Support Vector Machines Machines: Exercises, II

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In this exercise I will attempt to look into the least squares support vector machine formulations using the LS-SVM Matlab toolbox, particularly function estimation and time series prediction. Unlike normal SVM, LS-SVM is intended to fit a numerical predictive function to the data.

Unlike linear regression, LS-SVM uses only a subset of points to decide the optimal hyperplane. These are the points corresponding to the support vectors, that are outside the ϵ tube, and changing which would change the optimal hyperplane. By contrast, changing any data point within a training set used for a linear regression classifier would change the classifier.

```
rng('default')
rng(333)
```

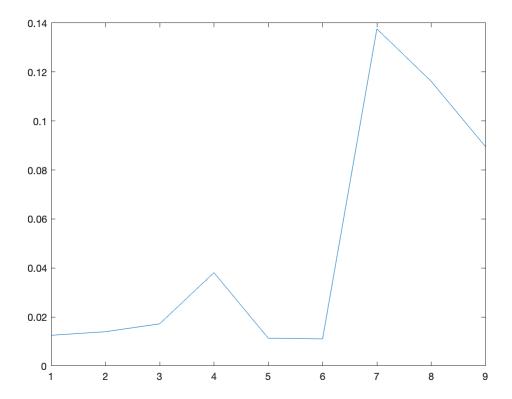
sinc regression

We can construct an example dataset using a noisy sinc function. Sinc is thus the true data generating process, and the task of an LS-SVM classifier will be to approximate this function without overfitting to replicate the noise.

```
X = transpose(-3:0.01:3);
Y = sinc(X) + 0.1 * randn(length(X), 1);
Xtrain = X(1:2: end); Ytrain = Y(1:2: end);
Xtest = X(2:2: end); Ytest = Y(2:2: end);
```

We can attempt approximation using the RBF kernel, iterating over a small parameter space.

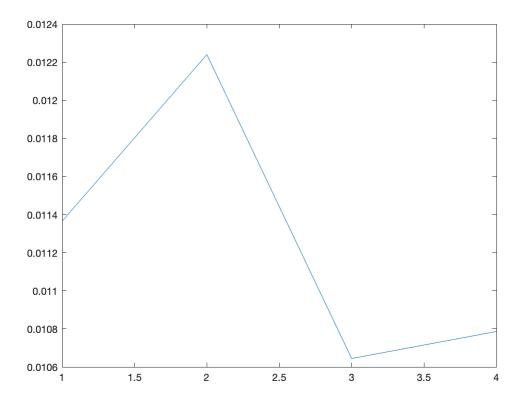
```
gams = [10, 10e3, 10e6]; sigmas = [0.01, 1, 100];
[sigmasMesh, gamsMesh] = meshgrid(sigmas, gams);
parameterSpace = num2cell([gamsMesh(:), sigmasMesh(:)], 2);
```



It seems that the fifth and sixth models are the best fitting on training set. Their parameters are:

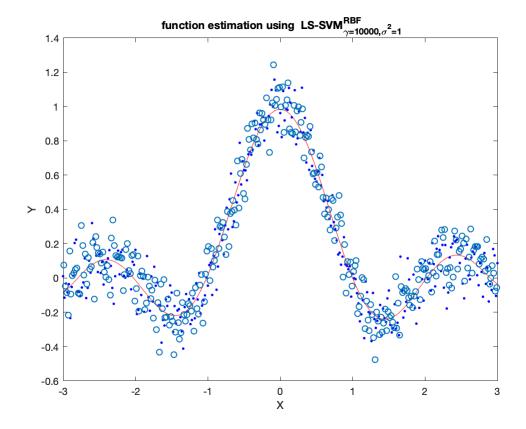
We can choose between them, as well as the first two models which are relatively well fitting, using the AUC of test set performance.

```
niceParams = cellfun(@(index) parameterSpace{index}, {1 2 5 6}, 'UniformOutput', false);
niceModelSpecs = cellfun(@(cell) { Xtrain , Ytrain , 'f', ...
    cell(:, 1), cell(:, 2), 'RBF_kernel'}, niceParams, 'UniformOutput', false);
niceModels = cellfun(@(cell) trainlssvm(cell), niceModelSpecs, 'UniformOutput', false);
niceSpecAndModel = cellfun(@(index) {niceModelSpecs{index}, ...
    niceModels{index}}, {1 2 3 4}, 'UniformOutput', false);
[Yest, Zt] = cellfun(@(cell) simlssvm(cell{1}, ...
    {cell{2}.alpha, cell{2}.b}, Xtest), niceSpecAndModel, 'UniformOutput', false);
test_mses = cellfun(@(cell) immse(cell, Ytest), Yest);
plot(test_mses)
```



It seems the fifth model fits the best on the test case. We may visualise the fifth model on the test data points.

```
modelSpec= {Xtrain, Ytrain, 'f', parameterSpace{5}(1), parameterSpace{5}(2), 'RBF_kernel'};
model = trainlssvm(modelSpec);
Yest = simlssvm(modelSpec, {model.alpha, model.b}, Xtest)
Yest = 300 \times 1
  -0.0855
  -0.0777
  -0.0695
  -0.0609
  -0.0521
  -0.0430
  -0.0338
  -0.0245
  -0.0151
  -0.0058
figure;
plotlssvm(modelSpec, {model.alpha, model.b});
Start Plotting...
finished
hold on;
scatter(Xtest, Ytest)
hold off;
```



Since the RBF kernel function estimation SVM is quite flexible, there should exist a pair of parameters that are optimal in the sense that, given these parameters, the resulting SVM is the best approximation of the underlying data-generating function possible. However, as we typically do not have direct access to the data generating process, a broader optimality criterion for parameters is that the resulting SVM is the best performing on some test set among the set of all possible SVMs. Some exceptions to this are possible - for example, there may be multiple near equal maxima or minima in the parameter space. This would correspond to having two or more models that fit the data equally well.

We can compare the resulting model to automatic parameter tuning.

```
[gamSimp, sigSimp, costSimp] = tunelssvm({Xtrain, Ytrain, 'f', ...
    [], [], 'RBF_kernel'}, 'simplex', 'crossvalidatelssvm', {10, 'mse'});
  Determine initial tuning parameters for simplex...: # cooling cycle(s) 1

    Coupled Simulated Annealing results: [gam]

                                        [sig2]
                                                     0.30308
                                                     0.011061
                                        F(X) =
TUNELSSVM: chosen specifications:
2. optimization routine:
                                  simplex
   cost function:
                                  crossvalidatelssvm
   kernel function
                                  RBF_kernel
3. starting values:
                                     14.9105
                                                0.303075
                         min f(x)
Iteration
          Func-count
                                    log(gamma)
                                                  log(sig2)
                                                              Procedure
```

```
1
               3
                   1.106100e-02 2.7021
                                                -1.1938
                                                            initial
    2
                                                -1.1938
              5
                   1.106100e-02 2.7021
                                                          contract outside
    3
              7
                                                          contract inside
                   1.106100e-02 2.7021
                                                -1.1938
                                                         contract inside
contract outside
reflect
contract inside
contract outside
contract outside
reflect
contract inside
reflect
    4
              9
                   1.106100e-02 2.7021
                                                -1.1938
    5
            10
                   1.106100e-02 2.7021
                                                -1.1938
    6
             12
                   1.106100e-02 2.7021
                                                -1.1938
    7
             14
                   1.106100e-02 2.7021
                                               -1.1938
                                               -1.1938
    8
             16
                   1.106100e-02 2.7021
             17
    9
                   1.106100e-02 2.7021
                                                -1.1938
            19
                   1.106100e-02 2.7021
                                                -1.1938
   10
                   1.106100e-02 2.7021
             20
                                                -1.1938
   11
                    1.106093e-02
                                   2.5087
   12
             24
                                                -1.2383
                                                            shrink
                    1.106092e-02 2.5674
             26
                                                -1.2175
   13
                                                            contract outside
optimisation terminated sucessfully (MaxFunEvals criterion)
Simplex results:
X=13.032541 0.295968, F(X)=1.106092e-02
Obtained hyper-parameters: [gamma sig2]: 13.0325
                                               0.295968
```

```
[gamGrid, sigGrid, costGrid] = tunelssvm({Xtrain, Ytrain, 'f', ...
    [], [], 'RBF_kernel'}, 'gridsearch', 'crossvalidatelssvm', {10, 'mse'});
  Determine initial tuning parameters for simplex...: # cooling cycle(s) 1

    Coupled Simulated Annealing results: [gam]

                                              7129.7485
                                              0.79574
                                   [sig2]
                                              0.010974
                                   F(X) =
TUNELSSVM: chosen specifications:
2. optimization routine: gridsearch
   cost function:
                             crossvalidatelssvm
   kernel function
                             RBF_kernel
3. starting values:
                               354.9693
                                         0.06531841
   cost of starting values: 0.011754
   time needed for 1 evaluation (sec):0.06
   limits of the grid: [gam] 354.969276
                                              1058148,4984
                      [sig2] 0.065318 9.6941
OPTIMIZATION IN LOG SCALE...
grain = 7
FIRST ITERATION:
  X=9.872
           -0.22848 ,F(X)=0.010955;
ITERATION: 2
 dF=4.9462e-07, dX=0.45169, X=9.4231 -0.2779, F(X)=0.010954;
```

It appears that we have by chance stumbled upon a slightly better model than determined by these parameters, since the test MSE of our fifth model is better than even the train MSEs found by automated tuning. Both methods produce similar results. Doing more iterations in both algorithms, over a larger space, could probably tune into the value we have found.

Obtained hyper-parameters: [gamma sig2]: 12370.3438 0.757372403