SGD draft

May 9, 2016

0.1 Problem Setting and Algorithm

Stochastic Gradient Descent (SGD) is a simple yet very efficient approach to discriminative learning of linear classifiers under convex loss functions such as (linear) Support Vector Machines and Logistic Regression. Even though SGD has been around in the machine learning community for a long time, it has received a considerable amount of attention just recently in the context of large-scale learning. The advantages of Stochastic Gradient Descent are: Efficiency, Ease of implementation (lots of opportunities for code tuning). The disadvantages of Stochastic Gradient Descent include: SGD requires a number of hyperparameters such as the regularization parameter and the number of iterations, SGD is sensitive to feature scaling.

Given a set of training examples $(x_1, y_1), \cdots, (x_n, y_n)$ where $x_i \in R^n$ $y_i \in -1, 1$, the goal of stochastic gradient descent is to learn a linear scoring function $f(x) = w^T x + b$ with model parameters $w \in R^m$ and intercept $b \in R$. In order to make predictions, we simply look at the sign of $f(x)$. The regularized training error is

$$E(w, b) = \frac{1}{n} \sum_{i=1}^{n} L(y_i, f(x_i)) + \alpha R(w)$$

where L is a loss function and R is a penalty term for model complexity; $\alpha > 0$ is a non-negative parameter.

Different choices for L entail different classifiers such as Hinge: (soft-margin) Support Vector Machines, Log: Logistic Regression, Least-Squares: Ridge Regression, Epsilon-Insensitive: (soft-margin) Support Vector Regression. All of the above loss functions can be regarded as an upper bound on the misclassification error (Zero-one loss).

The choices for regularization terms include: L2 normm $R(w) := \frac{1}{2} \sum w_i^2$, L1 norm $R(w) := \sum |w_i|$, and elastic net $R(w) := \frac{\rho}{2} \sum w_i^2 + (1 - \rho) \sum |w_i|$. At each time step, w and b are updated as follows

$$w \leftarrow w - \eta_t (\alpha \frac{\partial R(w)}{\partial w} + \frac{\partial L(w^T x_i + b, y_i)}{\partial w})$$
$$b \leftarrow b - \eta_t (\frac{\partial L(w^T x_i + b, y_i)}{\partial b})$$

The algorithm is guaranteed to converge if η_t satisfies the Robbins-monro conditions

$$\sum_{t=1}^{\infty} \eta_t = \infty, \sum_{t=1}^{\infty} \eta_t^2 < \infty$$

In this paper we will assume a Hinge loss function, a L2 norm regularization term and

$$\eta_t = \frac{1}{\alpha(t_0 + t)}$$

for Scikit learn t_0 is based on a heuristic proposed by Leon Bottou. This is the normal SVM problem.

0.2 Implementation in Python

In [1]:
```
class Lossfunction:
    def loss(self, p, y):
        return 0
    def dloss(self, p, y):
        return 0
```

In [2]:
```
class Hinge(Lossfunction):
    def __init__(self, threshold=1):
        self.threshold=threshold
    def loss(self, p, y):
        z=p*y

        if z<=self.threshold:
            return (self.threshold-z)
        return 0
    def _dloss(self, p ,y):
        z= p*y
        if z<=self.threshold:
            return -y
        return 0
```

In [3]:
```
import numpy as np
class sgddata:
    def __init__(self, X, Y, sample_weights=0,seed=None):
        if len(X)!=len(Y):
            raise IndexError('X, Y not same length')
        self.X = np.array(X)
        self.Y = np.array(Y)
        self.sample_weights = sample_weights
        self.n_samples = self.X.shape[0]
        self.n_features = self.X.shape[1]
        self.current_index = -1
    def __next__(self):
        self.current_index += 1
        return self.X[self.current_index], self.Y[self.current_index]
    def _reset(self):
        self.current_index = -1
    def shuffle(self ,seed=None):
        np.random.seed(seed)
        idx = np.random.permutation(self.n_samples)
        self.X = self.X[idx]
        self.Y = self.Y[idx]
    def __str__(self):
        return '{},{}'.format(str(self.X), str(self.Y))
```

In [4]:
```
from time import time
def sgd( weights,
               intercept,
               loss,
               penalty_type,
               alpha,
               dataset,
               n_iter, fit_intercept=True,
```

```
                 verbose=False, shuffle=True, seed=None,
                 weight_pos=1, weight_neg=1,
                 eta0=0,
                 t=1.0,
                 intercept_decay=1.0):
    MAX_DLOSS = 1e12
    eta = eta0
    l1_ratio = 0.0
    sumlosslist = []
    n_samples=dataset.n_samples
    typw = np.sqrt(1.0 / np.sqrt(alpha))
    # computing eta0, the initial learning rate
    initial_eta0 = typw / max(1.0, loss.dloss(-typw, 1.0))
    # initialize t such that eta at first sample equals eta0
    optimal_init = 1.0 / (initial_eta0 * alpha)
    t_start = time()
    for epoch in range(n_iter):
        sumloss=0

        if shuffle:
            dataset.shuffle(seed)
        for i in range(n_samples):
            x_current,y_current = next(dataset)
            p = np.dot(x_current,weights) + intercept
            eta = 1.0 / (alpha * (optimal_init + t - 1))
            if y_current > 0.0:
                class_weight = weight_pos
            else:
                class_weight = weight_neg
            dloss = loss._dloss(p, y_current)
            # clip dloss with large values to avoid numerical
            # instabilities
            if dloss < -MAX_DLOSS:
                dloss = -MAX_DLOSS
            elif dloss > MAX_DLOSS:
                dloss = MAX_DLOSS
            update = -eta * dloss
            update *= class_weight
            weights *= (max(0, 1.0 - ((1.0 - l1_ratio) * eta * alpha)))
            if update != 0.0:
                weights += update*x_current
                if fit_intercept == 1:
                    intercept += update * intercept_decay
            dataset._reset()
            t += 1
        if verbose > 0:
            sumloss=0
            for i in range(n_samples):
                x_current,y_current = next(dataset)
                p = np.dot(x_current,weights) + intercept
                sumloss+=loss.loss(p,y_current)
#               print("loss={}".format(str(sumloss)))
            sumlosslist.append(sumloss)
            dataset._reset()
```

```
        print('time = {} second'.format(str(time()-t_start)))
        return weights, intercept,sumlosslist
```

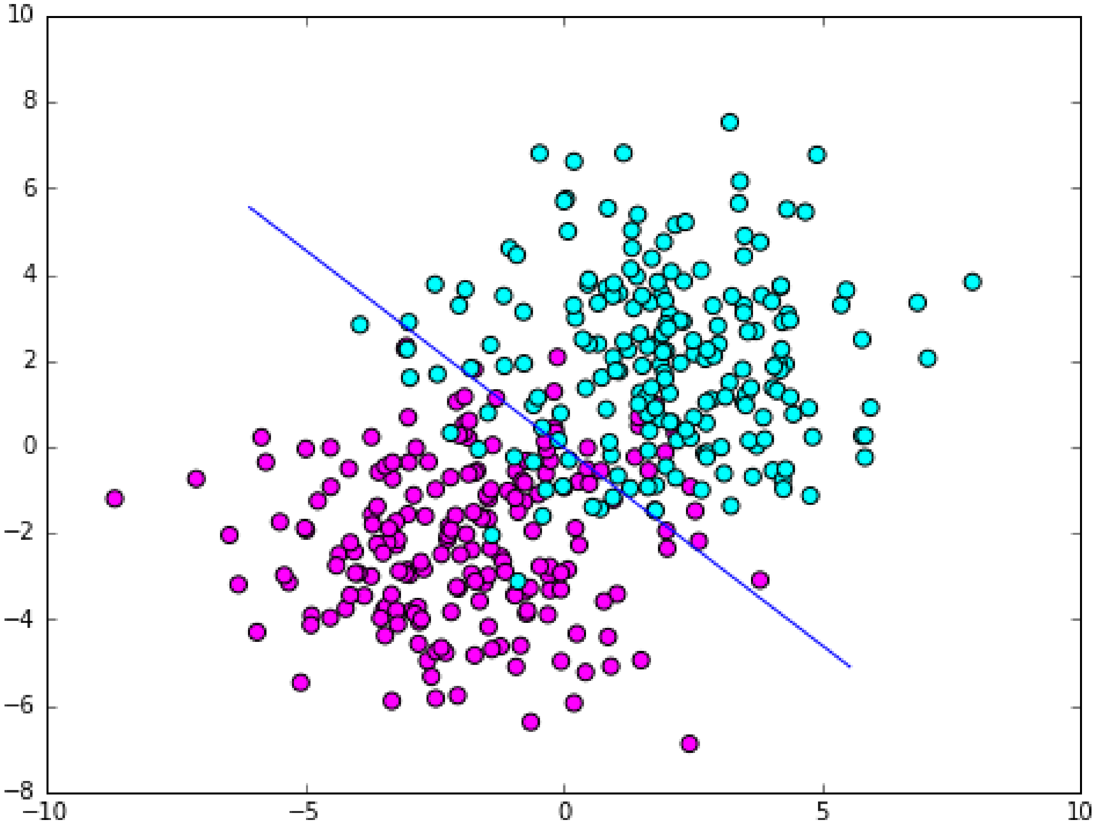
0.3 Running with Data

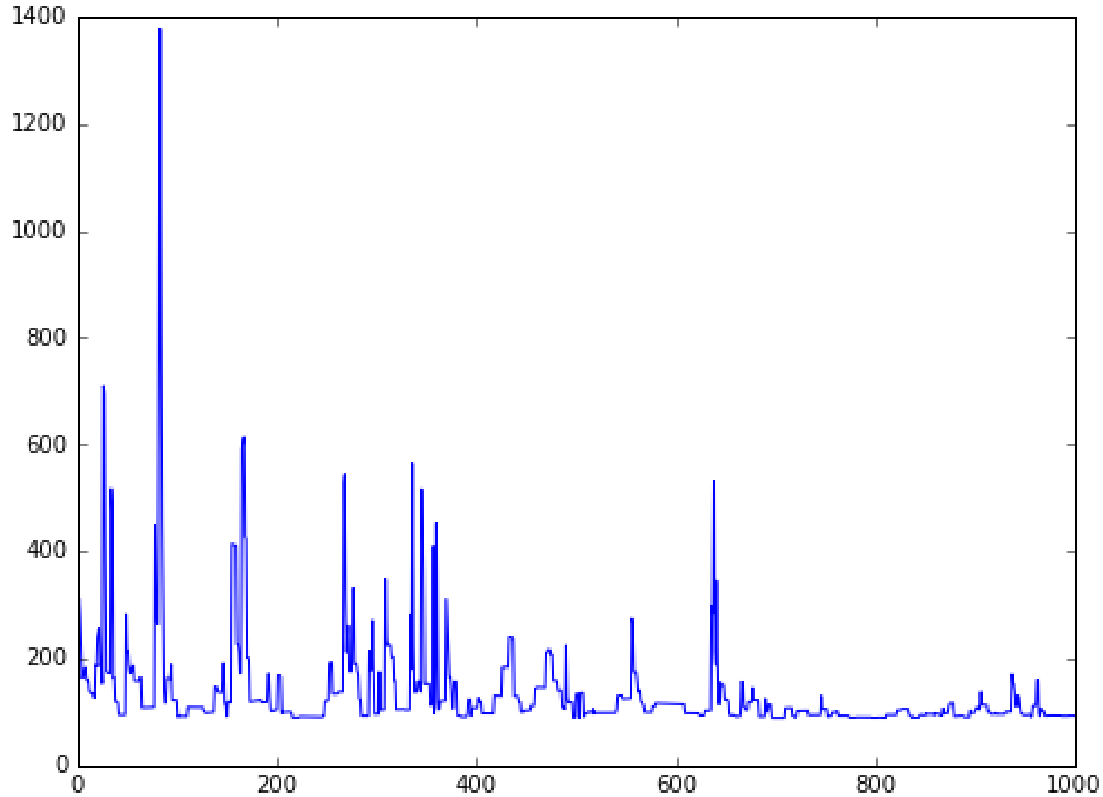
```
In [5]: from numpy import loadtxt
        train = loadtxt('data_stdev2_train.csv')
        X = train[:,0:2]
        Y = train[:,2:3]
```

```
In [6]: weight_init=np.array([0.,0.])
        intercept_init = 0.
        # X = [[0., 0.], [1., 1.],[2.,3.]]
        # y = [-1, 1, 1]

        dataset = sgddata(X,Y)
        loss=Hinge()
        n_iter = 1000
        verbose=True
        weights,intercept,sumlosslist=sgd(weight_init,intercept_init,loss,'L2',0.01,dataset,n_iter,verbo
        import pylab as pl
        %matplotlib inline
        pl.figure(0,figsize=(8, 6))
        pl.scatter(X[:, 0], X[:, 1], c=(1.-Y), s=50, cmap = pl.cm.cool)
        x1 = np.linspace(min(X[:, 0])*0.7,max(X[:, 0])*0.7,10)
        x2 = -(weights[0]*x1+intercept)/weights[1]
        pl.plot(x1,x2)
        if verbose:
            pl.figure(1,figsize=(8, 6))
            pl.plot(range(n_iter),sumlosslist)
```

```
time = 12.75475263595581 second
```


10
8
6
4
2
0
−2
−4
−6
−8
−10
−5
0
5
10



We see from the top figure that the SGD algorithm arrived a reasonable conclusion. Our bottom plot shows the stochastic nature of the process of convergence. Setting α to a smaller value increases the step size and leads to higher fluctuations.

0.4 Scikit Learn Optimizations

Scikit learn optimizes SGD using Cython. The optimizations mostly happen in three areas: 1. The loss function, 2. The data structure that stores the data, 3. The datastructure that stores and updates the weight vector and 4. The implementation of SGD itself.

0.4.1 Optimizations in Loss Function

The hinge loss function is implemented in Cython at lines 138-167, copied below. Besides the **init** function all other functions are cdef functions. Static typing is used throughout the implementation.

```
In [ ]: cdef class Hinge(Classification):
            """Hinge loss for binary classification tasks with y in {-1,1}
            Parameters
            ----------
            threshold : float > 0.0
                Margin threshold. When threshold=1.0, one gets the loss used by SVM.
                When threshold=0.0, one gets the loss used by the Perceptron.
            """

            cdef double threshold
```

```
    def __init__(self, double threshold=1.0):
        self.threshold = threshold

    cdef double loss(self, double p, double y) nogil:
        cdef double z = p * y
        if z <= self.threshold:
            return (self.threshold - z)
        return 0.0

    cdef double _dloss(self, double p, double y) nogil:
        cdef double z = p * y
        if z <= self.threshold:
            return -y
        return 0.0

    def __reduce__(self):
        return Hinge, (self.threshold,)
```

0.4.2 Optimizations in Data Storage

Scikit-learn first convert the data into a ArrayDataset object, which is also implemented in Cython. The code that converts the raw input data to a ArrayDataset is linked here.

First, we look at how ArrayDataSet is initialized. At lines 195-196 we see that ArrayDataSet creates memoryvies to the numpy array X and Y and assign their pointers to X_data_ptr and Y_data_ptr.

```
In [ ]: self.X_data_ptr = <double *>X.data
        self.Y_data_ptr = <double *>Y.data
```

The SGD algorithm goes through the dataset samples one-by-one. This is called in the SGD algorithm at lines 606-607, copied below. We see that this is implemented within the ArrayDataSet object

```
In [ ]: dataset.next(&x_data_ptr, &x_ind_ptr, &xnnz,
                                  &y, &sample_weight)
```

We take a closer look at the .next() function. The .next function is implemented at lines 20-46 of seq_dataset.pyx. The ArrayDataSet object keeps a data index, which .next() calls, advancing the index by one, and then calls the ._sample function,

```
In [ ]: cdef void _sample(self, double **x_data_ptr, int **x_ind_ptr,
                          int *nnz, double *y, double *sample_weight,
                          int current_index) nogil:
            cdef long long sample_idx = self.index_data_ptr[current_index]
            cdef long long offset = sample_idx * self.X_stride

            y[0] = self.Y_data_ptr[sample_idx]
            x_data_ptr[0] = self.X_data_ptr + offset
            x_ind_ptr[0] = self.feature_indices_ptr
            nnz[0] = self.n_features
            sample_weight[0] = self.sample_weight_data[sample_idx]
```

We see that the _sample function takes x_data_ptr and y and make it so they point to the pointer to the start of X_i. x_data_ptr and y are then used by the rest of the SGD algorithm to access the current sample.

0.4.3 Optimizations in Weights

The weight vector is stored in a WeightVector object at line 551 in sgd_fast.pyx

```
In [ ]: cdef WeightVector w = WeightVector(weights, average_weights)
```

The WeightVector object is defined here. Its mechanism of data storage is similar to ArrayDataset, relevant lines below

```
In [ ]: cdef double *wdata = <double *>w.data

                if w.shape[0] > INT_MAX:
                    raise ValueError("More than %d features not supported; got %d."
                                     % (INT_MAX, w.shape[0]))
                self.w = w
                self.w_data_ptr = wdata
```

All operations that update the weight vector is done within the WeightVector object. In particular we look at the add function, which scales sample x by constant c and add it to the weight vector. SGD calls it byWe copy the add function below

```
In [ ]: cdef void add(self, double *x_data_ptr, int *x_ind_ptr, int xnnz,
                          double c) nogil:
                """Scales sample x by constant c and adds it to the weight vector.
                This operation updates ``sq_norm``.
                Parameters
                ----------
                x_data_ptr : double*
                    The array which holds the feature values of ``x``.
                x_ind_ptr : np.intc*
                    The array which holds the feature indices of ``x``.
                xnnz : int
                    The number of non-zero features of ``x``.
                c : double
                    The scaling constant for the example.
                """
                cdef int j
                cdef int idx
                cdef double val
                cdef double innerprod = 0.0
                cdef double xsqnorm = 0.0

                # the next two lines save a factor of 2!
                cdef double wscale = self.wscale
                cdef double* w_data_ptr = self.w_data_ptr

                for j in range(xnnz):
                    idx = x_ind_ptr[j]
                    val = x_data_ptr[j]
                    innerprod += (w_data_ptr[idx] * val)
                    xsqnorm += (val * val)
                    w_data_ptr[idx] += val * (c / wscale)

                self.sq_norm += (xsqnorm * c * c) + (2.0 * innerprod * wscale * c)
```

Getting values from X_i is done using x_data_ptr[j], modifying the weight vector is done similarly. Note the “nogil” argument, this declares that the function is safe to call without GIL.

0.4.4 Optimizations in SGD algorithm

The raw code for the SGD algorithm in scikit-learn is here. Since we're assuming OPTIMAL leraning rate, hinge loss and L2 regularization, we copy the relevant parts of the code below

In [ ]:
```
def _plain_sgd(np.ndarray[double, ndim=1, mode='c'] weights,
               double intercept,
               np.ndarray[double, ndim=1, mode='c'] average_weights,
               double average_intercept,
               LossFunction loss,
               int penalty_type,
               double alpha, double C,
               double l1_ratio,
               SequentialDataset dataset,
               int n_iter, int fit_intercept,
               int verbose, bint shuffle, np.uint32_t seed,
               double weight_pos, double weight_neg,
               int learning_rate, double eta0,
               double power_t,
               double t=1.0,
               double intercept_decay=1.0,
               int average=0):

    # get the data information into easy vars
    cdef Py_ssize_t n_samples = dataset.n_samples
    cdef Py_ssize_t n_features = weights.shape[0]

    cdef WeightVector w = WeightVector(weights, average_weights)
    cdef double* w_ptr = &weights[0]
    cdef double *x_data_ptr = NULL
    cdef int *x_ind_ptr = NULL
    cdef double* ps_ptr = NULL

    # helper variables
    cdef bint infinity = False
    cdef int xnnz
    cdef double eta = 0.0in
    cdef double p = 0.0
    cdef double update = 0.0
    cdef double sumloss = 0.0
    cdef double y = 0.0
    cdef double sample_weight
    cdef double class_weight = 1.0
    cdef unsigned int count = 0
    cdef unsigned int epoch = 0
    cdef unsigned int i = 0
    cdef int is_hinge = isinstance(loss, Hinge)
    cdef double optimal_init = 0.0
    cdef double dloss = 0.0
    cdef double MAX_DLOSS = 1e12

    # q vector is only used for L1 regularization
    cdef np.ndarray[double, ndim = 1, mode = "c"] q = None
    cdef double * q_data_ptr = NULL
```

```
if penalty_type == L2:
    l1_ratio = 0.0


if learning_rate == OPTIMAL:
    typw = np.sqrt(1.0 / np.sqrt(alpha))
    # computing eta0, the initial learning rate
    initial_eta0 = typw / max(1.0, loss.dloss(-typw, 1.0))
    # initialize t such that eta at first sample equals eta0a
    optimal_init = 1.0 / (initial_eta0 * alpha)

t_start = time()
with nogil:
    for epoch in range(n_iter):
        if verbose > 0:
            with gil:
                print("-- Epoch %d" % (epoch + 1))
        if shuffle:
            dataset.shuffle(seed)
        for i in range(n_samples):
            dataset.next(&x_data_ptr, &x_ind_ptr, &xnnz,
                         &y, &sample_weight)

            p = w.dot(x_data_ptr, x_ind_ptr, xnnz) + intercept
            if learning_rate == OPTIMAL:
                eta = 1.0 / (alpha * (optimal_init + t - 1))

            if verbose > 0:
                sumloss += loss.loss(p, y)

            if y > 0.0:
                class_weight = weight_pos
            else:
                class_weight = weight_neg


            dloss = loss._dloss(p, y)
            # clip dloss with large values to avoid numerical
            # instabilities
            if dloss < -MAX_DLOSS:
                dloss = -MAX_DLOSS
            elif dloss > MAX_DLOSS:
                dloss = MAX_DLOSS

            update = -eta * dloss

            update *= class_weight * sample_weight

            if penalty_type >= L2:
                # do not scale to negative values when eta or alpha are too
                # big: instead set the weights to zero
                w.scale(max(0, 1.0 - ((1.0 - l1_ratio) * eta * alpha)))
            if update != 0.0:
                w.add(x_data_ptr, x_ind_ptr, xnnz, update)
```

```
                if fit_intercept == 1:
                    intercept += update * intercept_decay


            t += 1
            count += 1

        # report epoch information
        if verbose > 0:
            with gil:
                print("Norm: %.2f, NNZs: %d, "
                      "Bias: %.6f, T: %d, Avg. loss: %.6f"
                      % (w.norm(), weights.nonzero()[0].shape[0],
                         intercept, count, sumloss / count))
                print("Total training time: %.2f seconds."
                      % (time() - t_start))

        # floating-point under-/overflow check.
        if (not skl_isfinite(intercept)
            or any_nonfinite(<double *>weights.data, n_features)):
            infinity = True
            break

    if infinity:
        raise ValueError(("Floating-point under-/overflow occurred at epoch"
                          " #%d. Scaling input data with StandardScaler or"
                          " MinMaxScaler might help.") % (epoch + 1))

    w.reset_wscale()

    return weights, intercept, average_weights, average_intercept
```

Besides the performance benefits from ArrayDataSet and WeightVector, the Cython implementation has a few properties that further speeds it up. Nearly all variables are defined using cdef and static typing. The main part of the algorithm is done under with nogil.