logistic-regression

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1 1 Loading the Dataset

Extract instances showing "3" or "8", append a column of "1s" and create a vector of ground-truth labels where 1 corresponds to 3 and -1 to 8.

```
In [5]: X = data[np.logical_or(target == 3, target == 8)]
    y = target[np.logical_or(target == 3, target == 8)]

X = np.concatenate((X, np.ones([len(y),1])), axis = 1)

y[y==3] = 1
    y[y==8] = -1
```

2 1.1 Classification with sklearn

```
logistic = LogisticRegression(C = C)
            curr_scores = cross_val_score(logistic, X, y, cv = num_splits)
            scores[i,0] = np.average(curr_scores)
            scores[i,1] = np.std(curr_scores)
In [8]: import pandas as pd
       pd.options.display.float_format = '{:,.4f}'.format
In [9]: display(pd.DataFrame(
                data = scores,
                index = lambdas,
                columns = ['mean','std'])
                .rename_axis('C', axis = 'columns'))
С
            mean
                     std
0.0010
         0.9688 0.0531
         0.9691 0.0464
0.0100
0.1000
          0.9860 0.0288
1.0000
         0.9860 0.0288
10.0000 0.9803 0.0283
100.0000 0.9775 0.0304
1,000.0000 0.9747 0.0341
```

The accuracy of the prediction varies only very slowly when modifying the regularization parameter. The best accuracy is obtained for $\lambda=0.1,1,10$, thus a very large range. In the following we will proceed using $\lambda=1$.

3 1.2 Optimization Methods

```
In [10]: def sigmoid(z):
    return 1 / (1 + np.exp(-z))

In [11]: def predict(beta, X):
    # if X*beta > 0 --> y=1, if X*beta < 0 --> y=-1
    y = (X.dot(beta) >= 0) * 2 - 1
    return y

In [12]: def zero_one_loss(y_prediction, y_truth):
    return np.sum(np.not_equal(y_prediction, y_truth))

In [13]: def gradient(beta, X, y, lambda_ = 1):
    # distinguish the cases of one single / several training instances
    if np.isscalar(y):
        grad = beta / lambda_ - sigmoid(-X.dot(beta) * y) * y * X
    else:
        grad = beta / lambda_ - np.average((sigmoid(-X.dot(beta) * y) * y)[:,None] *:
    return grad
```

To sample single random instances, we do sampling without replacement since we want to avoid computing the gradient from the same instance repetitively. Instead, we want to use as much different samples as possible to compute the gradient. Only in the case of mini-batches, we do sampling with replacement since the training set is not large enough to sample 150 times a mini-batch witout replacing "old" samples.

```
In [15]: from sklearn.utils import shuffle
         def SGD(X, y, beta, tau_0, gamma, m):
             X, y = shuffle(X,y)
             for i in range(m):
                 tau = tau_0 / (1 + gamma * i)
                 beta = beta - tau * gradient(beta, X[i,:], y[i])
             return beta
In [16]: def SG_minibatch(X, y, beta, tau_0, gamma, m, B = 1):
             # here we do not replace the samples since there would not be enough samples
             # to perform m=150 optimization steps for larger B
             for i in range(m):
                 X, y = shuffle(X,y)
                 tau = tau_0 / (1 + gamma * i)
                 beta = beta - tau * gradient(beta, X[:B,:], y[:B])
             return beta
In [17]: def SG_momentum(X, y, beta, tau_0, gamma, mu, m):
             X, y = shuffle(X,y)
             # initialize g
             g = np.zeros(len(beta))
             for i in range(m):
                 tau = tau_0 / (1 + gamma * i)
                 g = mu * g + (1 - mu) * gradient(beta, X[i,:], y[i])
                 beta = beta - tau * g
             return beta
In [18]: def ADAM(X, y, beta, m, tau=10**-4, mu1=0.9, mu2=0.999, eps=10**-8):
             X, y = shuffle(X,y)
             # initialize q, q
             g = np.zeros(len(beta))
             q = np.zeros(len(beta))
             for i in range(m):
                 grad = gradient(beta, X[i,:], y[i])
                 g = mu1 * g + (1 - mu1) * grad
                 q = mu2 * q + (1 - mu2) * np.square(grad)
                 beta = beta - tau / (np.sqrt(q) + eps) * g
             return beta
```

```
In [19]: # so wie im Skript
                    def Newton_Raphson(X, y, beta, m, lambda_=0.001):# hier muss lambda kleiner gewählt w
                             N,D = X.shape
                             for _ in range(m):
                                      z = X.dot(beta)
                                      y_{tilde} = y / sigmoid(-y * z)
                                      W = np.diag(lambda_ / N * sigmoid(z) * sigmoid(-z))
                                      inv = np.linalg.inv(1 / lambda_ * np.identity(D) + np.dot(X.T, np.dot(W, X)))
                                      beta = beta + np.dot(inv, np.dot(X.T, np.dot(W, y_tilde)) - beta / lambda_)
                             return beta
In [20]: # so wie auf dem Zettel
                    def Newton_Raphson1(X, y, beta, m, lambda_=0.001):
                             N,D = X.shape
                             for _ in range(m):
                                      z = X.dot(beta)
                                      y_{tilde} = y / sigmoid(-y * z)
                                      W = lambda_ / N * np.diag(sigmoid(z) * sigmoid(-z))
                                      inv = np.linalg.inv(np.identity(D) + np.dot(X.T, np.dot(W, X)))
                                      beta = np.dot(inv, np.dot(X.T, W)).dot(z + y_tilde)
                             return beta
In [21]: def dual_coordinate_ascent(X, y, m, lambda_=1):
                             # initialization:
                             N = X.shape[0]
                             alpha = np.random.uniform(size=N)
                             beta = lambda_ * np.average((alpha * y)[:,None] * X, axis=0)
                             X, y = shuffle(X, y)
                             for i in range(m):
                                      f_{prime} = y[i] * np.dot(X[i,:], beta) + np.log(alpha[i] / (1 - alpha[i]))
                                      f_2prime = lambda_ / N * np.dot(X[i,:], X[i,:].T) + 1 / (alpha[i] * (1 - alpha[i]) + 1 / (alpha[i]) + 1 / 
                                      alpha_old = alpha[i].copy()
                                      alpha[i] = max(0, min(1, alpha[i] - f_prime / f_2prime))
                                      beta += lambda_ / N * y[i] * X[i,:] * (alpha[i] - alpha_old)
                             return beta
In [22]: def SAGD(X, y, beta_init, tau_0, gamma, m, lambda_ = 0.001):
                             #init
                             try:
                                     X, y = shuffle(X, y)
                                            = X.shape[0]
                                      beta = beta_init
                                     g_stored = np.zeros(N)
                                                       = np.zeros(N)
                                      g_vec
                                      for i in range(N):
                                               \#print(sigmoid(\neg y[i] * np.dot(X[i,:],beta)))
                                               g_{\text{stored}}[i] = -y[i] * X[i, :] * sigmoid(-y[i] * np.dot(X[i,:],beta))
                                      g = np.average(g_stored)
```

```
#iterate
                 for i in range(m):
                     g_{vec[i]} = -y[i] * X[i,:] * sigmoid(-y[i] * np.dot(X[i,:],beta))
                           = g + 1. / N * (g_vec[i] - g_stored[i])
                     tau_t = tau_0 / (1 + gamma * i)
                     g_stored[i] = g_vec[i]
                     beta = beta * (1 - tau_t / lambda_) - tau_t * g
                 return beta
             except:
                 raise NotImplementedError('Not yet implemented')
dual coordinate ascent
In [23]: X_train, X_test, y_train, y_test = train_test_split (X, y, test_size = 0.3 ,random_state
         beta = dual_coordinate_ascent(X_train, y_train, 150)
         errors = zero_one_loss(predict(beta, X_test), y_test)
         print(errors / len(y_test))
0.027777777778
SAGD
In [24]: X_train, X_test, y_train, y_test = train_test_split (X, y, test_size = 0.3 ,random_state
        beta = np.zeros(65)
         tau_0 = 0.001
         gamma = 0.0001
         beta = SAGD(X_train, y_train, beta, tau_0, gamma, 150)
         errors = zero_one_loss(predict(beta, X_test), y_test)
         print(errors / len(y_test))
        ValueError
                                                  Traceback (most recent call last)
        <ipython-input-22-028ad3c55fc7> in SAGD(X, y, beta_init, tau_0, gamma, m, lambda_)
                        #print(sigmoid(-y[i] * np.dot(X[i,:],beta)))
    ---> 11
                        g_{stored[i]} = -y[i] * X[i, :] * sigmoid(-y[i] * np.dot(X[i,:],beta))
                  g = np.average(g_stored)
         12
        ValueError: setting an array element with a sequence.
```

During handling of the above exception, another exception occurred:

```
Traceback (most recent call last)
        NotImplementedError
        <ipython-input-24-f91d9cc6115d> in <module>()
          3 tau_0 = 0.001
          4 \text{ gamma} = 0.0001
    ----> 5 beta = SAGD(X_train, y_train, beta, tau_0, gamma, 150)
          7 errors = zero_one_loss(predict(beta, X_test), y_test)
        <ipython-input-22-028ad3c55fc7> in SAGD(X, y, beta_init, tau_0, gamma, m, lambda_)
         20
                    return beta
         21
                except:
    ---> 22
                    raise NotImplementedError('Not yet implemented')
        NotImplementedError: Not yet implemented
GD
In [25]: X_train, X_test, y_train, y_test = train_test_split (X, y, test_size = 0.3 ,random_st
         beta = np.zeros(65)
         beta = GD(X_train, y_train, beta, 0.001, 0.0001, 10)
         errors = zero_one_loss(predict(beta, X_test), y_test)
         print(errors / len(y_test))
0.0185185185185
Newton Raphson
In [26]: X_train, X_test, y_train, y_test = train_test_split (X, y, test_size = 0.3 ,random_st
         beta = np.zeros(65)
         beta = Newton_Raphson(X_train, y_train, beta, 150)
         errors = zero_one_loss(predict(beta, X_test), y_test)
         print(errors / len(y test))
0.0185185185185
In [27]: X_test.shape
Out[27]: (108, 65)
```

SGD w/o replacement

0.0185185185185

ADAM

0.0185185185185

4 1.3 Comparison

```
/usr/local/lib/python3.6/site-packages/sklearn/cross_validation.py:41: DeprecationWarning: This module will be removed in 0.20.", DeprecationWarning)
```

```
In [32]: optimizers = ['GD', 'SGD', 'SGD_mini', 'SGD_mom', 'ADAM', 'DualCA', 'NR']
         #tbd: 'SAGD'
         class LogisticRegression:
             def __init__(self, X, y, type_, beta_0):
                 self.X = X
                 self.y = y
                 self.type = type_
                 self.beta = beta_0
             def compare_parameters(self, tau_0_, mu_, gamma_, iter_ = 150, num_results_shown =
                 if num_results_shown is None:
                      num_results_shown = len(tau_0_)*len(mu_)*len(gamma_)
                 if self.type in ['NR', 'GD']:
                      iter_{=} = 10
                 X_tr, X_test, y_tr, y_test = train_test_split (self.X, self.y, test_size = 0.3
                 cross_val_results = []
                 beta = self.beta
                 for (tau_0, mu, gamma) in itertools.product(tau_0_, mu_, gamma_):
                      kf = KFold(y_tr.shape[0], n_folds=10)
                      errors = 0
                      for train_idx, val_idx in kf:
                          if self.type == 'SGD':
                              beta = SGD(X_tr[train_idx], y_tr[train_idx], beta, tau_0, gamma,
                          elif self.type == 'GD':
                              beta = GD(X_tr[train_idx], y_tr[train_idx], beta, tau_0, gamma, i
                          elif self.type == 'SGD_mini':
                              \#print('SGD\ minibatch\ running\ with\ B=',\ B)
                              beta = SG_minibatch(X_tr[train_idx], y_tr[train_idx], beta, tau_0
                          elif self.type == 'SGD_mom':
                              beta = SG_momentum(X_tr[train_idx], y_tr[train_idx], beta, tau_0,
                          elif self.type == 'ADAM':
                              \#ADAM(X, y, beta, m, tau=10**-4, mu1=0.9, mu2=0.999, eps=10**-8):
                              beta = ADAM(X_tr[train_idx], y_tr[train_idx], beta, iter_)
                          elif self.type == 'DualCA':
                              beta = dual_coordinate_ascent(X_tr[train_idx], y_tr[train_idx], i
                          elif self.type == 'NR':
                              beta = Newton_Raphson(X_tr[train_idx], y_tr[train_idx], beta, ite
                          elif self.type == 'SAGD':
                              \#beta = self.type(X_tr[train_idx], y_tr[train_idx], beta, tau_0, y_tr[train_idx], beta, tau_0, y_tr[train_idx]
                              raise NotImplementedError('tbd')
                          errors += zero_one_loss(predict(beta, X_tr[val_idx]), y_tr[val_idx])
```

```
cross_val_results.append((tau_0, mu, gamma, errors))
                 sort = np.array(sorted(cross_val_results, key = itemgetter(3)))
                 print('\nUsing ' , self.type, ' optimizer.')
                 print('Listing results starting with lowest error score: \n')
                 display(pd.DataFrame(
                     data = sort[:num results shown - 1, :3],
                     index = sort[:num_results_shown - 1, -1],
                     columns = ['tau 0', 'mu', 'gamma'])
                     .rename_axis('errors', axis = 'columns'))
                 return sort[0]
                 #print(sorted(cross_val_results, key = itemgetter(3)))
In [33]: tau, mu, gamma = [0.001, 0.01, 0.1], [0.1, 0.2, 0.5], [0.0001, 0.001, 0.01]
         LR = LogisticRegression(X, y, 'SGD', np.zeros(65))
         LR.compare_parameters(tau, mu, gamma)
Using SGD optimizer.
Listing results starting with lowest error score:
                  mu gamma
errors tau_0
0.0000 0.0010 0.1000 0.0100
0.0000 0.0010 0.5000 0.0100
1.0000 0.0010 0.2000 0.0100
2.0000 0.0010 0.2000 0.0010
3.0000 0.0010 0.5000 0.0010
4.0000 0.0010 0.1000 0.0001
4.0000 0.0010 0.1000 0.0010
4.0000 0.0010 0.2000 0.0001
5.0000 0.0010 0.5000 0.0001
11.0000 0.0100 0.5000 0.0100
16.0000 0.0100 0.2000 0.0100
18.0000 0.0100 0.2000 0.0010
21.0000 0.0100 0.1000 0.0100
27.0000 0.0100 0.5000 0.0001
28.0000 0.0100 0.1000 0.0010
38.0000 0.0100 0.5000 0.0010
40.0000 0.1000 0.5000 0.0100
47.0000 0.0100 0.2000 0.0001
62.0000 0.0100 0.1000 0.0001
65.0000 0.1000 0.2000 0.0100
66.0000 0.1000 0.5000 0.0001
73.0000 0.1000 0.1000 0.0100
78.0000 0.1000 0.2000 0.0010
```

```
78.0000 0.1000 0.5000 0.0010
87.0000 0.1000 0.2000 0.0001
96.0000 0.1000 0.1000 0.0010
Out[33]: array([ 0.001,  0.1 ,  0.01 ,  0. ])
listing the n best results of each optimizer
In [34]: def list_n_best(X, y, n, opti_list, tau, mu, gamma):
             overview = np.empty([7], dtype=[('opt', 'U10'), ('tau', 'f4'), ('mu', 'f4'), ('gar
             for i, opt in enumerate(opti_list):
                 LR = LogisticRegression(X, y, opt, np.zeros(65))
                 best = LR.compare_parameters(tau, mu, gamma, num_results_shown=n)
                 overview['opt'][i] = opt
                 overview['tau'][i] = best[0]
                 overview['mu'][i] = best[1]
                 overview['gamma'][i] = best[2]
             print("\n \n Overall best parameters: \n")
             display(pd.DataFrame(
                     data = overview, index=overview['opt'],
                     columns = ['tau','mu', 'gamma']).rename_axis('optimizer', axis = 'columns
             return overview
In [35]: params = list_n_best(X, y, 10, optimizers, tau, mu, gamma)
Using GD optimizer.
Listing results starting with lowest error score:
errors tau_0
                 mu gamma
3.0000 0.0010 0.1000 0.0100
3.0000 0.0010 0.2000 0.0001
3.0000 0.0010 0.2000 0.0010
3.0000 0.0010 0.2000 0.0100
3.0000 0.0010 0.5000 0.0001
3.0000 0.0010 0.5000 0.0010
3.0000 0.0010 0.5000 0.0100
3.0000 0.0100 0.1000 0.0001
3.0000 0.0100 0.1000 0.0010
Using SGD optimizer.
Listing results starting with lowest error score:
```

errors tau_0 mu gamma
0.0000 0.0010 0.5000 0.0001
1.0000 0.0010 0.2000 0.0010
1.0000 0.0010 0.5000 0.0100
2.0000 0.0010 0.1000 0.0010
2.0000 0.0010 0.1000 0.0100
2.0000 0.0010 0.2000 0.0100
5.0000 0.0010 0.2000 0.0001
6.0000 0.0010 0.1000 0.0001
6.0000 0.0010 0.5000 0.0010

Using SGD_mini optimizer. Listing results starting with lowest error score:

errors tau_0 mu gamma
1.0000 0.0010 0.2000 0.0001
2.0000 0.0010 0.1000 0.0010
2.0000 0.0010 0.5000 0.0010
2.0000 0.0010 0.5000 0.0100
3.0000 0.0010 0.1000 0.0001
3.0000 0.0010 0.1000 0.0100
3.0000 0.0010 0.2000 0.0100
3.0000 0.0010 0.2000 0.0100
3.0000 0.0010 0.5000 0.0001

Using SGD_mom optimizer. Listing results starting with lowest error score:

errors tau_0 mu gamma
1.0000 0.0010 0.1000 0.0100
1.0000 0.0010 0.2000 0.0010
1.0000 0.0010 0.2000 0.0100
1.0000 0.0010 0.5000 0.0100
2.0000 0.0010 0.2000 0.0011
2.0000 0.0010 0.5000 0.0010
3.0000 0.0010 0.5000 0.0010
4.0000 0.0100 0.5000 0.0001

Using ADAM optimizer.

Listing results starting with lowest error score:

errors tau_0 mu gamma
1.0000 0.0100 0.1000 0.0100
1.0000 0.1000 0.5000 0.0001
2.0000 0.0010 0.2000 0.0010
2.0000 0.0100 0.2000 0.0010
2.0000 0.0100 0.2000 0.0100
2.0000 0.0100 0.2000 0.0100
2.0000 0.0100 0.5000 0.0001
2.0000 0.1000 0.1000 0.0001
2.0000 0.1000 0.2000 0.0010

Using DualCA optimizer.
Listing results starting with lowest error score:

errors tau_0 mu gamma
14.0000 0.0010 0.1000 0.0001
16.0000 0.0100 0.5000 0.0100
17.0000 0.1000 0.5000 0.0001
18.0000 0.1000 0.2000 0.0001
19.0000 0.0100 0.1000 0.0001
19.0000 0.0100 0.5000 0.0001
19.0000 0.1000 0.5000 0.0001
19.0000 0.1000 0.5000 0.0100
21.0000 0.0010 0.1000 0.0100

Using NR optimizer.

Listing results starting with lowest error score:

errors tau_0 mu gamma 27.0000 0.0010 0.1000 0.0001 27.0000 0.0010 0.1000 0.0010 27.0000 0.0010 0.2000 0.0010 27.0000 0.0010 0.2000 0.0010 27.0000 0.0010 0.2000 0.0010 27.0000 0.0010 0.2000 0.0100 27.0000 0.0010 0.5000 0.0010 27.0000 0.0010 0.5000 0.0010 27.0000 0.0010 0.5000 0.0010

Overall best parameters:

```
optimizer
             tau
                     mu gamma
GD
          0.0010 0.1000 0.0100
SGD
          0.0010 0.5000 0.0001
SGD_mini
          0.0010 0.2000 0.0001
SGD_mom
          0.0010 0.1000 0.0100
ADAM
          0.0100 0.1000 0.0100
DualCA
          0.0010 0.1000 0.0001
NR
          0.0010 0.1000 0.0001
   ## speed test
In [105]: import matplotlib.pyplot as plt
          %matplotlib inline
          data = np.empty(7, dtype=[ ('opt', 'U10'),
                                       ('tau', 'f4'),
                                       ('mu', 'f4'),
                                       ('gamma', 'f4'),
                                       ('compC', 'i8'),
                                       ('iterdata', '(8, 4)f4')]) #use for iterations-training
          #do iterations from 1 = 2^0 to 256=2^8 in steps of x2 as standard, ergo 9 steps. for
          # iterations from 1 to 17 in steps of +2
          for i, struct in enumerate(data):
                  struct['opt'] = params['opt'][i]
                  struct['tau'] = params['tau'][i]
                  struct['mu'] = params['mu'][i]
                  struct['gamma'] = params['gamma'][i]
                  if 0:#struct['opt'] in ['NR', 'GD']:
                      struct['iterdata'] = [[1.,0.,0.,0.],
                                             [5.,0.,0.,0.],
                                             [9.,0.,0.,0.],
                                             [13.,0.,0.,0.],
                                             [17.,0.,0.,0.],
                                             [21.,0.,0.,0.],
                                             [25.,0.,0.,0.],
                                             [29.,0.,0.,0.]]
                  else:
                      struct['iterdata'] = [[1.,0.,0.,0.],
```

```
[4.,0.,0.,0.]
                                   [8.,0.,0.,0.],
                                   [16.,0.,0.,0.],
                                   [32.,0.,0.,0.],
                                   [64.,0.,0.,0.],
                                   [128.,0.,0.,0.]]
#insert computational complexiies
D = 65
N = 357
B = 10
data['compC'] = D
data['compC'][data['opt'] == 'GD'] = N*D
data['compC'][data['opt'] == 'SGD_mini'] = B*D
data['compC'][data['opt'] == 'NR'] = N*D**2
X_tr, X_test, y_tr, y_test = train_test_split (X, y, test_size = 0.3 ,random_state =
for i, struct in enumerate(data):
        beta = np.zeros(65)
        tau_0 = struct['tau']
        mu = struct['mu']
        gamma = struct['gamma']
        for j, iterdata in enumerate(struct['iterdata']):
            iter_ = int(iterdata[0])
            errors = 0
            if struct['opt'] == 'SGD':
                beta = SGD(X_tr, y_tr, beta, tau_0, gamma, iter_)
            elif struct['opt'] == 'GD':
                beta = GD(X_tr, y_tr, beta, tau_0, gamma, iter_)
            elif struct['opt'] == 'SGD_mini':
                \#print('SGD\ minibatch\ running\ with\ B=',\ B)
                beta = SG_minibatch(X_tr, y_tr, beta, tau_0, gamma, iter_, B = 10)
            elif struct['opt'] == 'SGD_mom':
                beta = SG_momentum(X_tr, y_tr, beta, tau_0, gamma, mu, iter_)
            elif struct['opt'] == 'ADAM':
                \#ADAM(X, y, beta, m, tau=10**-4, mu1=0.9, mu2=0.999, eps=10**-8):
                beta = ADAM(X_tr, y_tr, beta, iter_)
            elif struct['opt'] == 'DualCA':
                beta = dual_coordinate_ascent(X_tr, y_tr, iter_)
            elif struct['opt'] == 'NR':
                beta = Newton_Raphson(X_tr, y_tr, beta, iter_)
            elif struct['opt'] == 'SAGD':
                \#beta = self.type(X_tr, y_tr, beta, tau_0, gamma, mu, iter_)
                raise NotImplementedError('tbd')
```

[2.,0.,0.,0.],

```
iterdata[1] = zero_one_loss(predict(beta, X_tr), y_tr)/len(y_tr)
   iterdata[2] = zero_one_loss(predict(beta, X_test), y_test)/len(y_test)
   iterdata[3] = iterdata[0]*struct['compC']

#print(struct['iterdata'][:,3])

#print(struct['iterdata'])

plt.figure()

plt.semilogx(struct['iterdata'][:,3],struct['iterdata'][:,1],label='training

plt.semilogx(struct['iterdata'][:,3],struct['iterdata'][:,2],label='test_'+si

plt.ylabel('error')

plt.xlabel('estimated T')

plt.legend()

#plt.plot(iterdata[3],iterdata[2],label='test')
```













