# learnFromWL

March 2, 2017

## 1 A point analysis of weak learning models

#### 1.1 1. Introduction.

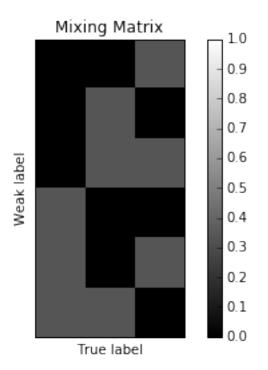
In this notebook we analyze the behavior of sample based estimates of a C-dimensional probability vector  $\eta$  from binary vector instances.

The main goal is to compare the behavior of a "supervised" estimate, based on a set of labels  $\{\mathbf{y}_k, k = 0, \dots, K-1\}$  generated from  $\boldsymbol{\eta}$ , and estimates based on weak labels,  $\{\mathbf{b}_k, k = 0, \dots, K-1\}$ , generated from some related distribution  $\mathbf{q} = \mathbf{M}\boldsymbol{\eta}$ , where  $\mathbf{M}$  is called a mixing matrix and contains conditional probabilities.

To do so, we will generate a dataset of labels drawn from  $\eta$ , and one or more datasets of weak labels drawn from  $\mathbf{q}$ .

First we define some configurable parameters:

```
plt.imshow(M, interpolation='nearest', cmap="gray", clim=(0.0, 1.0))
        plt.colorbar()
        plt.title('Mixing Matrix')
        plt.xlabel('True label')
        plt.ylabel('Weak label')
        plt.xticks([], [])
        plt.yticks([], [])
        plt.show()
Mixing matrix:
[[ 0.
               0.
                           0.33333333]
 [ 0.
               0.33333333 0.
 [ 0.
               0.33333333 0.333333333]
 [ 0.33333333 0.
                           0.
                                     ]
                           0.33333333]
 [ 0.33333333 0.
 [ 0.33333333  0.33333333  0.
                                     ]]
```



### 1.1.1 1.1. Dataset generation.

In the following we will generate a dataset of labels and their corresponding weak labels

```
In [3]: # Generate true labels
    I = np.eye(C)
    iy = np.random.choice(np.arange(0, C), size=K, p=eta)
    y = I[iy]

# Generate weak label indices
    iz = wlw.generateWeak(iy, M, C)
```

#### 1.1.2 1.2. Supervised, sample based estimation.

In the supervised setting,  $\mathbf{y}$  is observed an the optimal sample based estimate of  $\boldsymbol{\eta}$  (minimizing any Bregmann divergence) based on the observed labels is the sample average

### 1.1.3 1.3. Learning from weak labels.

There are many ways to estimate  $\eta$  from the weak labels. We consider here a representative sample of them:

**1.3.1.** Averaging virtual labels If z is a sample from distribution q, and V is any left inverse of the mixing matrix (so that VM = I then it can be shown that  $\mathbb{E}\{v\} = \eta$ . Therefore, we can estimate  $\eta$  as the average of virtual labels:

```
In [5]: # v = wlw.computeVirtual(iz, C, method='quasi_IPL')
        v = wlw.computeVirtual(iz, C, M=M, method='Mproper')
        print "Virtual labels are:"
        print v
        f_v = np.mean(v, axis=0)
        print "Virtual label estimate: {0}".format(f_v)
        e2 = np.sum((f_v - eta)**2)
        print "Square error: {0}".format(e2)
Virtual labels are:
[[0.9 - 0.6 0.9]
 [-0.3 \quad 1.2 \quad -0.3]
 [-0.6 \quad 0.9 \quad 0.9]
 [1.2 - 0.3 - 0.3]
 [ 0.9 0.9 -0.6]
 [0.9 \ 0.9 \ -0.6]]
Virtual label estimate: [ 0.52161  0.19116  0.28911]
Square error: 0.000663729799996
```

1.3.2. Maximum Likelihood Estimate The expected value of a virtual label vector can be shown to be equal to the minimizer of the expected log likelihood. This implies that, on average, the average of the virtual label vector and the ML estimate shuld be assymptotically equivalent. However, for a finite sample size, they can lead to different results.

The following function computes the ML estimate by means of the EM algorithm.

```
In [7]: def computeML(iz, M, f0=None, max_iter=1e10, echo='off'):
    """
    Compute the ML estimate of a probability vector based on weak labels in iz and the mixing m
    The estimation method is based on Expectation Maximization.
    """

# Initialize the estimate.
    if f0 is None:
```

```
f_ml = np.ones(C)/C
            else:
                f_ml = f0
            # Recursive estimation
            iterate = True
            count = 0
            while iterate:
                fi = np.dot(np.diag(f_ml), M.T)[:,iz.astype(int)]
                fi = fi / np.sum(fi, axis=0)
                f_new = np.mean(fi, axis=1)
                count += 1
                iterate = np.any(f_new != f_ml) and count < max_iter</pre>
                f_ml = np.copy(f_new)
            if echo=='on':
                if count>= max_iter:
                    print "Stopped before convergence after {0} iterations".format(max_iter)
                    print "Converged in {0} iterations".format(count)
            return f_ml
        def computeNLL(iz, M, f):
            Compute the Log-Likelihood function for an estimate f.
            I = np.eye(M.shape[0])
            z = I[iz.astype(int)]
            NLL = - np.dot(np.mean(z, axis=0), np.log(np.dot(M, f)))
            return NLL
  We can verify that the EM steps monotonically decrease the NLL
In [9]: n_{it} = 10000
        f = None
        NLL = []
        MSE = []
        K\Gamma = []
        MSE\_EM = []
        I = np.eye(M.shape[0])
        z = I[iz.astype(int)]
        q = np.mean(z, axis=0)
        f_lim = computeML(iz, M, f, max_iter=10000, echo='on')
        for i in range(n_it):
            f_new = computeML(iz, M, f, max_iter=1)
```

C = M.shape[1] # No. of classes

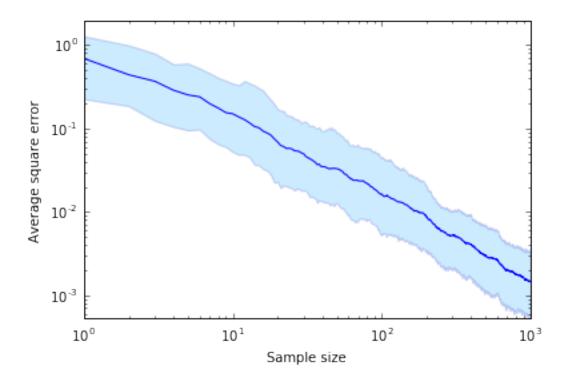
```
if f is not None and np.all(f_new == f):
                break
            else:
                f = np.copy(f_new)
            # NLL.append(computeNLL(iz, M, f) + np.dot(q, np.log(q)))
            NLL.append(computeNLL(iz, M, f) + np.dot(q, np.log(np.dot(M, f_lim))))
            MSE.append(np.sum((f - eta)**2))
            KL.append(- np.dot(eta, np.log(f)) + np.dot(eta, np.log(eta)))
            MSE_EM.append(np.sum((f - f_lim)**2))
        print "eta = {0}".format(eta)
        print "f_ml = \{0\}".format(f)
        print f_v = \{0\} format(f_v)
        its = range(len(NLL))
        plt.loglog(its, NLL, label= "Normalized NLL")
        plt.loglog(its, MSE, label= "MSE")
        plt.loglog(its, MSE_EM, label= "MSE_EM")
        plt.loglog(its, KL, label= "KL divergence")
        plt.legend(loc='best')
        plt.axis('tight')
        plt.xlabel('Iteration')
        plt.ylim((1e-14, plt.ylim()[1]))
        plt.show()
        print "The final estimate is {0}".format(f)
        print "The true label is {0}".format(eta)
Converged in 56 iterations
eta = [0.5 \ 0.2 \ 0.3]
f_ml = [0.52020299 \ 0.19300616 \ 0.28679085]
f_v = [0.52161 \ 0.19116 \ 0.28911]
           10-2
           10-3
           10<sup>-4</sup>
           10-5
           10-5
           10-7
           10<sup>-8</sup>
```

### 1.2 2. Statistical analysis of the MSE.

We will compute all estimates multiple times in order to compare the distribution of the MSE.

First, to make sure that the WLL estimate is working properly, we plot the convergence of the estimate with the number of iterations

```
In [11]: n_sim = 100
         mse = {'wll': []}
         K = 1000
         for n in range(n_sim):
             if (n+1)/1*1 == n+1:
                 print '\r Simulation {0} out of {1}'.format(str(n+1), n_sim),
             # Generate true labels
             iy = np.random.choice(np.arange(0, C), size=K, p=eta)
             # Generate weak label indices
             iz = wlw.generateWeak(iy, M, C)
             # Estimation with virtual labels
             v = wlw.computeVirtual(iz, C, method='Mproper', M=M)
             f_v = np.cumsum(v, axis=0) / np.arange(1, K+1)[:,np.newaxis]
             mse_n = np.sum((f_v - eta)**2, axis=1)
             mse['wll'].append(mse_n)
Simulation 100 out of 100
In [12]: mse_mean = np.mean(mse['wll'], axis=0)
         d = mse['wll'] - mse_mean
         mse_std_u = np.sqrt(np.sum(d**2*(d >=0), axis=0)/np.sum((d >=0), axis=0))
         mse_std_d = np.sqrt(np.sum(d**2*(d <=0), axis=0)/np.sum((d <=0), axis=0))
         plt.fill_between(range(K), mse_mean - mse_std_d, mse_mean + mse_std_u,
             alpha=0.2, edgecolor='#1B2ACC', facecolor='#089FFF',
             linewidth=1, linestyle='solid', antialiased=True)
         plt.loglog(range(K), mse_mean)
         plt.axis('tight')
         plt.xlabel('Sample size')
         plt.ylabel('Average square error')
         plt.show()
```



### 1.2.1 2.1. Supervision vs partial supervision

In the following we test, for a fixed sample size, the estimation of  $\eta$  as the average of virtual labels, in comparison with a complete supervision, as the average of the true labels.

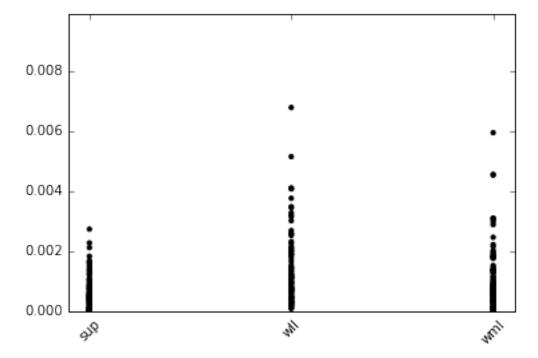
```
In [13]: n_sim = 100
         mse = {'sup': [], 'wll': [], 'wml': []}
         I_C = np.eye(C)
         for n in range(n_sim):
             if (n+1)/1*1 == n+1:
                 print '\r Simulation {0} out of {1}'.format(str(n+1), n_sim),
             # Generate true labels
             iy = np.random.choice(np.arange(0, C), size=K, p=eta)
             y = I_C[iy]
             # Generate weak label indices
             iz = wlw.generateWeak(iy, M, C)
             # Supervised estimation
             f = np.mean(y, axis=0)
             mse['sup'].append(np.sum((f - eta)**2))
             # Estimation with virtual labels
             # v = wlw.computeVirtual(iz, C, method='quasi_IPL')
             v = wlw.computeVirtual(iz, C, method='Mproper', M=M)
```

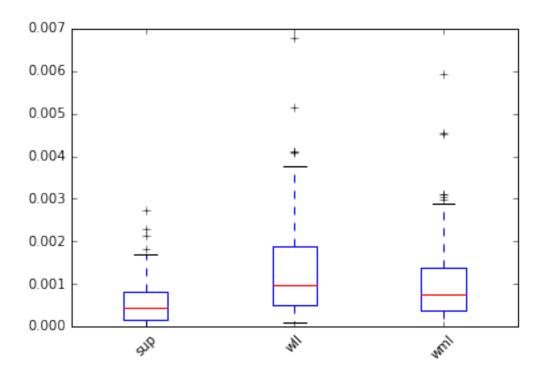
```
f_v = np.mean(v, axis=0)
mse['wll'].append(np.sum((f_v - eta)**2))

# Estimation with ML-EM
f_ml = computeML(iz, M, f0=None, max_iter=1000, echo='off')
mse['wml'].append(np.sum((f_ml - eta)**2))
```

Simulation 100 out of 100

The following error plots shows, that, under very weak supervision, there is a significant performance degradation caused by the use of weak labels.





### 1.3 3. Combination of datasets

In the following experiments we explore the combination of a fully labeled dataset with a weakly labeled dataset. We show that the beharior of the estimate based on virtual label depends on the choice of the virtual label vector.

The experiment demonstrates that, though different virtual label matrices can be asymptotically equivalent for the estimation of the probability vector, they show a different behavior under finite samples.

### 1.3.1 3.1. Weighting samples

In the following experiments we explore virtual matrices  $\mathbf{V}$  which are a combination of virtual matrices from the original datasets, i.e. they have the form  $\mathbf{V} = (w\mathbf{V}_0, (1-w)\mathbf{V}_1)$  where  $\mathbf{V}_0$  and  $\mathbf{V}_1$  are virtual matrices for the original datasets. We show that the empirical mse depends on w, and there is an optimal choice for w.

Note that the experiment does not explore all possible virtual matrices (i.e. all left inverses of the mixing matrix), but only those that are a composition of two virtual matrices.

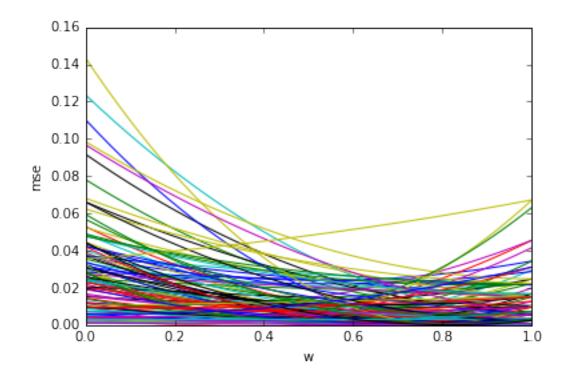
```
In [15]: n_sim = 100
    K = 50

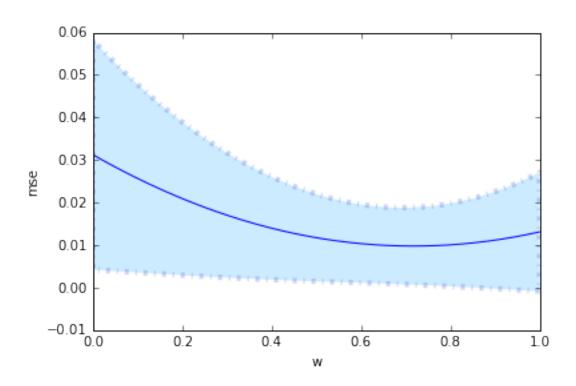
mse = []
    for n in range(n_sim):

    if (n+1)/1*1 == n+1:
        print str(n+1),

# Generate fully labeled dataset
    iy = np.random.choice(np.arange(0, C), size=K, p=eta)
```

```
y = I_C[iy]
             # Generate weakly labeled dataset
             iy = np.random.choice(np.arange(0, C), size=K, p=eta)
             iz = wlw.generateWeak(iy, M, C)
             # Supervised estimation
             f = np.mean(y, axis=0)
             # Estimation with virtual labels
             # v = wlw.computeVirtual(iz, C, method='quasi_IPL')
             v = wlw.computeVirtual(iz, C, method='Mproper', M=M)
             f_v = np.mean(v, axis=0)
             # Combination of virtual labels.
             # Al values of w provide consistent virtual matrices. However, the msw for a finite sample
             w = np.arange(0, 1, 0.001)[:, np.newaxis]
             f_{est} = f * w + f_v * (1 - w)
             mse_n = np.sum((f_est - eta)**2, axis=1)
             mse.append(mse_n)
         plt.plot(w.flatten(), np.array(mse).T)
         plt.xlabel('w')
         plt.ylabel('mse')
         plt.show()
         mse_mean = np.mean(np.array(mse), axis=0)
         mse_std = np.std(np.array(mse), axis=0)
         plt.plot(w.flatten(), mse_mean)
         plt.fill_between(w.flatten(), mse_mean - mse_std, mse_mean + mse_std,
             alpha=0.2, edgecolor='#1B2ACC', facecolor='#089FFF',
             linewidth=4, linestyle='dashdot', antialiased=True)
         plt.xlabel('w')
         plt.ylabel('mse')
         plt.show()
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 3
```



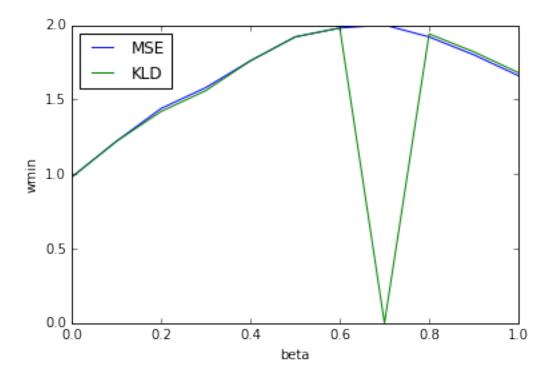


#### 1.3.2 3.2. Optimal weight versus noise level

The following experiment shows that the relation between the noise level and the optimal weight might be non-trivial.

```
In [16]: C = 3
                          # Number of classes
         Ktrue = 4000
                            # Number of clean labels
        Kweak = 4000
                            # Number of weak labels
         qTrue = float(Ktrue)/(Ktrue + Kweak)
         qWeak = float(Kweak)/(Ktrue + Kweak)
         eta = np.array([0.5, 0.2, 0.3]) # True probability vector
         beta_set = np.linspace(0, 1, 11)
         n_sim = 100
                          # Number of experiments for each value of eta.
         wmse = []
         wkld = []
         w = np.linspace(0, 1, 101)[:, np.newaxis]/ qTrue
         for beta in beta_set:
             print "\rBeta = {0}".format(beta),
             # Mixing matrix
             M = wlw.computeM(C, beta=beta, method='noisy')
             # Compute virtual matrix (this is to compute virtual labels in a more efficient way
             # than the current implementation of ComputeVirtual in WLweakener)
             V = np.linalg.pinv(M)
             np.random.seed(0)
             mse = []
             kld = []
             for n in range(n_sim):
                 # Generate fully labeled dataset
                 iy = np.random.choice(np.arange(0, C), size=Ktrue, p=eta)
                 y = I_C[iy]
                 # Generate weakly labeled dataset
                 iy2 = np.random.choice(np.arange(0, C), size=Kweak, p=eta)
                 iz2 = wlw.generateWeak(iy2, M, C)
                 # Supervised estimation
                 f = np.mean(y, axis=0)
                 # Estimation with virtual labels
                 # v = wlw.computeVirtual(iz, C, method='Mproper', M=M)
                 v = V.T[iz2.astype(int)]
                 f_v = np.mean(v, axis=0)
                 if np.any(f_v \le 0):
                     print f_v
                 # Weighted average
                 f_{est} = f * w * qTrue + f_v * (1 - w * qTrue)
```

```
\# f_{-est} = f * w + f_{-}v * (1 - w)
                                                     mse_n = np.sum((f_est - eta)**2, axis=1)
                                                     mse.append(mse_n)
                                                     kld_n = - np.dot(eta, np.log(f_est.T))
                                                     kld.append(kld_n)
                                         mse_mean = np.mean(np.array(mse), axis=0)
                                         imin = np.argmin(mse_mean)
                                         wmse.append(w[imin])
                                         kld_mean = np.mean(np.array(kld), axis=0)
                                         imin = np.argmin(kld_mean)
                                         wkld.append(w[imin])
Beta = 0.7 [ 0.77 -0.035 0.265]
[ 0.715  0.3  -0.015]
/Users/jcid/anaconda/lib/python 2.7/site-packages/ipykernel/\_main\_.py:55: RuntimeWarning: invalid value with the contraction of the contraction 
[ 0.435 -0.14 0.705]
[ 0.67 -0.08 0.41]
[ 0.73 -0.14 0.41]
[ 0.475 -0.02 0.545]
Γ0.6
                     -0.055 0.455]
[ 0.73  0.31 -0.04]
[ 0.59 -0.01 0.42]
[ 0.525 -0.005 0.48 ]
[ 0.69 -0.01 0.32]
[ 0.515 -0.04 0.525]
Beta = 1.0
In [17]: plt.plot(beta_set, np.array(wmse).flatten(), label="MSE")
                            plt.plot(beta_set, np.array(wkld).flatten(), label="KLD")
                            plt.xlabel('beta')
                            plt.ylabel('wmin')
                            plt.legend(loc='best')
                            plt.show()
```



The last experiment shows several important issues:

- The optimal weights could be independent on the choice of the proper loss
- The average of the virtual labels can be out of the probability simplex. In this respect, the optimal probability estimate should be computed with the constraint that the estimate lies inside the probability simplex. (Negative values are the cause of the anomalies in the KL divergence weighs).

### 1.3.3 3.3. A comparison between EM, virtual labels and the optimal weights

The following section shows that, despite ML-EM and weak losses may lead to different results, they can show very similar performance, though the results may depend on the selection of the configurable parameters (in particular, label proportions and mixing matrix).

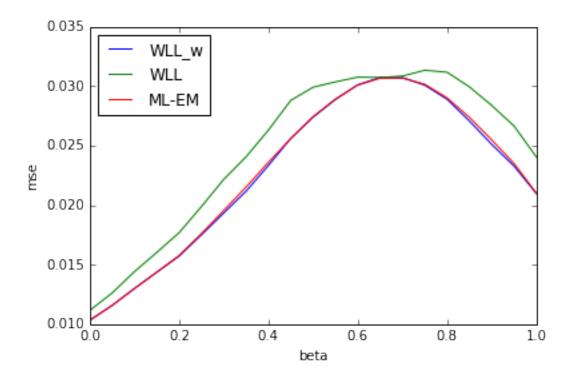
```
In [21]: C = 3
                          # Number of classes
         Ktrue = 20
                          # Number of clean labels
         Kweak = 40
                          # Number of weak labels
         qTrue = float(Ktrue)/(Ktrue + Kweak)
         qWeak = float(Kweak)/(Ktrue + Kweak)
         eta = np.array([0.5, 0.2, 0.3])
                                            # True probability vector
         beta_set = np.linspace(0, 1, 21)
                           # Number of experiments for each value of eta.
         n_sim = 1000
         wmse = []
         w = np.linspace(0, 1, 101)[:, np.newaxis]/ qTrue
         mse_w = []
         mse_v = []
         mse_ml = []
         wtest = []
```

```
wpseudo = []
for beta in beta_set:
   print "\rBeta = {0}".format(beta),
   # Mixing matrix
   # M = wlw.computeM(C, beta=beta, method='quasi_IPL')
   M = wlw.computeM(C, beta=beta, method='noisy')
   # Compute virtual matrix (this is to compute virtual labels in a more efficient way
    # than the current implementation of ComputeVirtual in WLweakener)
   V = np.linalg.pinv(M)
    # Compute combined mixing matrix
   M2 = np.vstack((qTrue*np.eye(C), qWeak*M))
   V2 = np.linalg.pinv(M2)
   np.random.seed(0)
   mse_wn = []
   mse_vn = []
   mse_mln = []
   for n in range(n_sim):
        # ###################
        # ## Dataset generation
        # Generate fully labeled dataset
        iy = np.random.choice(np.arange(0, C), size=Ktrue, p=eta)
        y = I_C[iy]
        # Generate weakly labeled dataset
        iy2 = np.random.choice(np.arange(0, C), size=Kweak, p=eta)
        iz = wlw.generateWeak(iy2, M, C)
        # Join datasets
        iz2 = np.hstack((iy, iz + C))
        # #########################
        # ## Weighted combination
        # Supervised estimation with dataset 0
        f = np.mean(y, axis=0)
        # Estimation with virtual labels and dataset 1
        # v = wlw.computeVirtual(iz, C, method='Mproper', M=M)
        v = V.T[iz.astype(int)]
        f_v = np.mean(v, axis=0)
        # Weighted average
        f_{est} = f*w*qTrue + f_v*(1-w*qTrue)
       mse_wn.append(np.sum((f_est - eta)**2, axis=1))
```

```
# ########################
                 # ## (pinv) M-proper loss
                 v2 = V2.T[iz2.astype(int)]
                 f_v2 = np.mean(v2, axis=0)
                 mse_vn.append(np.sum((f_v2 - eta)**2))
                 # #############
                 # ## ML estimate
                 f_ml = computeML(iz2, M2, f0=None, max_iter=1000, echo='off')
                 mse_mln.append(np.sum((f_ml - eta)**2))
             mse_mean = np.mean(np.array(mse_wn), axis=0)
             imin = np.argmin(mse_mean)
             wmse.append(w[imin])
             mse_w.append(np.min(mse_mean))
             mse_v.append(np.mean(np.array(mse_vn), axis=0))
             mse_ml.append(np.mean(np.array(mse_mln), axis=0))
             F11 = qWeak**2 * np.linalg.norm(np.dot(M, V), 'fro')**2
             F10 = qWeak**2 * np.linalg.norm(M, 'fro')**2
             F01 = qTrue**2 * np.linalg.norm(V, 'fro')**2
             F00 = qTrue**2*C
             w0= qTrue*C/(F00 + F10)
             wtest.append(qTrue*(F11 + F01) / (qTrue**2*(F11+F01) + qWeak**2*(F00+F10)))
             wpseudo.append((w0/qTrue-1))
Beta = 1.0
In [22]: beta_set = np.linspace(0, 1, 21)
         wtest = []
         wpseudo = []
         for beta in beta_set:
             # Mixing matrix
             # M = wlw.computeM(C, beta=beta, method='quasi_IPL')
             M = wlw.computeM(C, beta=beta, method='noisy')
             # Compute virtual matrix (this is to compute virtual labels in a more efficient way
             # than the current implementation of ComputeVirtual in WLweakener)
             V = np.linalg.pinv(M)
             # Compute combined mixing matrix
             M2 = np.vstack((qTrue*np.eye(C), qWeak*M))
             V2 = np.linalg.pinv(M2)
             F11 = qWeak**2 * np.linalg.norm(np.dot(M, V), 'fro')**2
             F10 = qWeak**2 * np.linalg.norm(M, 'fro')**2
             F01 = qTrue**2 * np.linalg.norm(V, 'fro')**2
             F00 = qTrue**2*C
             w0= qTrue*C/(F00 + F10)
             wtest.append(qTrue*(F11 + F01) / (qTrue**2*(F11+F01) + qWeak**2*(F00+F10)))
```

```
wpseudo.append(w0/qTrue-1)
```

```
In [23]: plt.plot(beta_set, np.array(mse_w).flatten(), label="WLL_w")
         plt.plot(beta_set, np.array(mse_v).flatten(), label="WLL")
         plt.plot(beta_set, np.array(mse_ml).flatten(), label="ML-EM")
         plt.xlabel('beta')
         plt.ylabel('mse')
         # plt.ylim((0, np.max(mse_w)+0.001))
         plt.legend(loc='best')
         plt.show()
         plt.plot(beta_set, np.array(wmse).flatten(), label="Empirical")
         plt.plot(beta_set, np.array(wtest).flatten(), label="Prediction")
         plt.plot(beta_set, np.array(wpseudo).flatten(), label="Pseudo-pred")
         plt.xlabel('beta')
         plt.ylabel('wmin')
         plt.legend(loc="best")
         plt.show()
         print np.array(wmse).flatten()
```



```
3.0
                Empirical
                Prediction
   2.5
                Pseudo-pred
   2.0
wwin
  1.5
   1.0
  0.5 L
0.0
                   0.2
                                 0.4
                                               0.6
                                                             0.8
                                                                           1.0
                                       beta
```