regularized_regression

December 10, 2017

```
In [1]: import numpy as np
        import pandas as pd
        from matplotlib import pyplot as plt
        from scipy import sparse as sp
        from scipy.sparse.linalg import lsqr
        from scipy.ndimage import gaussian_filter
        from scipy.optimize import minimize, least_squares
        import time
        from sklearn.model_selection import KFold
        from sklearn.datasets import load_digits
        %pylab inline
```

```
Populating the interactive namespace from numpy and matplotlib
```

1 Question 1: Ridge regression

$$\hat{\beta} = \text{argmin}_{\beta} \quad f(\beta; X, y, \tau) \tag{1}$$

where $f(\beta; X, y, \tau) = ||X\beta - y||_F^2 + \tau||\beta||_2^2$. The minimum can be taken by setting the derivative of f with respect to β to 0.

$$\begin{aligned} 0 = \partial_{\beta} f &= 2X^T X\beta - 2X^T y + 2\tau\beta & (2)\\ &\Rightarrow (X^T X + \tau\mathbb{1})\beta = X^T y & (3)\\ &\Rightarrow \hat{\beta} = S_{\tau}^{-1} X^T y & (4)\\ &\Rightarrow \hat{\beta} = S_{\tau}^{-1} X^T (X\beta^* + \epsilon) & (5)\\ &\Rightarrow \hat{\beta} = S_{\tau}^{-1} S\beta^* + S_{\tau}^{-1} X^T \epsilon & (6) \end{aligned}$$

Now we can calculate the expected value

$$\begin{aligned} \mathbb{E}[\hat{\beta}] &= \mathbb{E}[S_{\tau}^{-1} S\beta^*] + \mathbb{E}[S_{\tau}^{-1} X^T \epsilon] & (7)\\ &= S_{\tau}^{-1} S\beta^* \quad \text{since } \mathbb{E}[\epsilon] = 0 & (8) \end{aligned}$$

For the variance, we get

$$\begin{aligned}
\mathrm{Var}[\hat{\beta}] &= \mathrm{Var}[S_\tau^{-1}X^T(X\beta^* + \epsilon)] && (9)\\
&= (S_\tau^{-1}X^T)\mathrm{Var}[X\beta^* + \epsilon](S_\tau^{-1}X^T)^T && (10)\\
&= (S_\tau^{-1}X^T)(\mathrm{Var}[X\beta^*] + \mathrm{Var}[\epsilon] + 2\mathrm{Cov}[X\beta^*, \epsilon])(S_\tau^{-1}X^T)^T && (11)\\
&= (S_\tau^{-1}X^T)(0 + \sigma^2 + 0)(S_\tau^{-1}X^T)^T \quad \text{since } X\beta^* \text{ is certain and not correlated to } \epsilon && (12)\\
&= \sigma^2 S_\tau^{-1}X^T X S_\tau^{-1,T} && (13)\\
&= \sigma^2 S_\tau^{-1} S S_\tau^{-1,T} && (14)
\end{aligned}$$

S is symmetric, because $S^T = (X^TX)^T = X^TX = S$. S_τ^{-1} is symmetric as well, because $\tau\mathbb{1}$ is also symmetric. Therefore, we get

$$\begin{aligned}
\mathrm{Var}[\hat{\beta}] &= \sigma^2 S_\tau^{-1} S S_\tau^{-1} && (15)\\
&= \sigma^2 S_\tau^{-1} S_\tau^{-1} S && (16)\\
&= \sigma^2 S_\tau^{-2} S && (17)\\
& && (18)
\end{aligned}$$

2 Question 2: Denoising of a CT image

```
In [2]: ### mostly the same as in exercise 5
        def construct_X(M, alphas, Np=None, tau=0):
            # calculating Np if not given
            if Np == None:
                Np_estimate = int(np.floor(np.sqrt(2)*M))
                Np = Np_estimate if Np_estimate % 2 == 1 else Np_estimate + 1
                print('Use Np={:d}'.format(Np))

            # defining the dimensions
            D = M*M
            N = Np * len(alphas)
            # creating the normal vectors
            n = np.array([[np.cos(alpha*np.pi/180), -np.sin(alpha*np.pi/180)] for alpha in alpl
            # coordinates of detector rotation center
            # M - 1, because indexing starting from 0
            s0 = np.array([(M-1)/2, (M-1)/2])

            beta_flat_index = np.arange(D) # just an array with all indices of beta

            # C contains the vector from center of rotation to beta element
            C = np.empty((2, D)) # create C
            C[0,:] = -s0[0] + np.mod(beta_flat_index, M) # x-value: x(beta) = modulo
            C[1,:] = -s0[1] + np.floor_divide(beta_flat_index, M) #y-value: y(beta) = floor_di


            # np.tensordot gives the projected length of C vectors on
```

```
# Since they are measured from the rotation center, 0 corresponds to the rotation c
p = (Np-1)/2 - np.tensordot(n, C, axes=((1), (0)))
# TODO: what to do with values smaller than 0?

# calculate weights and indices
# detector_index_1 is the integral part of p, i.e. the first (most left) sensor th
# beta is contributing to detector_index_1 with weight_1 = 1 - weight_2, where wei
# therefore weight_2 is the fractional part of p
# the neighbouring element of detector_index_2 is the one right of it, so just + 1
weight_2, detector_index_1 = np.modf(p)
weight_1 = 1 - weight_2
detector_index_2 = detector_index_1 + 1

# now it can happen, that some are out of bounds. Here we just replace these value
# TODO: performance?
mask_detector_index_1 = np.logical_or(detector_index_1 < 0, detector_index_1 >= Np)
weight_1[mask_detector_index_1] = 0
detector_index_1[mask_detector_index_1] = 0 # just to avoid later errors
mask_detector_index_2 = np.logical_or(detector_index_2 < 0, detector_index_2 >= Np)
weight_2[mask_detector_index_2] = 0
detector_index_2[mask_detector_index_2] = 0 # just to avoid later index errors


# merge arrays
weights = np.array([])
weights = np.append(weights, [weight_1[angle_index] for angle_index in range(len(al
weights = np.append(weights, [weight_2[angle_index] for angle_index in range(len(al
# this is what is called i_indices
detector_indices = np.array([])
detector_indices = np.append(detector_indices, [Np*angle_index + detector_index_1[a
detector_indices = np.append(detector_indices, [Np*angle_index + detector_index_2[a

# create j indices
beta_indices = np.array([])
# we have to flip the beta_flat_index array, because otherwise the picture is upsi
beta_indices = np.append(beta_indices, [beta_flat_index[::-1] for _ in range(len(al
beta_indices = np.append(beta_indices, [beta_flat_index[::-1] for _ in range(len(al

if tau != 0:
    # append to sparse matrix sqrt(Tau)*1
    # ... create diagonal elements with value sqrt(tau)
    weights = np.append(weights, [np.sqrt(tau) for _ in range(D)])
    # ... first index: have to start from N, because sqrt(Tau)*1 is appended
    detector_indices = np.append(detector_indices, np.arange(N, N+D))
    # ... second index: just start from 0 to D
    beta_indices = np.append(beta_indices, np.arange(D))
    # modify N to not modify sp.coo_matrix call
    N += D
```

```
        # i hope duplicate entries will sum
        X = sp.coo_matrix((weights, (detector_indices, beta_indices)), shape=(N, D), dtype
        return X
```

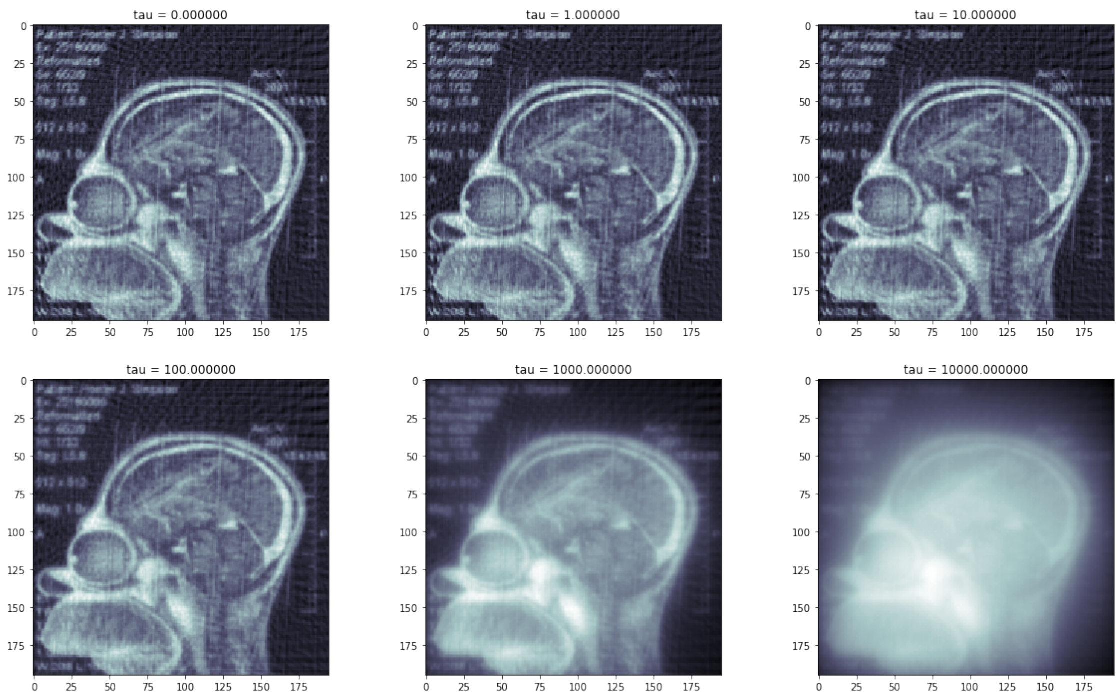
```
In [3]: def get_beta(M, Np, alphas, y, tau=0, error=1e-5):
            t0 = time.time()
            x = construct_X(M, alphas, Np, tau)
            t1 = time.time()
            print('Constructed X in {:f}s'.format(t1 - t0))
            print('Sparsity:', x.nnz/(x.get_shape()[0]*x.get_shape()[1]))
            t0 = time.time()
            if tau != 0:
                y = np.append(y, [0 for _ in range(M*M)])
            beta = lsqr(x, y, atol=error, btol=error)[0]
            t1 = time.time()
            print('Solved for beta in {:f}s'.format(t1 - t0))
            return beta
```

```
In [4]: alphas_195 = np.load('hs_tomography/alphas_195.npy')
        y_195 = np.load('hs_tomography/y_195.npy')
```

```
In [5]: sorted_alphas = np.argsort(alphas_195)

        fig, ax = plt.subplots(2, 3, figsize=(20, 12))

        for k, tau in enumerate([0, 1, 10, 100, 1000, 10000]):
            j = 3 # roughly 64 angles
            y_reduced = np.array([])
            y_reduced = np.append(y_reduced, [y_195[i*275:(i+1)*275] for i in range(0, len(alph
            beta = get_beta(195, 275, alphas_195[sorted_alphas][::j], y_reduced, tau=tau, erro
            ax[k//3, k %3].imshow(beta.reshape(195, 195), cmap='bone')
            ax[k//3, k %3].set_title('tau = {:f}'.format(tau), fontsize='12')
        plt.show()
```

```
Constructed X in 0.378474s
Sparsity: 0.007272727272727273
Solved for beta in 1.320373s
Constructed X in 0.470778s
Sparsity: 0.0022191655204034846
Solved for beta in 2.647175s
Constructed X in 0.458277s
Sparsity: 0.0022191655204034846
Solved for beta in 1.369626s
Constructed X in 0.450709s
Sparsity: 0.0022191655204034846
Solved for beta in 0.793385s
Constructed X in 0.450333s
Sparsity: 0.0022191655204034846
```

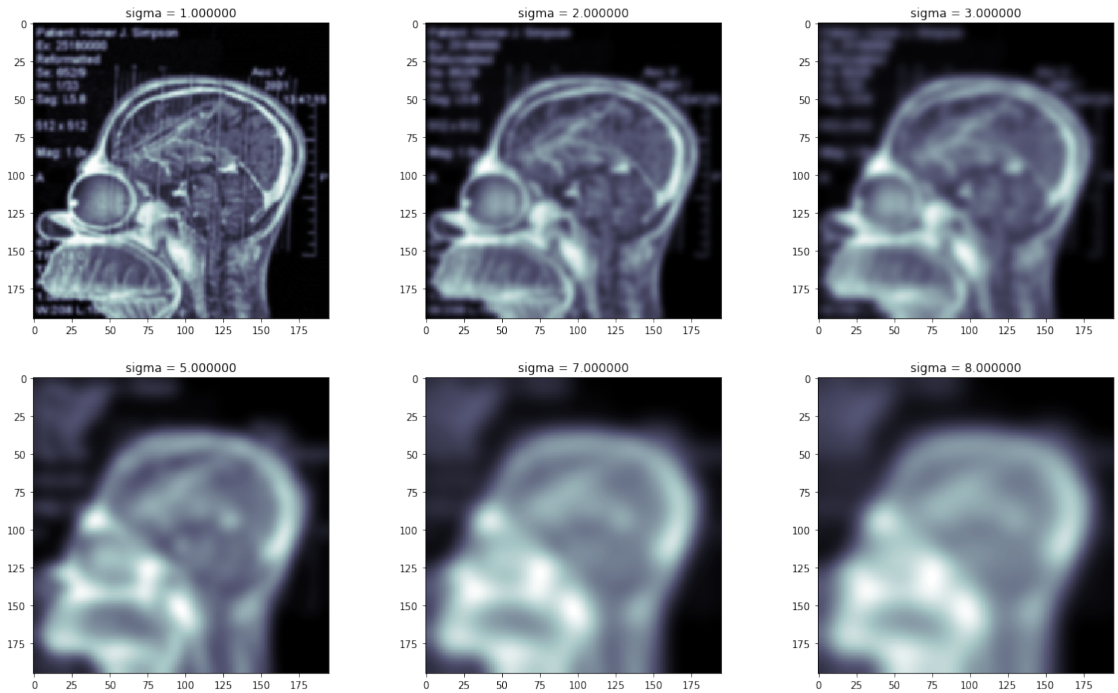
```
Solved for beta in 0.369708s
Constructed X in 0.425737s
Sparsity: 0.0022191655204034846
Solved for beta in 0.230858s
```



For me the pictures blur out and brightness is transported to already bright regions resulting in a shining of the image.

```
In [6]: beta = get_beta(195, 275, alphas_195, y_195, tau=0, error=1e-4)

        fig, ax = plt.subplots(2, 3, figsize=(20, 12))

        for k, sigma in enumerate([1, 2, 3, 5, 7, 8]):
            ax[k//3, k %3].imshow(gaussian_filter(beta.reshape(195, 195), sigma), cmap='bone')
            ax[k//3, k %3].set_title('sigma = {:f}'.format(sigma), fontsize='12')
        plt.show()
```

```
Constructed X in 0.946661s
Sparsity: 0.007272727272727273
Solved for beta in 4.636954s
```



This filter just blur out.

3 Question 3: Automatic feature selection for regression

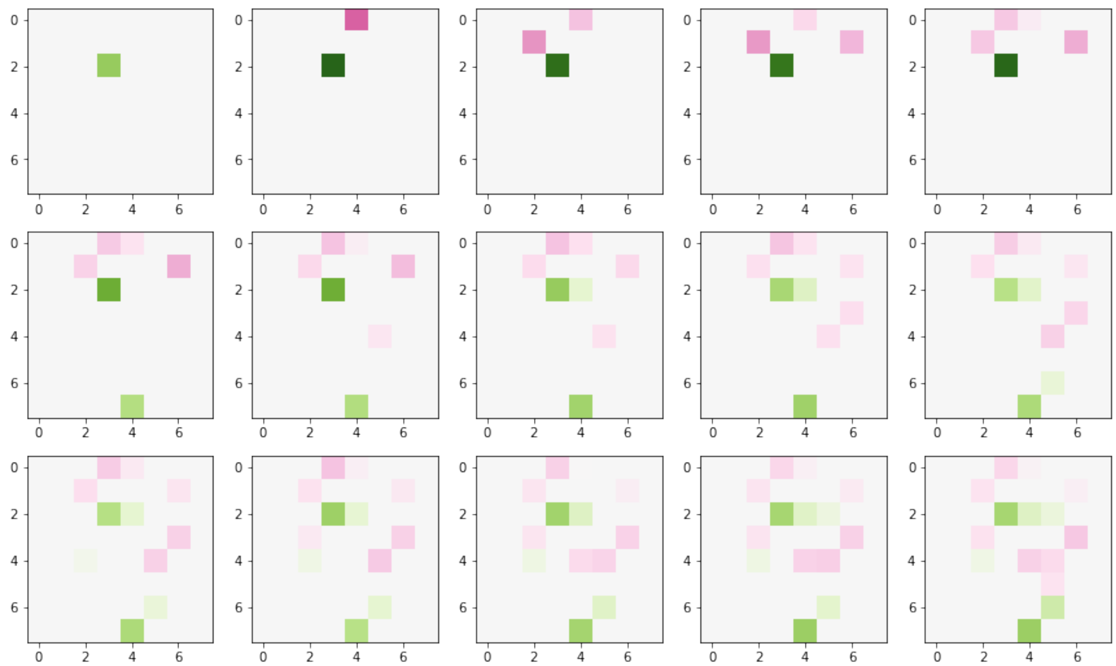
In [7]:
```
digits = load_digits()
data = digits["data"]
images = digits["images"]
target = digits["target"]
target_names = digits["target_names"]
# use only 1 and 7 for this exercise
mask_all = np.logical_or(target == 1, target == 7)
X_all = data[mask_all]
X_all /= np.max(data)
y_all = target[mask_all]
y_all[y_all == 7] = -1
```

In [8]:
```
def frob_squared(beta, args):
    # add a star before args if using least_squares. Scipy is inconsistent here.
    # args = (X_t, y)
    return np.sum((np.dot(args[0], beta) - args[1]) ** 2)
def omp_regression(X, y, T):
    N = X.shape[0]
    D = X.shape[1]

    A = set([])
```

```
    B = set(np.arange(D))
    r = y

    beta = np.empty((D, T))
    beta[:, -1] = np.zeros((D)) # for optimization only, will be overwritten

    X_t = np.zeros(X.shape, dtype=X.dtype)

    for t in range(T):
        # calculate correlation
        corr = np.abs(np.dot(X.transpose(), r))

        j_choices = np.argsort(corr) # ascending order...
        not_used = np.array([j not in A for j in j_choices])
        j_best = j_choices[not_used][-1] # ...therefore use the last one

        # add to A and remove from B
        A.add(j_best)
        B.remove(j_best)

        # update X_t
        X_t[:, j_best] = X[:, j_best]

        # optimization
        # least squares is stable, but super slow.
        # minimize throws some errors, but should be okay. If you have problems, uncom
        # or use least_squares
        # beta_hat = least_squares(frob_squared, beta[:,t - 1], args=[X_t, y], xtol = 
        beta_hat = minimize(frob_squared, beta[:,t - 1], args=[X_t, y])

        # check if somehow failed
        # if not beta_hat["success"]:
        #     raise ValueError('Minimizing failed. Original: {:s}'.format(beta_hat["mes
        # save beta
        beta[:,t] = beta_hat["x"]
        # update residue
        r = y - np.dot(X_t, beta_hat["x"])

    return beta
```

In [11]:
```
T = 15

beta_hat = omp_regression(X_all, y_all, T)

plot_cols = 5

plot_rows = int(np.ceil(T / plot_cols))
fig, ax = plt.subplots(plot_rows, plot_cols, figsize=(3*plot_cols, plot_rows*3))
```

```
for i in range(plot_cols*plot_rows):
    if i >= T:
        ax[i//plot_cols][i%plot_cols].axis('off')
    else:
        ax[i//plot_cols][i%plot_cols].imshow(beta_hat[:,i].reshape(8, 8), cmap='PiYG'
plt.show()
```



In the plot green indicates positive values and pink negative ones. A good distinction between both is to check if the value in β is larger or smaller than 0.

As you can see in the plot (t = 7), the most important pixels for digit 1 are (2,3), (7,4) and (2,4). The most important digits for digit 7 are (1,2), (0,4) and (1,6). In exercise 2 I chosed the pixels upon the difference of the average images for all 1s and 7s in the dataset. There I chosed for digit 1 (2,3), (2,4) and (7,4) and for digit 7 (1,2), (0,5) and (1,6). For digit 1 this matches exactly the results for β. For digit 7, they do not, but you can see in the plot, that they appear later und that the noise is much higher for digit 7.

3.1 One against the rest classification

```
In [12]: def create_aux_labels(target_names, target):
             y = {}
             for j in target_names:
                 aux_labels = np.ones(target.shape)
                 aux_labels[target != j] = -1
                 y[j] = aux_labels
             return y
```

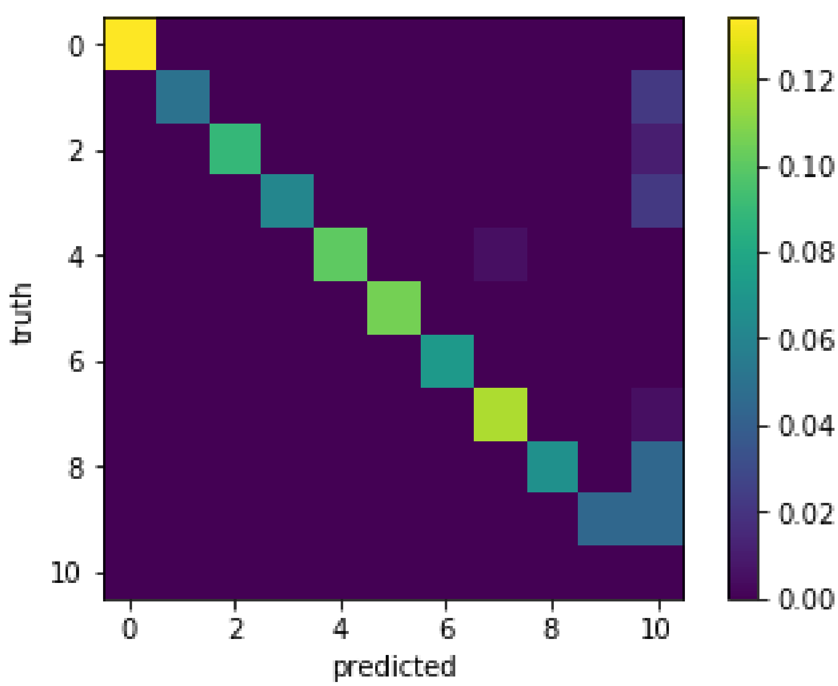
```
def progress(percent, prefix, length = 50):
    sharps = int(percent * length/100)
    print(prefix, '[{:s}{:s}] {:.1f}%'.format(sharps*'#', (length-sharps)*' ', percen
    if percent == 100:
        print('\n')

# create a kfold instance
kf = KFold(n_splits=10, shuffle=True)

X = data/np.max(data)
y = target
# from here on we assume, that the values of target are only the indices for target_n
aux_labels = create_aux_labels(target_names, y)
```

```
In [13]: def get_confusion_matrix(predicted, truth, possible_labels=[0, 1, 2, 3, 4, 5, 6, 7, 8
             conf = np.empty((len(possible_labels), len(possible_labels)))
             # first dimension is pred, second is truth
             for i, k in enumerate(possible_labels):
                 items, counts = np.unique(predicted[truth == k], return_counts=True)
                 count_array = np.zeros(len(possible_labels))
                 for fd in items:
                     count_array[fd] = counts[items == fd]
                 conf[i] = count_array
             return conf/len(predicted)
```

Disclaimer: the following will take forever.

```
In [14]: T = 20
         error_rates = []

         total_workload = len(target_names)*kf.n_splits
         counter = 0

         progress(counter*100/total_workload, '')

         for train, test in kf.split(X):

             pred = np.empty((len(target_names) + 1, len(test))) # +1 to get default
             pred[-1] = np.zeros(len(test))

             # run this without default category: just delete +1 and comment out pred[-1] = ..

             for k, aux_ts in aux_labels.items():

                 classifier = omp_regression(X[train], aux_ts[train], T)[:,-1]
                 pred[k] = np.dot(X[test], classifier)

                 counter += 1
```

```
                progress(counter*100/total_workload, '')

            pred = np.argmax(pred, axis=0) # chooses automatically the default if all others
            error_rates.append(np.count_nonzero(pred - y[test])/pred.shape[0])

            if counter == total_workload:
                conf = get_confusion_matrix(pred, y[test])
                fig, ax = plt.subplots(1, 1)
                cax = ax.imshow(conf)
                ax.set_xlabel('predicted')
                ax.set_ylabel('truth')
                plt.colorbar(cax)
                plt.show()

        mean_error = np.mean(error_rates)
        std_error = np.std(error_rates)

        print('Mean error rate on 10 folds: {:f} (std: {:f})'.format(mean_error, std_error))

[##################################################] 100.0%
```



```
Mean error rate on 10 folds: 0.190854 (std: 0.038546)
```

The problem of the classification is that a lot of instances are classified as unknown (default). The number of unknown samples decreases with T. The default category enables a much smaller false positive classification, because the algorithm does not have to decide where it is uncertain. However, I get much better performance without the default category.

```
In [ ]:
```