ITCS 5356: Introduction to Machine Learning

Linear Algebra and Optimization in Python

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Python Programming Stack

- 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 plotting library.

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()
  - also np.ndarray.
- 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(),

NumPy: Broadcasting

- Broadcasting describes how numpy treats arrays with different shapes during arithmetic operations.
- The smaller array is "broadcast" across the larger array s.t. 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.
  - When no dimension is left in one array, it is viewed as 1.

- http://scipy.github.io/old-wiki/pages/EricsBroadcastingDoc
- https://docs.scipy.org/doc/numpy-dev/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

import scipy

- scipy.sparse.coo_matrix()

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

Implementation: Vectorization

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

$$\sum_{n=1}^{N}(h_n - y_n)\mathbf{x}_n$$

```
grad = np.zeros(K)
for n in range(N):
    h = sigmoid(w.dot(X[:, n])
    temp = h − y[n]
    for k in range(K):
      grad(k) = grad(k) + temp * X[k,n]
```

Implementation: Vectorization

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

$$\sum_{n=1}^{N} (h_n - y_n)\mathbf{x}_n$$

```
grad = np.zeros(K)
for n in range(N):
    grad = grad + (sigmoid(w.dot(X[:, n])) − y[n]) * X[:, n]
```

Implementation: Vectorization

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

$$\sum_{n=1}^{N} (h_n - y_n)\mathbf{x}_n$$

grad = X.dot(sigmoid(**w**.dot(X)) − **t**)

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