Regularised regression

Our original squared loss function in matrix/vector notation is:

$$L = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{t}-\mathbf{X}\mathbf{w})^T(\mathbf{t}-\mathbf{X}\mathbf{w})$$

Here's another loss function:

$$L = \lambda\mathbf{w}^T\mathbf{w} + \frac{1}{N}\sum_{n=1}^{N}(\mathbf{t}-\mathbf{X}\mathbf{w})^T(\mathbf{t}-\mathbf{X}\mathbf{w})$$

Recall that we're minimising this function and so (if $\lambda > 0$) this additional term will penalise large positive and negative values in $\mathbf{w}$. λ controls how much influence this new term has over the original squared error term.

Differentiating this with respect to $\mathbf{w}$ and then setting to zero (this is a good exercise to do) results in:

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\mathbf{w} = \mathbf{X}^T\mathbf{t}$$

where $\mathbf{I}$ is a square matrix with ones on the diagonal and zeros elsewhere (the identity matrix).

To demonstrate the effect of this additional term, we will generate some synthetic data by using a quadratic function and assing some random (normal / Gaussian) noise.

In [13]:

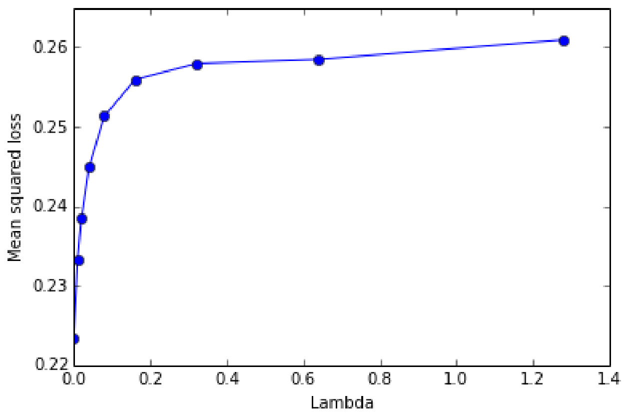
```
import urllib
urllib.urlretrieve('https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv', 'winequality-red.csv')
import numpy as np
with open('winequality-red.csv') as f:
    lines = (line for line in f)
    data = np.loadtxt(lines, delimiter=';', skiprows=1)
%matplotlib inline
import pylab as plt
from numpy.linalg import inv

#np.random.shuffle(data)
N = data.shape[0] #get tupple (numRows, numCols)

train = data[:int(N*0.7)]
test = data[int(N*0.7):]
X_train = train[:,:11]
X_train = np.c_[np.ones(train.shape[0]), X_train] # append 1s as first column
q_train = train[:,11]

X_test = test[:,:11]
X_test = np.c_[np.ones(test.shape[0]), X_test]
q_test = test[:,11]

lambs = [0,0.01,0.02,0.04,0.08,0.16,0.32,0.64, 1.28]
errors = []
for lamb in lambs:
    XtX = np.dot(X_train.T, X_train)
    XtXlam = XtX + X_train.shape[0]*lamb*np.identity(12)
    XtXlamI = inv(XtXlam)
    XtXIXt = np.dot(XtXlamI, X_train.T)
    w = np.dot(XtXIXt, q_train)

#     w = np.linalg.solve(np.dot(X_train.T,X_train) + lamb*np.identity(12),np.dot(X_train.T,q_train))
    f_test = np.dot(X_test,w)
    meanSquareError = ((q_test-f_test)**2).mean()/2.0
#     meanSquareError = (sum((q_test-f_test)**2) + lamb*np.dot(w.T,w))/float(2*X_test.shape[0])
    #print meanSquareError
    errors += [meanSquareError]
    print "lampda", lamb, "Mean Square Error =", meanSquareError
    #plt.figure()
    #plt.scatter(f_test,q_test, color='blue')
```

```
plt.legend()
plt.xlabel('Lambda')
plt.ylabel('Mean squared loss')
plt.plot(lambs, errors, '-o')
```

```
lampda 0 Mean Square Error = 0.223480575369
lampda 0.01 Mean Square Error = 0.233248626626
lampda 0.02 Mean Square Error = 0.238444290646
lampda 0.04 Mean Square Error = 0.244910826995
lampda 0.08 Mean Square Error = 0.251326923632
lampda 0.16 Mean Square Error = 0.255929947365
lampda 0.32 Mean Square Error = 0.257959899459
lampda 0.64 Mean Square Error = 0.258487108554
lampda 1.28 Mean Square Error = 0.260936238138
```

Out[13]:

```
[<matplotlib.lines.Line2D at 0x6726cb0>]
```



As λ increases, high values in $\mathbf{w}$ are more heavily penalised which leads to *simpler* functions. Why do lower values correspond to simpler functions?

Firstly, what does *simpler* mean?

I would argue that simpler functions have smaller derivatives (first, second, etc) as they typically change more slowly. In our polynomials, the derivatives are dependent on the values of $\mathbf{w}$. In particular our polynomial is:

$$t = \sum_{d=0}^{D} w_d x^d$$

and the first derivative is:

$$\frac{dt}{dx} = \sum_{d=1}^{D} d w_d x^{d-1}$$

and second is:

$$\frac{d^2 t}{dx^2} = \sum_{d=2}^{D} d(d-1) w_d x^{d-2}$$

which in both cases increases with increasing values of w_d. So penalising high (positive and negative) values decreases (in general) the gradients (and gradients of gradients, etc).

In [12]:

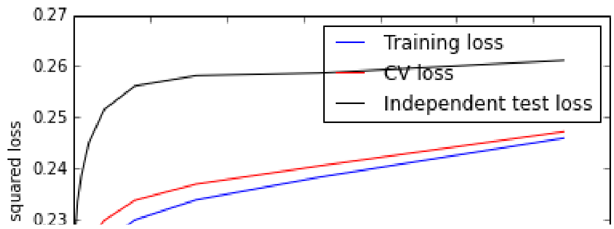
```
N = train.shape[0]
K = 10
sizes = np.tile(np.floor(N/10),(1,K))
sizes[-1] = sizes[-1] + N - sizes.sum()
c_sizes = np.hstack((0,np.cumsum(sizes)))
X = np.copy(train[:,:11])
X = np.c_[np.ones(train.shape[0]), X]
t = np.copy(train[:,11])
X_test = np.copy(test[:,:11])
X_test = np.c_[np.ones(test.shape[0]), X_test]
t_test = np.copy(test[:,11])
lambs = [0,0.01,0.02,0.04,0.08,0.16,0.32,0.64, 1.28]
```

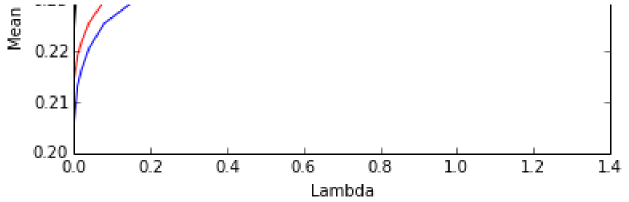
```
cv_loss = np.zeros((K, len(lambs)))
ind_loss = np.zeros((K, len(lambs)))
train_loss = np.zeros((K, len(lambs)))

k = 0
for lamb in lambs:
    for fold in range(K):
        X_fold = X[c_sizes[fold]:c_sizes[fold+1],:]
        X_train = np.delete(X,np.arange(c_sizes[fold],c_sizes[fold+1],1),0)

        t_fold = t[c_sizes[fold]:c_sizes[fold+1]]
        t_train = np.delete(t,np.arange(c_sizes[fold],c_sizes[fold+1],1),0)
        XtX = np.dot(X_train.T, X_train)
        XtXlam = XtX + X_train.shape[0]*lamb*np.identity(12)
        XtXlamI = inv(XtXlam)
        XtXIXt = np.dot(XtXlamI, X_train.T)
        w = np.dot(XtXIXt, t_train)

#         w = np.linalg.solve(np.dot(X_train.T,X_train) + lamb*np.identity(12),np.dot(X_train.T,t_train
))
        fold_pred = np.dot(X_fold,w)
        cv_loss[fold,k] = ((fold_pred - t_fold)**2).mean()/2.0
        ind_pred = np.dot(X_test,w)
        ind_loss[fold,k] = ((ind_pred - t_test)**2).mean()/2.0
        train_pred = np.dot(X_train,w)
        train_loss[fold,k] = ((train_pred - t_train)**2).mean()/2.0

#         cv_loss[fold,k] = (sum((fold_pred-t_fold)**2) + lamb*np.dot(w.T,w))/float(2*X_fold.shape[0])
#         ind_pred = np.dot(X_test,w)
#         ind_loss[fold,k] = (sum((ind_pred-t_test)**2) + lamb*np.dot(w.T,w))/float(2*X_test.shape[0])
#         train_pred = np.dot(X_train,w)
#         train_loss[fold,k] = (sum((train_pred-t_train)**2) + lamb*np.dot(w.T,w))/float(2*X_train.shap
e[0])
    k += 1

print "Mean cv_loss error", cv_loss.min()
print "Mean train_loss", train_loss.min()
print "Mean ind_loss", ind_loss.min()
plt.figure()
plt.plot(lambs,train_loss.mean(axis=0),'b-',label="Training loss")
plt.plot(lambs,cv_loss.mean(axis=0),'r-',label="CV loss")
plt.plot(lambs,ind_loss.mean(axis=0),'k',label="Independent test loss")
plt.legend()
plt.xlabel('Lambda')
plt.ylabel('Mean squared loss')

plt.figure()
plt.plot(lambs,train_loss.mean(axis=0),'b-',label="Training loss")
plt.legend()
plt.xlabel('Lambda')
plt.ylabel('Mean squared loss')
plt.figure()
plt.plot(lambs,cv_loss.mean(axis=0),'r-',label="CV loss")
plt.legend()
plt.xlabel('Lambda')
plt.ylabel('Mean squared loss')
plt.figure()
plt.plot(lambs,ind_loss.mean(axis=0),'k',label="Independent test loss")
plt.legend()
plt.xlabel('Lambda')
plt.ylabel('Mean squared loss')
```

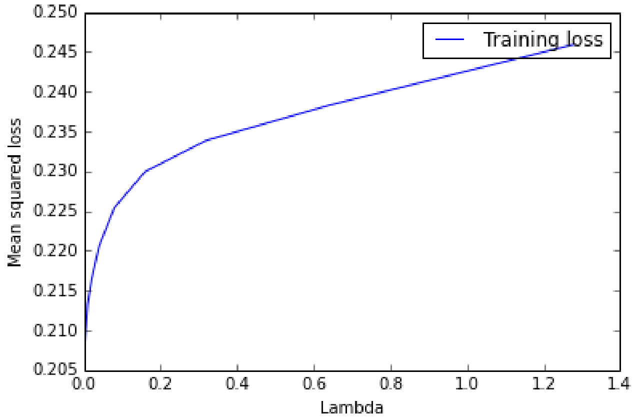
```
Mean cv_loss error 0.187886244788
Mean train_loss 0.202688764111
Mean ind_loss 0.220361053166
```

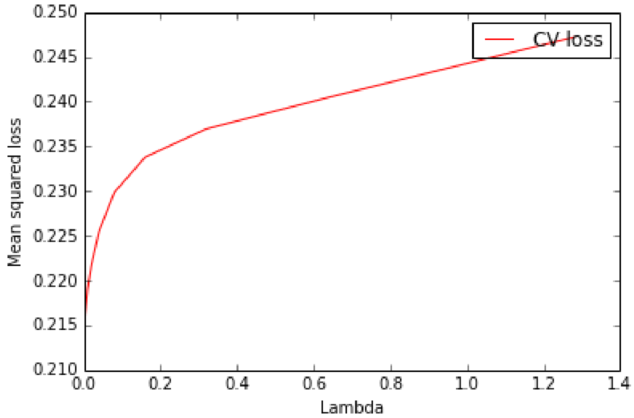
Out[12]:

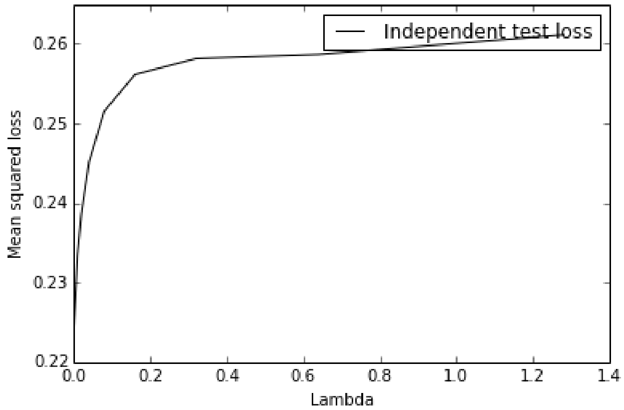
```
<matplotlib.text.Text at 0x6607b30>
```




Mean
0.22
0.21
0.20
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
Lambda


Training loss
Mean squared loss
0.250
0.245
0.240
0.235
0.230
0.225
0.220
0.215
0.210
0.205
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
Lambda


CV loss
Mean squared loss
0.250
0.245
0.240
0.235
0.230
0.225
0.220
0.215
0.210
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
Lambda


Independent test loss
Mean squared loss
0.26
0.25
0.24
0.23
0.22
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
Lambda

In [ ]:

In [ ]: