Kernel Ridge Regression Example

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This is a walkthrough example of how to use a kernel ridge regression (KRR) method in Matlab. This specific example attempts to model a function (with added gaussian noise) in R^3 space using the gaussian kernel trick. This example can be expanded to data with higher dimensionality.

Process Inputs

Import and normalize data

```
clear all;clc;
addpath('../');
data=zscore(csvread('gaussian_data.csv'));
x=data(:,1:end-1);
y=data(:,end);
```

Randomly shuffle samples

```
N = length(y);
shuffled_indexes = randperm(N);

x = x(shuffled_indexes,:);
y = y(shuffled_indexes,:);
```

Create a test/train split

```
t_split = 0.6;

N_train = N*t_split;
N_test = N-N_train;

x_test = x(N_train+1:end,:);
x_train = x(1:N_train,:);

y_test = y(N_train+1:end,:);
y_train = y(1:N_train,:);
```

Create Model

Create a 2D gaussian kernel that will represent the multidimensional data. This kernel will be based on the train sample data *x* and *y*. The following is the kernel formula:

```
K_{i,j} = \exp(-||x_j - x_i||)
```

```
K=zeros(N_train,N_train);
for j=1:N_train
  for i=1:N_train
    K(i,j)=exp(-norm(x_train(j,:)-x_train(i,:)));
end
end
```

Apply the kernel to the test data. This is done using the ridge regression formula:

```
\hat{y} = y^T (K + \lambda I)^{-1} K
```

Notice that in the code we keep λ constant. λ is a hyperparameter that is normaly tunned to achieve higher accuracy. A higher value of λ signifies that we trust our data less and helps counter overfitting.

```
y_predicted_sample=zeros(N_train,1);
lambda=0.1;

for i=1:N_train
    if mod(i,10) == 0
        fprintf('Training on Sample: %d of %d\n',i,N_train);
    end
    y_predicted_sample(i,1)= y_train'*((K+ lambda*eye(N_train))\K(i,:)');
end

Training on Sample: 10 of 120
Training on Sample: 20 of 120
```

```
Training on Sample: 30 of 120
Training on Sample: 40 of 120
Training on Sample: 50 of 120
Training on Sample: 60 of 120
Training on Sample: 70 of 120
Training on Sample: 80 of 120
Training on Sample: 90 of 120
Training on Sample: 100 of 120
Training on Sample: 110 of 120
Training on Sample: 120 of 120
Training on Sample: 120 of 120
```

```
in_sample_error = 0.0287
```

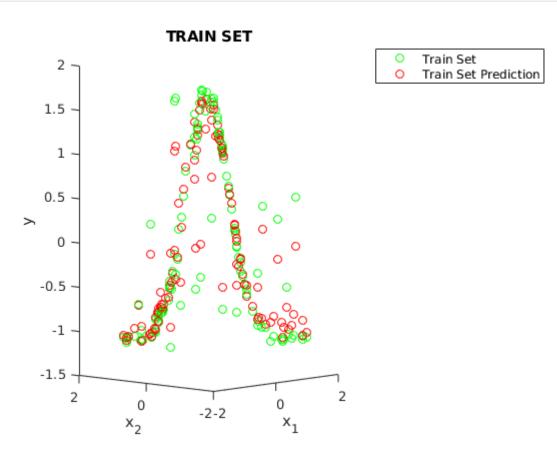
The resulting fit should be good, as we are testing our model against the same data it was trained on

```
figure
hold on

scatter3(x_train(:,1),x_train(:,2),y_train,'g')
scatter3(x_train(:,1),x_train(:,2),y_predicted_sample,'r')

title('TRAIN SET')
```

```
xlabel({'x_1'})
ylabel({'x_2'})
zlabel('y')
view([-47.1 4.4])
legend('Train Set','Train Set Prediction')
hold off
```



Testing Model

Now, we can use the kernel we created in the previous step and apply it to a novel x' and y'. The following equations outline how we will make a prediction:

$$k_{i,j} = \exp(-\|x_i - x_j'\|)$$
$$\hat{y}' = y^T (K + \lambda I)^{-1} \kappa$$

```
k=zeros(N_test,N_train);
for j=1:N_train
  for i=1:N_test
      k(i,j)=exp(-norm(x_train(j,:)-x_test(i,:)));
  end
end

y_predicted=zeros(N_test,1);
```

```
for i=1:N_test
    y_predicted(i,1) = y_train'*((K+ lambda*eye(N_train))\k(i,:)');
end

out_sample_error = norm(y_predicted-y_test)^2/N_test
```

out_sample_error = 0.2261

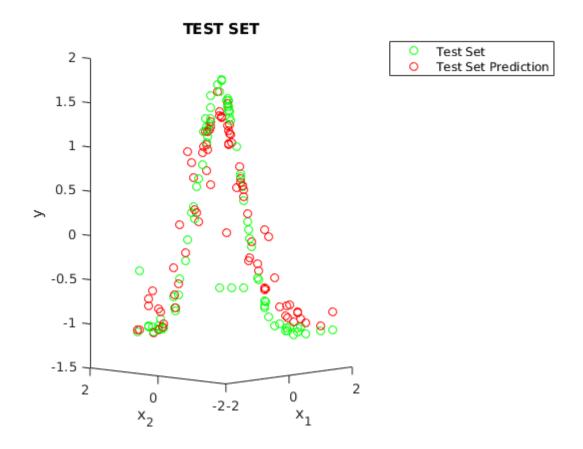
This new visualization shows the predicted \hat{y}' compared to y'. This is infinately more significant than the original plot as these \hat{y}' values were obtained with no knowledge of the corresponding y' values.

```
figure
hold on

scatter3(x_test(:,1),x_test(:,2),y_test,'g')
scatter3(x_test(:,1),x_test(:,2),y_predicted,'r')

title('TEST SET')
xlabel({'x_1'})
ylabel({'x_2'})
zlabel('y')
view([-47.1 4.4])
legend('Test Set','Test Set Prediction')

hold off
```



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