ex06_nico

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Ullrich Köthe: Fundamentals of Machine Learning, Winter Semester 2017/18 Notebook created by Nicolas Roth

1 Solutions for Exercise 6

2 1.) Bias and variance of ridge regression

Probably on blackboard so everyone can follow the calculations...

Ridge regression solves:

$$\hat{\beta}_{\tau} = \operatorname{argmin}_{\beta} ||X\beta - \tau||_F^2 + \tau ||\beta||_2^2 \tag{1}$$

$$= \operatorname{argmin}_{\beta} (X\beta - y)^T (X\beta - y) + \tau ||\beta||_2^2 \tag{2}$$

Prove, that:

$$\mathbb{E}[\hat{\beta}_{\tau}] = S_{\tau}^{-1} S \beta^* \tag{3}$$

$$Var[\hat{\beta}_{\tau}] = S_{\tau}^{-2} S \sigma^2 \tag{4}$$

with scatter matrices $S = X^T X$ and $S_{\tau} = X^T X + \tau \mathbb{H}$

Find the minimum by calculating $\partial_{\beta} \text{Loss} \stackrel{!}{=} 0$:

$$2X^T X \hat{\beta}_{\tau} - 2X^T y + 2\tau \hat{\beta}_{\tau} = 0 \tag{5}$$

$$(X^T X + \tau \mathbb{1})\hat{\beta}_{\tau} = X^T y \tag{6}$$

$$\hat{\beta}_{\tau} = S_{\tau}^{-1} X^T y \tag{7}$$

(8)

True model: $y = X\beta^* + \epsilon$

$$\hat{\beta}_{\tau} = S_{\tau}^{-1} X^{T} (X \beta^* + \epsilon) \tag{9}$$

$$\hat{\beta}_{\tau} = S_{\tau}^{-1} S \beta^* + S_{\tau}^{-1} X^T \epsilon \tag{10}$$

Now, take the expectancy value:

$$\mathbb{E}[\hat{\beta}] = \mathbb{E}[S_{\tau}^{-1}S\beta^*] + \mathbb{E}[S_{\tau}^{-1}X^T\epsilon] \tag{11}$$

$$= S_{\tau}^{-1} S \beta^* + S_{\tau}^{-1} X^T \mathbb{E}[\epsilon]$$
 (12)

$$=S_{\tau}^{-1}S\beta^* \quad \Box \tag{13}$$

Calculate Covariance:

$$Cov[\hat{\beta}_{\tau}] = Cov[\hat{\beta}_{\tau}, \hat{\beta}_{\tau}] = \mathbb{E}[(\hat{\beta}_{\tau} - \mathbb{E}[\hat{\beta}_{\tau}]) \cdot (\hat{\beta}_{\tau} - \mathbb{E}[\hat{\beta}_{\tau}])^{T}]$$
(14)

$$= \mathbb{E}\left[(\hat{\beta}_{\tau} - S_{\tau}^{-1} S \beta^*) \cdot (\hat{\beta}_{\tau} - S_{\tau}^{-1} S \beta^*)^T \right] \tag{15}$$

$$= \mathbb{E}\left[(S_{\tau}^{-1} X^{T} \epsilon) \cdot (S_{\tau}^{-1} X^{T} \epsilon)^{T} \right] \tag{16}$$

$$= \mathbb{E}\left[S_{\tau}^{-1} X^{T} \epsilon \epsilon^{T} X S_{\tau}^{-1T}\right] \tag{17}$$

$$= S_{\tau}^{-1} S S_{\tau}^{-1T} \mathbb{E}[\epsilon \epsilon^T] \tag{18}$$

$$=S_{\tau}^{-2}S\sigma^{2}\quad \Box \tag{19}$$

BUT: Why is $[S, S_{\tau}^{-1T}] = 0$?

$$[S, S_{\tau}] = [S, S] + \tau [S, \mathbb{1}] = 0 \tag{20}$$

$$[S, \mathbb{1}] = [S, S_{\tau}S_{\tau}^{-1}] = 0 \tag{21}$$

$$\Rightarrow [S, S_{\tau}^{-1}] = 0 \tag{22}$$

$$\Rightarrow [S, S_{\tau}^{-1}] = 0$$

$$\stackrel{sym}{\Rightarrow} [S, S_{\tau}^{-1T}] = 0$$

$$(22)$$

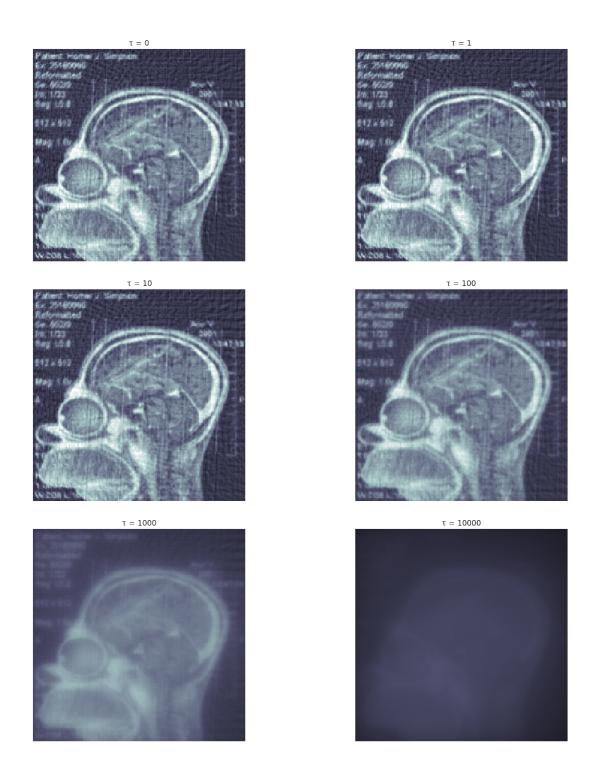
2.) Denoising of a CT image

Use solution from last week - with only one small tweak...

```
No = len(alphas)
# flattened output coordinates
j = np.mgrid[0:D].astype(np.int32)
# coordinate matrix for the output pixels
M2 = (M-1) / 2
qrid = np.mqrid[-M2:M-M2,-M2:M-M2].swapaxes(1,2).reshape(2,D)
# collect indices and corresponding values for all iterations
i indices = []
j_indices = []
weights = []
for k, alpha in enumerate(alphas):
    # convert angle and prepare projection vector
    alph_rad = np.radians(alpha)
    proj_vec = np.array([np.cos(alph_rad), -np.sin(alph_rad)])
    # project coordinates
    proj = np.dot(proj_vec, grid) + Np // 2
    # compute sensor indices and weights below the projected points
    i = np.floor(proj)
    w = (i+1) - proj
    # make sure rays falling outside the sensor are not counted
    clip = np.logical\_and(0 \le i, i \le Np-1)
    i_indices.append((i + k*Np)[clip])
    j_indices.append(j[clip])
    weights.append(w[clip])
    # compute sensor indices and weights above the projected points
    w = proj - i
    i_indices.append((i+1 + k*Np)[clip])
    j_indices.append(j[clip])
    weights.append(w[clip])
# construct matrix X
i = np.concatenate(i_indices).astype(np.int32)
j = np.concatenate(j_indices).astype(np.int32)
w = np.concatenate(weights)
X = coo_{matrix}((w, (i,j)), shape = (No*Np, D), dtype = np.float32)
# append diag(sqrt(tau)) for regularization
if tau > 0:
    reg = np.sqrt(tau) *eye(M*M)
    X = vstack([X, req])
return X
```

Reconstruct the tomogram for 64 angles and variations of τ

```
In [3]: M = 195
        Np = 275
        y = np.load('hs_tomography/y_195.npy')
        alphas = np.load('hs_tomography/alphas_195.npy')
        # reconstruct for 64 angles
        index = [int(np.ceil(len(alphas) * p/64)) for p in range(64)]
        alphas sub = alphas[index]
        y_sub = []
        for j in index:
            y_sub.extend(y[j*Np : (j+1)*Np])
        y_sub = np.asarray(y_sub)
        y_sub_tau = np.hstack((y_sub, np.zeros(M**2)))
        tau = [0, 1, 10, 100, 1000, 10000]
        fig, axes = plt.subplots(3, 2, figsize = (16, 16))
        for i in range(len(tau)):
            X = construct_X(M, alphas_sub, Np, tau=tau[i]).tocsc()
            beta = lsqr(X, y_sub if tau[i] == 0 else y_sub_tau, atol = 1e-5, btol =
            axes.flat[i].imshow(beta, vmin = 0, vmax = 255, interpolation = 'neares
            axes.flat[i].set_title('\tau = \{\}'.format(tau[i]))
            axes.flat[i].axis('off')
            print('\tau = {}, shape of X = {}, mean GV = {}'.format(tau[i], X.shape, r
        fig.tight_layout()
        plt.show()
\tau = 0, shape of X = (17600, 38025), mean GV = 119.92763181263976
\tau = 1, shape of X = (55625, 38025), mean GV = 119.91782488461713
\tau = 10, shape of X = (55625, 38025), mean GV = 119.82967990942062
\tau = 100, shape of X = (55625, 38025), mean GV = 118.95303321615249
\tau = 1000, shape of X = (55625, 38025), mean GV = 110.7951105526207
\tau = 10000, shape of X = (55625, 38025), mean GV = 65.61257007577262
```

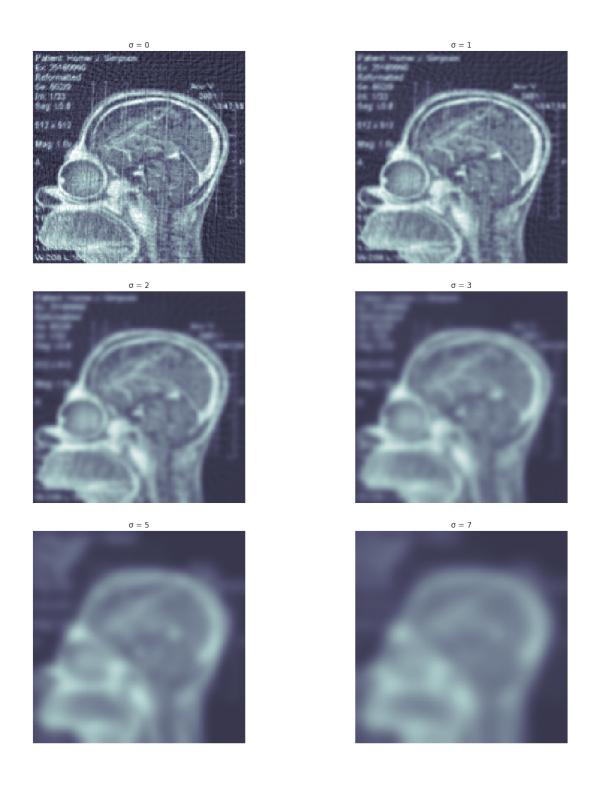


Compare this with gaussian filtering of different standard deviations:

$$g(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot e^{-\frac{x^2}{2\sigma^2}} \tag{24}$$

Apply 1d-filter in all dimensions (truncate filter after 4σ)

In [4]: from scipy.ndimage.filters import gaussian_filter X = construct_X(M, alphas_sub, Np, tau=0).tocsc() beta = lsqr(X, y_sub, atol = 1e-5, btol = 1e-5)[0].reshape(195,195) sigma = [0,1,2,3,5,7] fig, axes = plt.subplots(3, 2, figsize = (16,16)) for i in range(len(sigma)): beta_smooth = gaussian_filter(beta,sigma[i]) axes.flat[i].imshow(beta_smooth, vmin = 0, vmax = 255, interpolation = axes.flat[i].set_title('\sigma = {}'.format(sigma[i])) axes.flat[i].axis('off') #print(np.mean(beta_smooth)) fig.tight_layout() plt.show()



4 3.) Automatic feature selection for regression

4.1 3.1) Orthogonal Matching Pursuit

Implement OMP according to algorithm given in the lecture:

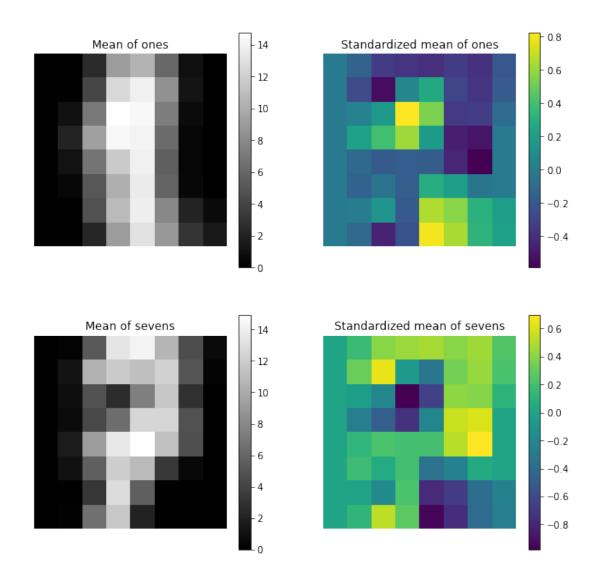
```
In [5]: from sklearn.datasets import load_digits
        from sklearn.model_selection import train_test_split
        from numpy.linalg import lstsq
        def omp_regression(X, y, T):
            H H H
            Orthogonal Matching Pursuit iterates T times to automatically find the
            1... T most relevant features in the training set X (standardized!) with
            It returns the optimal weight vector for every iteration with dimension
            # initialization
            dim = X.shape[1]
            beta_hat = np.zeros((dim,T))
            B = list(range(X.shape[1]))
            res = y
            # iteration
            for t in range(T): # do iteration
                cor = [np.abs(np.dot(X[:,j].T,res)) for j in B] # 1a.) correlations
                j_max = np.argmax(np.array(cor)) # 1b.) find maximum
                A.append(B.pop(j_max)) # 2.) move most important dim/feature to act
                X_active = X[:,A] # 3.) form the active matrix
                #print(A,len(B))
                beta = lstsq(X_active,y) # 4.) solve least squares problem n
                res = y - np.dot(X_active, beta[0]) # 5.) update the residual
                beta_hat[A,t] = beta[0]
                #print(y)
            return beta_hat
```

4.2 3.2) Classification with sparse LDA

Use results of OMP for linear discrimination - again with the digits 1&7 of the digits data set.

```
# Data filering
            mask = np.logical_or(target == num_1, target == num_2)
            data = data[mask] #/data.max()
            # data_std = (data -np.mean(data))/np.std(data) # standardize matrix B
            target = target[mask]
            # Relabel targets
            target[target == num_1] = 1
            target[target == num_2] = -1
            # Random Split
            x_training, x_test, y_training, y_test = train_test_split(data, target,
                                                                                rando
            train_std = np.std(x_training, axis=0)+1e-99
            train_mean = np.mean(x_training, axis=0)
            # standardize training data (for every dimension, respectively)
            x_training_std = (x_training - train_mean)/train_std
            # standardize test data in SAME WAY
            x_test_std = (x_test - train_mean)/train_std
            return x_training, x_training_std, x_test, x_test_std, y_training, y_te
        x_training, x_training_std, x_test, x_test_std, y_training, y_test = LDA_da
  Take a look at standardized data
In [7]: plt.figure(figsize=(10,10))
        plt.subplot(221)
        plt.imshow(np.array(np.mean(x_training[y_training==1],axis=0)).reshape((8,8)
        plt.title('Mean of ones')
```

```
in [7]: pit.rigure(rigsize=(10,10))
    plt.subplot(221)
    plt.imshow(np.array(np.mean(x_training[y_training==1],axis=0)).reshape((8,8)
    plt.title('Mean of ones')
    plt.axis('off'); plt.colorbar()
    plt.subplot(222)
    plt.title('Standardized mean of ones')
    plt.imshow(np.array(np.mean(x_training_std[y_training==1],axis=0)).reshape
    plt.axis('off'); plt.colorbar()
    plt.subplot(223)
    plt.title('Mean of sevens')
    plt.imshow(np.array(np.mean(x_training[y_training==-1],axis=0)).reshape((8,plt.axis('off'); plt.colorbar())
    plt.subplot(224)
    plt.title('Standardized mean of sevens')
    plt.imshow(np.array(np.mean(x_training_std[y_training==-1],axis=0)).reshape(plt.axis('off'); plt.colorbar())
    plt.show()
```



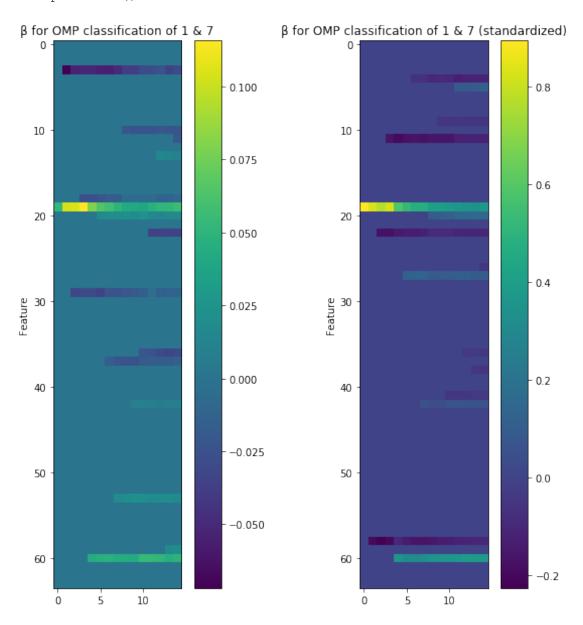
OMP regression for t = 1...15

```
In [8]: T = 15
    beta = omp_regression(x_training, y_training, T)
    beta_std = omp_regression(x_training_std, y_training, T)

plt.figure(figsize=(10,10))
    plt.subplot(121)
    plt.ylabel('Feature')
    plt.title('\beta for OMP classification of 1 & 7')
    plt.imshow(beta)
    plt.colorbar()

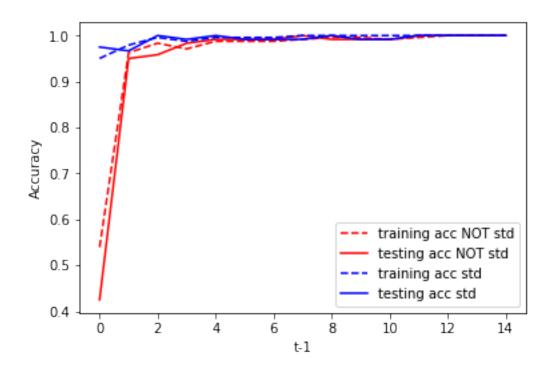
plt.subplot(122)
    plt.ylabel('Feature')
```

```
plt.imshow(beta_std) plt.title('\beta for OMP classification of 1 & 7 (standardized)') plt.colorbar() plt.show()
```



```
In [9]: def prediction_acc(testset, beta_vector, label):
    #print(testset.shape, beta_vector.shape)
    pred = np.dot(testset,beta_vector)
    pred[np.where(pred < 0)] = -1
    pred[np.where(pred > 0)] = 1
    return np.mean(pred == label)
```

```
accuracy = np.zeros((2,T))
       accuracy_std = np.zeros((2,T))
       for t in range(T):
           #print(str(t) +' Test acc: '+ str(prediction_acc(x_test,beta[:,t],y_test)
           accuracy[0,t] = prediction_acc(x_training,beta[:,t],y_training)
           accuracy[1,t] = prediction_acc(x_test,beta[:,t],y_test)
           accuracy_std[0,t] = prediction_acc(x_training_std,beta_std[:,t],y_train
           accuracy_std[1,t] = prediction_acc(x_test_std,beta_std[:,t],y_test)
       display(pd.DataFrame(
              data = accuracy,
              index = ['err_train', 'err_test'],
              columns = list(range(1, T+1))
              .rename_axis('not standard. | t =', axis = 'columns'))
       display(pd.DataFrame(
              data = accuracy_std,
              index = ['err_train', 'err_test'],
              columns = list(range(1,T+1))
              .rename_axis('standardized | t =', axis = 'columns'))
       plt.plot(accuracy[0,:],'r',linestyle='--', label='training acc NOT std')
       plt.plot(accuracy[1,:], 'r', label='testing acc NOT std')
       plt.plot(accuracy_std[0,:],'b',linestyle='--', label='training acc std')
       plt.plot(accuracy_std[1,:],'b', label='testing acc std')
       plt.ylabel('Accuracy')
       plt.xlabel('t-1')
       plt.legend()
       plt.show()
not standard. | t = 1
                       2
                            3
                                 4
                                      5
                                           6
                                               7
                                                   8
                                                             10
                  0.54 0.96 0.98 0.97 0.99 0.99 0.99 0.99 1.00 1.00 0.99
err_train
                  0.42 0.95 0.96 0.98 0.99 0.99 0.99 1.00 0.99 0.99
err_test
not standard. | t = 12
                        1.3
                             14
err_train
                  1.00 1.00 1.00 1.00
                  1.00 1.00 1.00 1.00
err_test
standardized | t = 1
                       2
                            3
                                     5
                                          6
                                                   8
                                                             10
                                 4
                                               7
                 err_train
                 err test
                            14
standardized | t = 12  13
                                 15
                 1.00 1.00 1.00 1.00
err_train
                 1.00 1.00 1.00 1.00
err_test
```

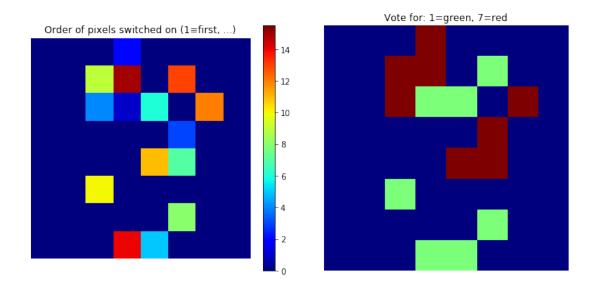


Standardization only makes a difference for small t, especially for t=1 (... which makes sense!)

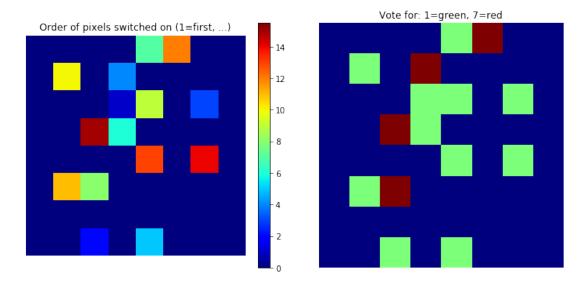
Order of the pixels switched to "active":

```
In [10]: def vis_pixel(beta, mean=np.ones(64)):
             Visualizes the order of pixels getting activated and for what number a
             'mean' only has to be given, if the data was standardized (otherwise :
             111
             old_idx = []
             im = np.zeros((8,8))
             im_v = np.zeros((8,8))
             for j in range(beta.shape[1]):
                 idx = np.where(beta[:,j]!=0)
                 for i in idx[0]:
                     if i not in old_idx:
                         new = i
                         iu = np.unravel_index(i, (8,8))
                         im[iu] = beta.shape[1]+1-j
                         old_idx.append(i)
                          if beta[i,j]*mean[i] > 0:
                              vote = 1
                              im_v[iu] = 1
                         else:
                              vote = 7
```

```
im_v[iu] = 2
        plt.figure()
        plt.subplot(121); plt.axis('off')
        plt.title('Add pixel {} = {}'.format(new,iu))
        plt.imshow(im, vmin=0, vmax=beta.shape[1]+1, cmap='jet')
        plt.subplot(122); plt.axis('off')
        plt.title('Votes for {}'.format(vote))
        plt.imshow(im_v, vmin=0, vmax=2, cmap='jet')
def vis_pixel_singleoutput(beta, mean=np.ones(64)):
    I = I = I
    Same as vis_pixel() but only one output image is generated
    (mostly for exporting to pdf)
    old_idx = []
    im = np.zeros((8,8))
    im_v = np.zeros((8,8))
    for j in range(beta.shape[1]):
        idx = np.where(beta[:, j]!=0)
        for i in idx[0]:
            if i not in old idx:
                new = i
                iu = np.unravel_index(i, (8,8))
                im[iu] = j+1
                old_idx.append(i)
                if beta[i,j] *mean[i] > 0:
                    vote = 1
                    im_v[iu] = 1
                else:
                    vote = 7
                    im_v[iu] = 2
    plt.figure(figsize=(12,12))
    plt.subplot(121); plt.axis('off')
    plt.title('Order of pixels switched on (1≡first, ...)')
    plt.imshow(im, vmin=0, vmax=beta.shape[1]+0.5, cmap='jet')
    plt.colorbar(fraction=0.05)
    plt.subplot(122); plt.axis('off')
    plt.title('Vote for: 1=green, 7=red')
    plt.imshow(im_v, vmin=0, vmax=2, cmap='jet')
vis_pixel_singleoutput(beta)
```



In [11]: vis_pixel_singleoutput(beta_std, np.array(np.mean(x_training_std[y_training_std))

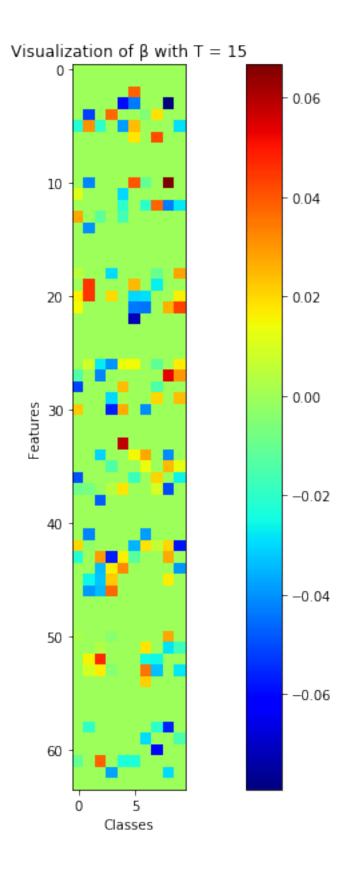


4.3 3.3) One-against-the-rest classification

Train C classifiers, trained on C auxillary training sets. Every classifier gives a score for the one class he is trained on. The test instance is assigned the class with the highest score.

In [12]: from sklearn.utils import shuffle # shuffle arrays in consistent way

```
def OAR_trainingdata(num, train_data, train_target):
             This function filters one digit from the trainingset (label = 1)
             and combines it with the same amount of other digits (label = -1)
             to the auxilary training set for "class = num"
             train_data, train_target = shuffle(train_data, train_target, random_st
             # Data filering for num
             data_num = train_data[train_target == num]
             target_num = train_target[train_target == num]
             # Data filering for other classes
             data_other = train_data[train_target != num]
             data_other = data_other[:data_num.shape[0],:] # slize for balanced tra
             target_other = train_target[train_target != num]
             target_other = target_other[:data_num.shape[0]]
             data_train = np.concatenate((data_num, data_other))
             target_train = np.concatenate((target_num, target_other))
             target train[target train != num] = -1
             target_train[target_train == num] = 1
             # Random shuffle
             x_training, y_training = shuffle(data_train, target_train, random_stat
             return x_training, y_training
In [13]: T OAR = 15 #also show for T OAR = 2, 10, 15
         C = target_names # = [0 1 2 3 4 5 6 7 8 9]
         X_training, X_test, Y_training, Y_test = train_test_split(data, target, te
         beta_classes = np.zeros((data.shape[1],len(C))) # (D x #classes) matrix
         # train every classifier with corresponding auxillary training set
         for k in C:
             x_temp, y_temp = OAR_trainingdata(k, X_training, Y_training)
             beta_OAR = omp_regression(x_temp, y_temp, T_OAR)
             beta_classes[:,k] = beta_OAR[:,T_OAR-1]
         plt.figure(figsize=(16,10))
         plt.imshow(beta classes, cmap='jet')
         plt.title('Visualization of \beta with T = '+str(T_OAR))
         plt.xlabel('Classes'); plt.ylabel('Features')
         plt.colorbar()
         plt.show()
```



If all scores for a test image are negative, assign it the class "unknown" ("unkn") to reduce the amount of false positives.

```
In [14]: C_u = np.hstack((C, 10))
         class_scores = np.zeros((X_test.shape[0],len(C_u)))
         for k in C:
             class_scores[:,k] = np.dot(X_test,beta_classes[:,k])
         y_predict_u = np.argmax(class_scores,axis=1)
         y_predict = np.argmax(class_scores[:,:len(C)],axis=1)
         acc = np.mean(y_predict == Y_test)
         acc_u = np.mean(y_predict_u == Y_test)
         confusion = np.zeros((len(C_u),len(C)))
         confusion_u = np.zeros((len(C_u),len(C)))
         for i in C_u:
             for j in C:
                 confusion_u[i,j] = np.sum((Y_test == j) * (y_predict_u == i)) / np.
                 confusion[i,j] = np.sum((Y_test == j) * (y_predict == i)) / np.sur
         print ('Accuracy of OAR classifier (T = {}) without introduction of "unknown
         display(
             pd.DataFrame(data = confusion[:len(C),:], index = C, columns = C)
             .rename_axis('w/o "unkn"', axis = 'columns')
             .style.apply(fade_zeros)
             .format('{0:.2f}%')
         )
         print('Accuracy of OAR classifier (T = {}) with introduction of "unknown":
         display(
             pd.DataFrame(data = confusion_u, index = np.hstack((C,np.nan)), column
             .rename_axis('w/ "unkn"', axis = 'columns')
             .style.apply(fade_zeros)
             .format('{0:.2f}%')
         )
Accuracy of OAR classifier (T = 15) without introduction of "unknown": 0.9276094276
<pandas.io.formats.style.Styler at 0x7f71819117b8>
Accuracy of OAR classifier (T = 15) with introduction of "unknown": 0.9276094276094
<pandas.io.formats.style.Styler at 0x7f716e61fdd8>
```

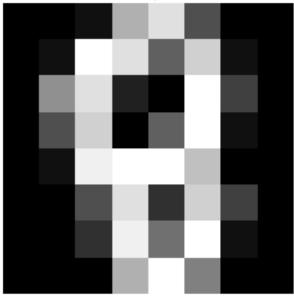
```
0.92% 0.00% 0.00% 0.00% 0.00% 0.00%
           2 0.00% 0.00%
           3 0.00% 0.00% 0.02% 0.91% 0.00% 0.00% 0.00% 0.00%
                                                            0.06% 0.02%
           4 0.00% 0.00% 0.00% 0.00% 0.94% 0.00% 0.00%
                                                      0.04%
           5 0.00% 0.00% 0.00% 0.00% 0.00% 0.92% 0.00% 0.00%
                                                            0.01%
                   0.02% 0.00% 0.00% 0.00%
                                          0.02% 1.00%
                                                            0.01%
           7 0.00% 0.00% 0.00% 0.00% 0.02% 0.00% 0.00% 0.91% 0.01% 0.02%
                   0.03% 0.03%
                               0.07% 0.02%
           9 0.00% 0.00% 0.00%
                               0.02% 0.02% 0.06% 0.00% 0.04% 0.00%
                                                                  0.92%
w/ "unkn"
                         2
                               3
                                     4
                                           5
                                                 6
                                                       7
                                                             8
                                                                   9
                     0.03% 0.00% 0.00% 0.00% 0.00% 0.00% 0.00% 0.00%
      0.0 1.00% 0.00%
         0.00% 0.95% 0.00% 0.00% 0.00% 0.00% 0.00% 0.02% 0.07% 0.00%
                     0.92% 0.00% 0.00% 0.00% 0.00% 0.00% 0.00% 0.00%
      3.0 0.00% 0.00% 0.02% 0.91% 0.00% 0.00% 0.00% 0.00%
                                                         0.06% 0.02%
      4.0 0.00% 0.00% 0.00% 0.00%
                                 0.94%
                                                   0.04%
      5.0 0.00% 0.00% 0.00% 0.00% 0.00%
                                       0.92%
                                                         0.01%
                                       0.02%
                                             1.00%
      7.0 0.00% 0.00% 0.00% 0.00% 0.02% 0.00%
                                                   0.91%
                                                         0.01%
                           0.05% 0.02%
               0.03%
                     0.03%
                                                         0.82%
                           0.02% 0.02% 0.06%
                                                   0.04%
                                                               0.92%
         0.00% 0.00% 0.00% 0.02% 0.00% 0.00% 0.00% 0.00%
                                                         0.01%
In [15]: unknowns = list(np.where(y_predict_u == C_u[-1])[0])
          for u in unknowns:
               plt.figure()
               plt.imshow(X_test[u,:].reshape(8,8), cmap='gray')
               plt.axis('off')
               plt.title('Test image {}, if not "unkn": prediction = {}, true label =
               plt.show()
```

0 1.00% 0.00% **0.03%** 0.00% 0.00% 0.00% 0.00% 0.00% 0.00%

1 0.00% **0.95%** 0.00% 0.00% 0.00% 0.00% **0.02% 0.07%** 0.00%

w/o "unkn"

Test image 156, if not "unkn": prediction = 6, true label = 8



Test image 509, if not "unkn": prediction = 8, true label = 3

