Project 3: Kernel SVM

"Just as we have two eyes and two feet,
duality is part of life."
--Carlos Santana

Files you'll edit:

`partners.txt`	If you work in a group, this file should contain the two wustlkeys of you and your group partner. These should be in two separate lines. There should be nothing else in this file. Please make sure that your partner also puts your wustlkey in his/her `partners.txt` file, as **project partnerships must be reciprocal**. If you don't have a partner then just leave the file blank.
`l2distance.m`	Computes the Euclidean distances between two sets of vectors. You can copy this function from previous assignments.
`computeK.m`	Computes a kernel matrix given input vectors.
`generateQP.m`	Generates all the right matrices and vectors to call the `qp` command in Octave.
`recoverBias.m`	Solves for the hyperplane bias *b* after the SVM dual has been solved.
`trainsvm.m`	Trains a kernel SVM on a data set and outputs a classifier.
`crossvalidate.m`	A function that uses cross validation to find the best kernel parameter and regularization constant.

`autosvm.m`	Take a look at this function. It takes as input a data set and its labels, cross validates over the hyper-parameters of your SVM and outputs a well-tuned classifier. You should "tune" this for the quality part of the project.

Files you might want to look at:

`visdecision.m`	This function visualizes the decision boundary of an SVM in 2d.
`extractpars.m`	This function extracts parameters. It is a helper function for visdecision.

Introduction

In this project, you will implement a kernel SVM solver. Remember that the SVM optimization has the following dual formulation:

$$\begin{aligned} \min_{\alpha_1,\cdots,\alpha_n} \ & \frac{1}{2}\sum_{i,j}\alpha_i\alpha_j y_i y_j \mathbf{K}_{ij} - \sum_{i=1}^{n}\alpha_i \\ \text{s.t.} \quad & 0 \le \alpha_i \le C \\ & \sum_{i=1}^{n}\alpha_i y_i = 0. \end{aligned}$$

This is equivalent to solving for the SVM primal

$$L(\mathbf{w}, b) = C\sum_{i=1}^{n}\max(1 - y_i(\mathbf{w}^\top\phi(\mathbf{x}_i) + b), 0) + ||w||_2^2$$

where $\mathbf{w} = \sum_{i=1}^{n} y_i\alpha_i\phi(\mathbf{x}_i)$ and $\mathbf{K}_{ij} = k(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^\top\phi(\mathbf{x}_j)$, for some mapping $\phi(\cdot)$. Please note that here all $\alpha_i \ge 0$. This is possible because we multiply by y_i in the definition of $\mathbf{w}$. One advantage of keeping all α_i non-negative is that we can easily identify non-support vectors as vectors with $\alpha_i = 0$.

Spiral data set

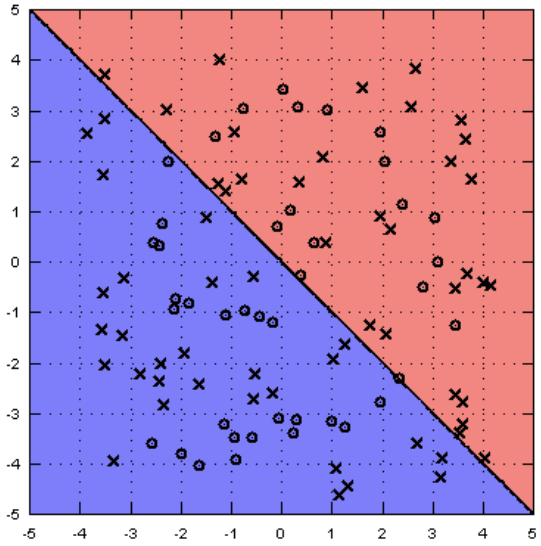
We provide you with a "spiral" data set. You can load it and visualize it with the following commands:

```
>> load spiral
>> whos
Variables in the current scope:

   Attr Name        Size                     Bytes  Class
   ==== ====        ====                     =====  =====
        xTe         2x242                     3872  double
        xTr         2x100                     1600  double
        yTe         1x242                     1936  double
        yTr         1x100                      800  double

Total is 1227 elements using 9808 bytes

>> dummy=@(X) sign(mean(X,1));
>> visdecision(xTr,yTr,dummy);
```



The function `visdecision` visualizes the data set and the decision boundary of a classifier. In this case the `dummy` classifier is not particularly powerful and only serves as a placeholder.

Implementing a kernelized SVM

1. First implement the kernel function

   ```
   computeK(ktype,X,Z,kpar)
   ```

   It takes as input a kernel type (ktype) and two data sets $\mathbf{X}$ in $\mathcal{R}^{d\times n}$ and $\mathbf{Z}$ in $\mathcal{R}^{d\times m}$ and outputs a kernel matrix $\mathbf{K} \in \mathcal{R}^{n\times m}$. The last input, `kpar` specifies the kernel parameter (e.g. the inverse kernel width γ in the RBF case or the degree p in the polynomial case.)
   1. For the linear kernel (`ktype='linear'`) svm, we use $k(\mathbf{x},\mathbf{z}) = x^T z$
   2. For the radial basis function kernel (`ktype='rbf'`) svm we use $k(\mathbf{x},\mathbf{z}) = \exp(-\gamma||x-z||^2)$ (gamma is a hyperparameter, passed a the value of kpar)
   3. For the polynomial kernel (`ktype='poly'`) we use $k(\mathbf{x},\mathbf{z}) = (x^T z + 1)^p$ (p is the degree of the polymial, passed as the value of kpar)

   You can use the function **`l2distance.m`** as a helperfunction.

2. Read through the specifications of the Matlab internal quadratic programming solver, quadprog.

   ```
   >> help quadprog
   [...]
    -- Function File:
    [X, OBJ, INFO, LAMBDA] = quadprog (H, q, A, b,Aeq,beq,lb,
   [...]
   ```

   Here, `x0` is any initial guess for your vector α. The quadprog solver is not very fast (in fact it is pretty slow) but for our purposes it will do. Write the function

   ```
   [H,q,Aeq,beq,lb,ub]=generateQP(K,yTr,C)
   ```

which takes as input a kernel matrix **K**, a label vector **yTr** and a regularization constant C and outputs the matrices `[H,q,Aeq,beq,lb,ub]` so that they can be used directly with the `quadprog` solver to find a solution to the SVM dual problem. (Be careful, the `b` here has nothing to do with the SVM hyper-plane bias b.)

Note: You can set additional parameters A,b in quadprog to Aeq.*0 and beq.*0 respectively.

You must turn off output from quadprog before submitting your code to the autograder. You can do this by creating an optimoptions object with the following line:

```
optimoptions(@quadprog,'Display','off');
```

You will then need to pass this as the options argument to quadprog. It may be helpful to see the qualprog output while developing and debugging your code, so we recummend only turning off this display when submitting your code to the autograder. But you must not forget to turn off the display, or your code will fail the autograder.

If Quadprog produces any warnings, we recommend fixing these. However, if you chose not to fix them, you must supress these messages before submitting your code by placing the following line before your call to quadprog:

```
warning('off','all');
```

3. Implement the function

```
[svmclassify,sv_i,alphas]=trainsvm(xTr,yTr,
```

It should use your functions **computeK.m** and **generateQP** to solve the SVM dual problem of an SVM specified by a training data set (**xTr,yTr**), a regularization parameter (C), a kernel type (`ktype`) and kernel parameter (`kpar`). For now ignore the first output `svmclassify` (you can keep the pre-defined solution that generates random labels) but make sure that `sv_i` corresponds to all the support vectors (up to numerical accuracy) and `alphas` returns an n-dimensional vector of alphas.

4. Now that you can solve the dual correctly, you should have the values for α_i. But you are not done yet. You still need to be able to classify new test points. Remember from class that $h(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b$. We need to obtain b. It is easy to show (and omitted here) that if $C > \alpha_i > 0$ (with strict $>$), then we must have that $y_i(\mathbf{w}^\top \phi(\mathbf{x}_i) + b) = 1$. Rephrase this equality in terms of α_i and solve for b. Implement

```
bias=recoverBias(K,yTr,alphas,C);
```

where `bias` is the hyperplane bias b (Hint: This is most stable if you pick an α_i that is furthest from C and 0.)

5. With the `recoverBias` function in place, you can now finish your function `trainsvm.m` and implement the remaining output, which returns an actual classifier `svmclassify`. This function should take a set of inputs of dimensions $d \times m$ as input and output predictions ($1 \times m$). You can evaluate it and see if you can match my testing and training error exactly:

```
>> load spiral
>> svmclassify=trainsvm(xTr,yTr,6,'rbf',0.25);
Generate Kernel
```

```
Generate Kernel ...
Generate QP ...
Solve QP ...
Recovering bias ...
Extracting support vectors ...
>> testerr=sum(sign(svmclassify(xTe))~=yTe(:))/length(yTe)
testerr =  0.29339
>> trainerr=sum(sign(svmclassify(xTr))~=yTr(:))/length(yTr)
trainerr = 0.13000
```

6. If you play around with your new SVM solver, you will notice that it is rather sensitive to the kernel and regularization parameters. You therefore need to implement a function

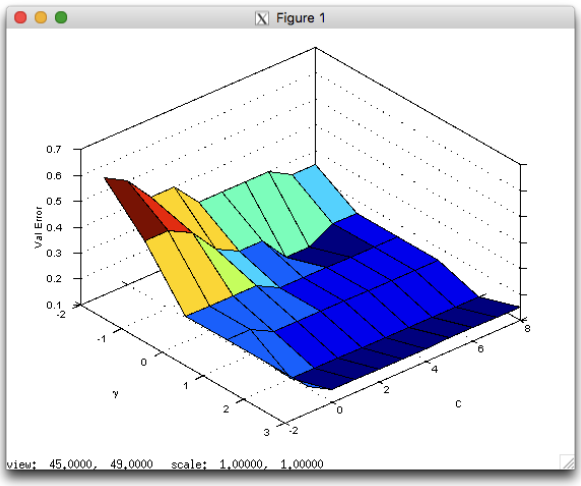
```
[bestC,bestP,bestvalerror]=crossvalidate(xTr,yTr,ktype,Cs,k
```

to automatically sweep over different values of C and kpars and output the best setting on a validation set (**`xTv,yTv`**). For example you could set `Cs=2.^[-5:5]` to try out different orders of magnitude. Cut off a section of your training data to generate a valication set.

If you did everything correctly, you should now be able to visualize your cross validation map:

```
>> load spiral
>> [bestC,bestP,bestval,allerrs]=crossvalidate(xTr,yTr,'rbf
>> [xx,yy]=meshgrid(-2:3,-1:8);
>> surf(xx,yy,allerrs);
>> xlabel('\gamma'); ylabel('C'); zlabel('Val Error');
```

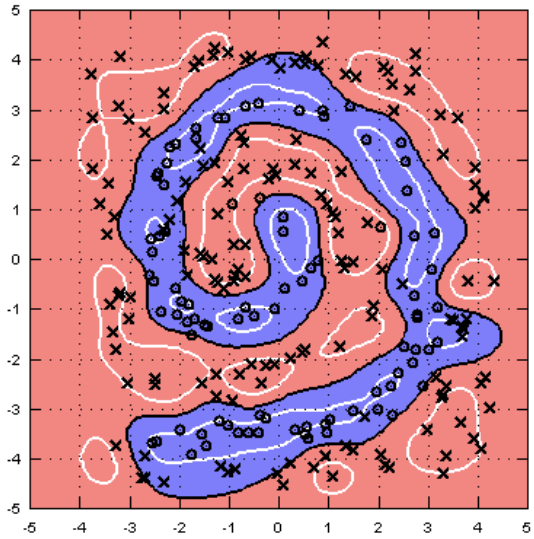
The result should look similar to this image(if you rotate the obtained image a bit):



You can now also take the best parameters and train your SVM. The following code trains the SVM with crass validated parameters, computes the test error and visualizes its decision boundary.

```
>> svmclassify=trainsvm(xTr,yTr,bestC,'rbf',bestP);
>> testerr=sum(sign(svmclassify(xTe))~=yTe(:))/length(yTe)
testerr =  0.15289
>> visdecision(xTe,yTe,svmclassify,'vismargin',true);
```

Your results should look very similar to the following image (test error and image may vary due to different implementations of cross validation):



Hints

Tests. To test your code you can run `example_tests.m`, which describes and partially implements several unit tests. Feel free to implement your own tests to better debug and test your implementation. Those tests are a subset of what we will use in the audograder to grade your submission.

It might help if you execute

```
>> more off
```

whenever you start on Matlab console, to see the output of your functions on the screen right away.

SVM Training (Quality Evaluation)

30% of the grade for your project3 submission will be assigned by how well your kernel SVM performs on a secret test set. Implement the function **`autosvm.m`**. Currently it takes a data set as input and tunes the hyper-parameters for the RBF kernel to perform best on a hold-out set (with your `crossvalidation.m` function). Can you improve it? (For example, you may look into adding new kernels to `computeK.m`, use telescopic cross validation, or use k-fold cross validation instead of a single validation set.)

Credits: Project adapted from Kilian Weinberger (Thanks for sharing!).