs.scipy.org/doc/numpy/user/basics.broadcasting.html

Other Numpy Functions

- np.dot(), np.vdot()
  - also np.ndarray.
- np.outer(), np.inner()

- **import numpy.random as random:**
  - randn(), randint(), uniform()

- **import numpy.linalg as la:**
  - la.norm(), la.det(), la.matrix_rank(), np.trace()
  - la.eig(), la.svd()
  - la.qr(), la.cholesky()

- https://docs.scipy.org/doc/numpy/reference/routines.linalg.html

Implementation: Vectorization of LR

- **Version 3**: Compute gradient, vectorized.

$$\nabla L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(\hat{y}_n - y_n)\mathbf{x}_n$$

grad = X.T @ sigmoid(X.dot(**w**) − **y**) / N

```
def sigmoid(x):
    return 1 / (1 + np.exp(−x))
```

import scipy

- scipy.sparse.coo_matrix()

```
groundTruth = coo_matrix((np.ones(N, dtype = np.uint8),
                          (labels, np.arange(N)))).toarray()
```

- scipy.optimize:
  - scipy.optimize.fmin_l_bfgs_b()

```
theta, _, _ = fmin_l_bfgs_b(softmaxCost, theta,
                  args = (numClasses, inputSize, decay, images, labels),
                  maxiter = 100, disp = 1)
```

  - scipy.optimize.fmin_cg()
  - scipy.minimize

https://docs.scipy.org/doc/scipy-0.10.1/reference/tutorial/optimize.html

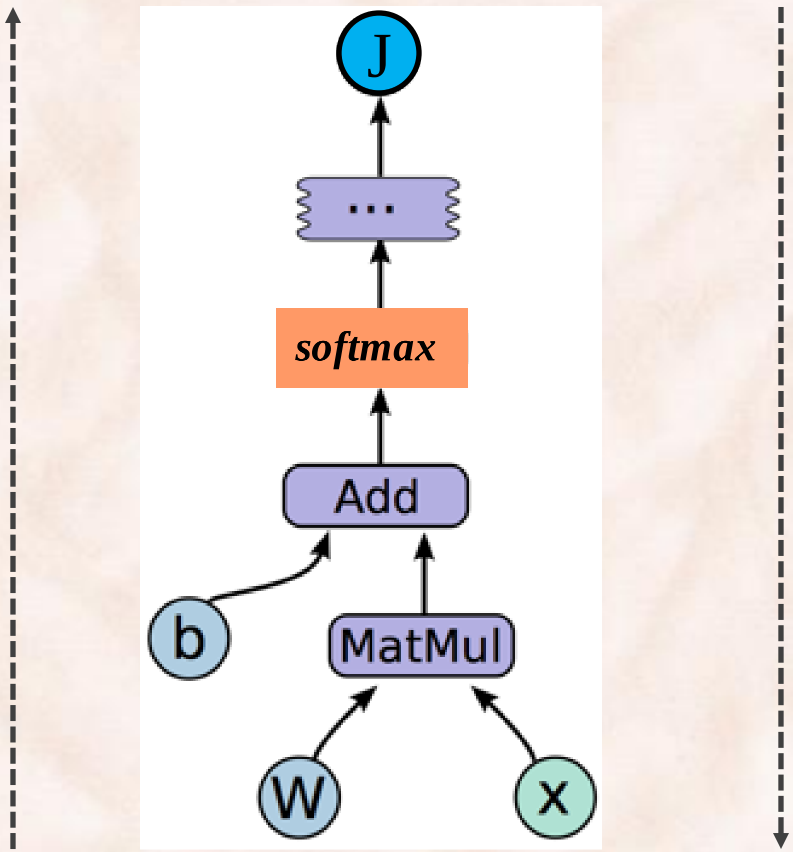
Towards PyTorch: Graphs of Computations

- A function J can be expressed by the **composition** of computational elements from a given set:
  - Mathematical operators:
    - multiplication and additions
  - Elementwise application of mathematical functions:
    - $\max(0, x)$, $\exp(x)$, …

- The function is defined by a graph of computations:
  - A directed acyclic graph, with one node per computational element.
  - Depth of architecture = depth of the graph = longest path from an input node to an output node.

Logistic Regression as a Computation Graph

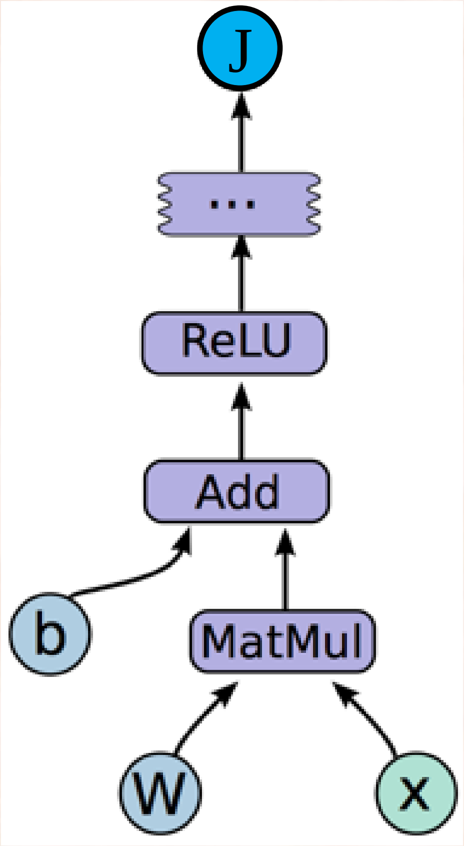
Inference =
Forward
Propagation



Learning =
Backward
Propagation

Neural Network as a Computation Graph

Inference =
Forward
Propagation



Learning =
Backward
Propagation

What is PyTorch

- A wrapper of **NumPy** that enables the use of GPUs.
  - **Tensors** similar to NumPy's *ndarray*, but can also be used on GPU.

- A flexible deep learning platform:
  - Deep Neural Networks built on a tape-based **autograd** system:
    - Building neural networks using and replaying a tape recorder.
    - **Reverse-mode auto-differentiation** allows changing the network at runtime:
      - The computation graph is created on the fly.
      - Backpropagation is done on the dynamically built graph.

http://pytorch.org/about/

Automatic Differentiation

https://pytorch.org/tutorials/beginner/blitz/autograd_tutorial.html

- Deep learning packages offer automatic differentiation.

- PyTorch has the *autograd* package:
  - *torch.Tensor* the main class; *torch.Function* class also important.
    - When *requires_grad* = *True*, it tracks all operations on this tensor (e.g. the parameters).
    - An acyclic graph is built **dynamically** that encodes the history of computations, i.e. compositions of functions.
      - TensorFlow compiles **static** computation graphs.
    - To compute the gradient, call *backward*() in a scalar valued Tensor (e.g. the *loss*).

Tensors

- PyTorch **tensors** support the same operations as NumPy.
  - Arithmetic.
  - Slicing and Indexing.
  - Broadcasting.
  - Reshaping.
  - Sum, Max, Argmax, …

- PyTorch tensors can be converted to NumPy tensors.
- NumPy tensors can be converted to PyTorch tensors.

http://pytorch.org/tutorials/beginner/blitz/tensor_tutorial.html

Autograd

- The **autograd** package provides automatic differentiation for all operations on Tensors.
  - It is a *define-by-run* framework, which means that the gradient is defined by how your code is run:
    - Every single **backprop** iteration can be different.

- **autograd.Tensor** is the central class of the package.
  - Once you finish your computation you can call **.backward()** and have all the gradients computed automatically.

http://pytorch.org/tutorials/beginner/blitz/autograd_tutorial.html

Tensor and Function

- A **Tensor** v has three important attributes:
  - v.**data** holds the raw tensor value.
  - v.**grad** is another Tensor which accumulates the gradient w.r.t. **v**:
    - The gradient of what?
      - The gradient of any variable *u* that uses *v* on which we call u.**backward**().
    - http://pytorch.org/docs/master/autograd.html
  - v.**grad_fn** stores the **Function** that has created the Tensor *v*:
    - http://pytorch.org/docs/master/autograd.html

Multivariate Chain Rule for Differentiation

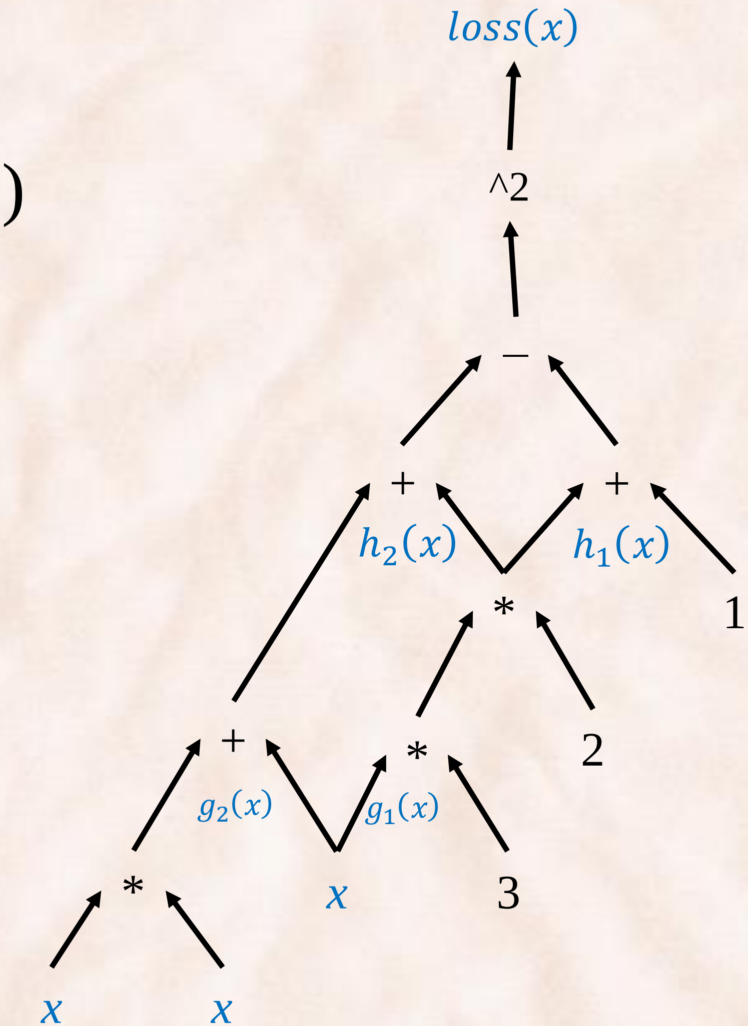
- Multivariate Chain Rule:

$$f = f(g_1(x), g_2(x), \ldots, g_n(x))$$

$$\frac{\partial f}{\partial x} = \sum_{i=1}^{n} \frac{\partial f}{\partial g_i} \frac{\partial g_i}{\partial x}$$

- Example 2:

$$loss(x) = (h_1(x) - h_2(x))^2$$
$$h_1(x) = 2g_1(x) + 1$$
$$h_2(x) = 2g_1(x) + g_2(x)$$
$$g_1(x) = 3x$$
$$g_2(x) = x^2 + x$$



$$loss(x) = \left(h_1(x) - h_2(x)\right)^2$$

$$h_1(x) = 2g_1(x) + 1 \longrightarrow 7$$

$$h_2(x) = 2g_1(x) + g_2(x) \longrightarrow 8$$

$$g_1(x) = 3x \longrightarrow 3$$

$$g_2(x) = x^2 + x \longrightarrow 2$$

$$\frac{\partial l}{\partial x} = \frac{\partial l}{\partial h_1} \cdot \frac{\partial h_1}{x} + \frac{\partial l}{\partial h_2} \cdot \frac{\partial h_2}{\partial x}$$

$$= 2\,(h_1 - h_2) \cdot \frac{\partial h_1}{\partial x} + 2\,(h_2 - h_1)\frac{\partial h_2}{\partial x}$$

$$= 2\,(h_1 - h_2)\left(\frac{\partial h_1}{\partial x} - \frac{\partial h_2}{\partial x}\right)$$

$$= 2\,(h_1 - h_2)\left(\frac{\partial h_1}{\partial g_1} \cdot \frac{\partial g_1}{\partial x} - \frac{\partial h_2}{\partial g_1}\frac{\partial g_1}{\partial x} - \frac{\partial h_2}{\partial g_2} \cdot \frac{\partial g_2}{\partial x}\right)$$

$$= 2\,(h_1 - h_2)\left(\cancel{2 \cdot 3} - \cancel{2 \cdot 3} - 1 \cdot (2x+1)\right) = 2\,(h_1 - h_2)(-2x - 1)$$

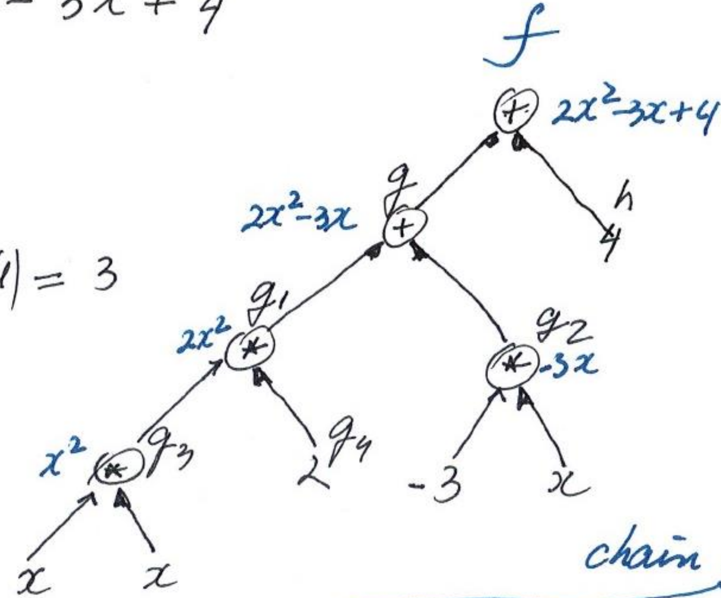
$$= 2\,(h_2 - h_1)(2x + 1)$$

$$x = 1 \Rightarrow \frac{\partial l}{\partial x} = 2\,(8 - 7)\,(3) = 6$$

$f(x) = 2x^2 - 3x + 4$

forward pass

$f(1) = 3$



$f'(x) = \frac{\partial f}{\partial x} = 4x - 3$

$x = 1$

backward() pass

$f'(1) = 1$

add(x, y) = x+y

chain rule of differentiation

$f = add(g, h)$

$\frac{\partial f}{\partial x} = \frac{\partial add}{\partial g} \cdot \frac{\partial g}{\partial x} + \frac{\partial add}{\partial h} \cdot \frac{\partial h}{\partial x}$

$= 1 \cdot \frac{\partial g}{\partial x} + 1 \cdot 0 = \frac{\partial g}{\partial x} = 4x - 3$

$g = add(g_1, g_2) \Rightarrow \frac{\partial g}{\partial x} = \frac{\partial g_1}{\partial x} + \frac{\partial g_2}{\partial x} = 4x - 3$

$\frac{\partial g_2}{\partial x} \to -3$

$\frac{\partial g_1}{\partial x} = \frac{\partial mul}{\partial g_3} \frac{\partial g_3}{\partial x} + \frac{\partial mul}{\partial g_4} \cdot \frac{\partial g_4}{\partial x} = 2 \cdot 2x + g_3 \cdot 0 = 4x$

PyTorch

- Install using Anaconda:
  - conda install pytorch torchvision -c pytorch
  - http://pytorch.org
- Install from sources:
  - https://github.com/pytorch/pytorch#from-source
- Tutorials:
  - http://pytorch.org/tutorials/
  - http://pytorch.org/tutorials/beginner/pytorch_with_examples.html