Machine Learning
ITCS 6156/8156

Python Stack
Linear Algebra and Optimization in NumPy
Computation Graphs in PyTorch

Razvan C. Bunescu
Department of Computer Science @ CCI

rbunescu@uncc.edu
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/](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:
  - 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](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](https://docs.scipy.org/doc/numpy/reference/routines.linalg.html)
Logistic Regression: Vectorization

- **Version 1**: Compute gradient component-wise.

\[ \nabla E(w) = \sum_{n=1}^{N} (h_n - t_n)x_n \]

```python
grad = np.zeros(K)
for n in range(N):
    h = sigmoid(w.dot(X[:, n]))
    temp = h - t[n]
    for k in range(K):
        grad(k) = grad(k) + temp * X[k, n]
```
Logistic Regression: Vectorization

- **Version 2**: Compute gradient, partially vectorized.

\[
\nabla E(w) = \sum_{n=1}^{N} (h_n - t_n) x_n
\]

\[
\text{grad} = \text{np.zeros}(K)
\]

for n in range(N):
    grad = grad + (sigmoid(w.dot(X[:, n])) - t[n]) * X[:, n]
Logistic Regression: Vectorization

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

\[
\nabla E(w) = \sum_{n=1}^{N} (h_n - t_n)x_n
\]

\[
\text{grad} = X @ (\text{sigmoid}(w \cdot X)) - t
\]

```python
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:
  – logic operators.
  – logistic operators.
  – multiplication and additions.

• 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](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](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:**
  \[ \text{loss}(x) = (h_1(x) - h_2(x))^2 \]
  \[ h_1(x) = 2g_1(x) + 1 \]
  \[ h_2(x) = 2g_1(x) + g_2(x) \]
  \[ g_1(x) = 3x \]
  \[ g_2(x) = x^2 + x \]
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