CPSC 340 Assignment 3 (due October 23rd)

Clustering, Item Recommendation, Linear Regression

- You can work in groups on the assignments. However, please hand in your own assignments and state the group members that you worked (as well as other sources of help like online material).
- Place your name and student number on the first page, and submit all answers as a single PDF file to handin.
- For questions that ask for code, you should include the relevant parts of the code in the appropriate place in the PDF file.
- Please organize your submission sequentially according to the sections used in this document.
- All Sections (1-5) are equally weighted.
- There may be updates/clarifications to the assignment after the first version is put online. Any modifications will be marked in red.

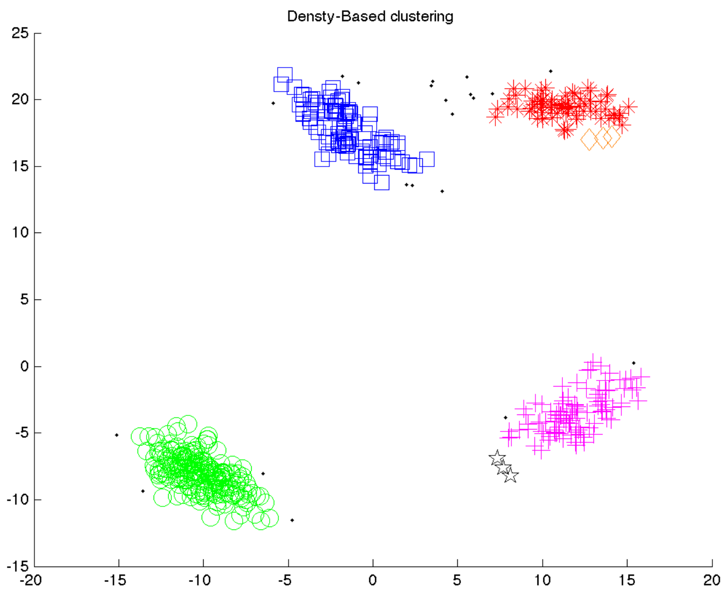
0 Unnoffiial Course Evaluation

To help improve the course as we go along, or to suggest of how things could be done differently, please fill out the survey here:
`https://survey.ubc.ca/surveys/37-7d0090012c11ea5c07f0bca610f/cpsc340-asst-3`

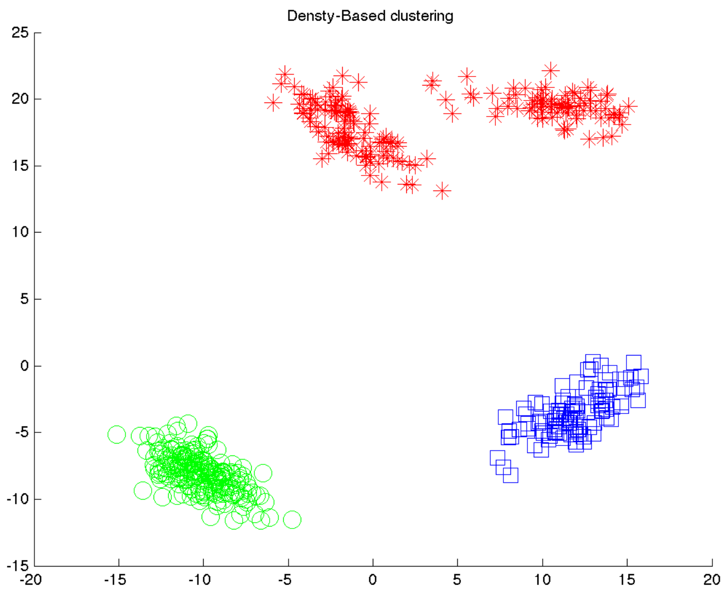
1 Non-Parametric Clustering

1.1 Effect of Parameters on DBSCAN

If you run the function *example_DBscan*, it will apply the basic density-based clustering algorithm to the dataset from the previous assignment. The final output should look like this:



Even though we know that each object was generated from one of four clusters, the algorithm finds 6 clusters and does not assign some objects to any cluster. However, the assignments will change if we change the parameters of the algorithm. Find and report values for the two parameters of the density-based clustering algorithm such that it finds the correct 4 clusters and assigns all points to their appropriate cluster. Further, find and report values for the two parameters such that the top two clusters are merged into one cluster, so that we have 3 clusters as in the figure below:



Answer:
There are many possible parameter settings that would work. I found that we didn't need to change the

minPoints. We could get the true clusters by changing the radius to 10, and we could get the '3 cluster' interpretation by setting it to 20.

1.2 K-Means vs. DBSCAN Clustering

If you run the function *example_animals*, it will load a dataset containing 85 attribute values for 50 animals. It will then apply a k-means clustering to the animals, and report the resulting clusters. The exact clustering will depend on the initialization of k-means and the value of k, but below is the result of one of the runs:

- Cluster 1: killer+whale blue+whale hippopotamus humpback+whale seal walrus dolphin
- Cluster 2: elephant ox sheep rhinoceros buffalo giant+panda pig cow
- Cluster 3: skunk mole hamster squirrel rabbit mouse raccoon
- Cluster 4: antelope horse moose spider+monkey gorilla chimpanzee giraffe zebra deer
- Cluster 5: grizzly+bear beaver dalmatian persian+cat german+shepherd siamese+cat tiger leopard fox bat wolf chihuahua rat weasel otter bobcat lion polar+bear collie

Some of these groupings make sense (cluster 1 contains fairly-large animals that live in or near the water) while others do not (grizzly bears and bats are both in cluster 5). Modify this demo to use the density-based clustering method, and report the clusters obtained if you set *minPoints* to 3 and the radius such that it finds 5 clusters.

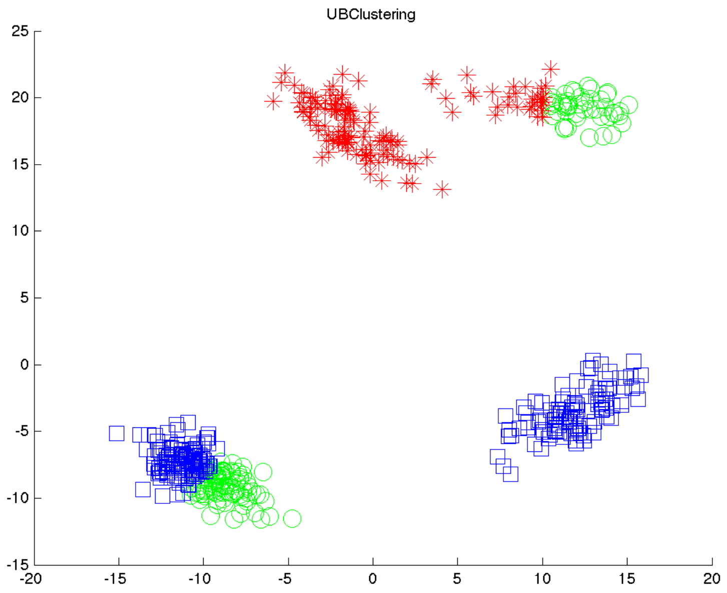
Answer:
The exact clustering could vary, but I found that a radius of 15 gave the following clustering:

- Cluster 1: antelope horse moose ox sheep giraffe buffalo zebra deer pig cow
- Cluster 2: dalmatian persian+cat german+shepherd siamese+cat mole tiger leopard fox hamster squirrel rabbit wolf chihuahua rat weasel bobcat mouse collie
- Cluster 3: hippopotamus elephant rhinoceros
- Cluster 4: blue+whale humpback+whale seal walrus dolphin
- Cluster 5: spider+monkey gorilla chimpanzee

These are much more interpretable: cluster 1 is medium-sized four-legged land animals, cluster 2 is furry friends and their wild counterparts, cluster 3 is huge african animals, cluster 4 is water-based mammals, and cluster 5 is primates.

1.3 UBClustering Algorithm

If you run the function *example_UBClustering.m*, it will load our usual synthetic clustering data. It will then apply k-means clustering 20 times, and use the mode of these clusterings as the final result. Due to the 'label switching' problem, this typically produces non-sensical clusterings like this one:



Modify this demo so that it puts two points in the same cluster if they appear together in at least 50% of the clusterings (merging the clusters of points that satisfy this property). Hand in your code and the plot that you obtain with this strategy.

Hint: Try to see if you can adapt the structure of the 'for' loop and the 'expand' functions from the DBSCAN algorithm in order to implement this new algorithm.

Answer:
I added the following extra code after fitting each of the k-means models:

```
% Find the number of times each pair of points was in the same cluster
for n1 = 1:N
    for n2 = 1:N
        D(n1,n2) = sum(clusters(n1,:)==clusters(n2,:))/nModels;
    end
end

% This will be the cluster of each object.
cluster = zeros(N,1);

% This variable will keep track of whether we've visited each object.
visited = zeros(N,1);

% K will count the number of clusters we've found
K = 0;
for i = 1:N
    if ~visited(i)
        % We only need to consider examples that have never been visited
        visited(i) = 1;
        neighbors = find(D(:,i) > 0.5);
        if length(neighbors) > 1
            % We found a new cluster
            K = K + 1;
            [visited,cluster] = expand(X,i,neighbors,K,D,visited,cluster);
        end
    end
end
```

I also copied and pasted the expand function from the DBSCAN code, modifying the following part:

```
if ~visited(n)
    visited(n) = 1;
    neighbors2 = find(D(:,n) > 0.5);
    if length(neighbors2) > 1
        neighbors = [neighbors;setdiff(neighbors2,neighbors)];
    end
end
```

For the last line, the *union* function would be a more elegant way to do it. With the new method, I found it often tends to return the true clustering, or it tends to return 3 clusters as in Question 1.1.

2 Item Recommendation

The file *newsgroups.mat* contains our usual newsgroups dataset, except that all the objects are placed together in a big matrix X, and (since we are focusing on unsupervised learning) there is no label y. In this question, we're going to build a 'word' recommendation system. That is, given a word, return a list of other words that are relevant (this could be used to direct a user to other relevant topics).

2.1 Amazon Recommendation Algorithm

In class, we discussed the recommendation algorithm used by Amazon. For each product/word j, it works with a vector x_j containing the users/posts that contain j. For the newsgroups data, this is simply $X(:,j)$. To make recommendations for a product/word i, it returns the K words that have the highest *cosine similarity*,

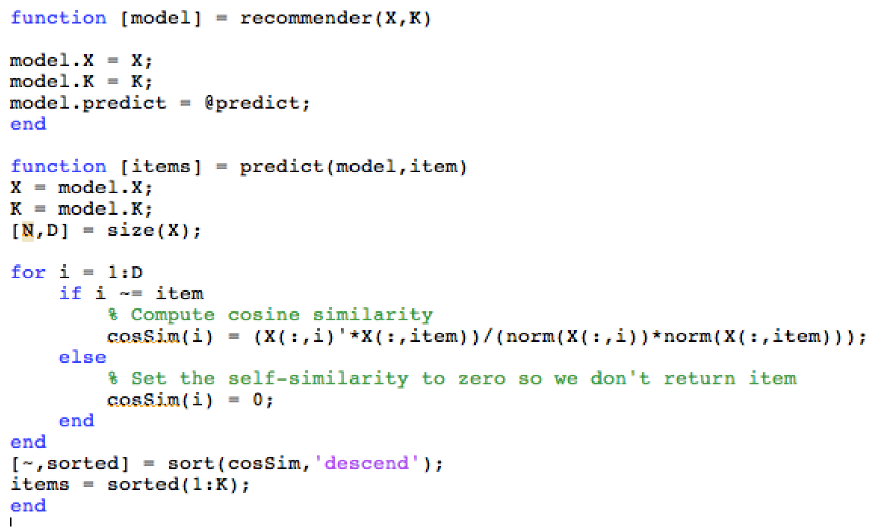
$$\cos(x_i, x_j) = \frac{x_i^T x_j}{\|x_i\|\|x_j\|}.$$

Write a function 'recommender', that has the following behaviour:

1. Calling 'model = recommender(X,K)' will do any 'training' the model requires (if necessary) and store relevant quantities used by the model to make predictions.
2. Calling 'wordNumbers = model.predict(model,j)' will return the K word numbers whose vectors have the highest cosine similarity with word number 'j'. Make sure to exclude 'j' from the output.

Hand in your implementation of the 'recommender' function. For each of the first 5 words, list the recommended words when $K = 5$.

Answer:
Here is one possible implementation:



```
function [model] = recommender(X,K)

model.X = X;
model.K = K;
model.predict = @predict;
end

function [items] = predict(model,item)
X = model.X;
K = model.K;
[N,D] = size(X);

for i = 1:D
    if i ~= item
        % Compute cosine similarity
        cosSim(i) = (X(:,i)'*X(:,item))/(norm(X(:,i))*norm(X(:,item)));
    else
        % Set the self-similarity to zero so we don't return item
        cosSim(i) = 0;
    end
end
[~,sorted] = sort(cosSim,'descend');
items = sorted(1:K);
end
```

Here are the first 5 words and their recommendations:

1. aids: health, diseases, patients, cancer, food.
2. baseball: players, games, league, season, team.
3. bible: god, jesus, christian, religion, fact.
4. bmw: car, engine, honda, oil, drive.
5. cancer: patients, disease, medicine, vitamin, health.

2.2 Fast Recommendation with Sparse Data

Let n be the number of rows in X and d be the number of columns. Computing a norm of a column costs $O(n)$, while computing the inner product between columns also costs $O(n)$. Thus, to make a recommendation the worst case cost of computing the cosine similarity between all d rows is $O(nd)$. This would be too slow for a company like Amazon, who has millions or users (n) and millions of products (d).

Consider an implementation that maintains the following two data structures for each product:

1. A *sorted list* of the user identification numbers for the users that bought the product.
2. An *list* of the products that have non-zero similarity with the product (i.e., have been bought by one of the same users).

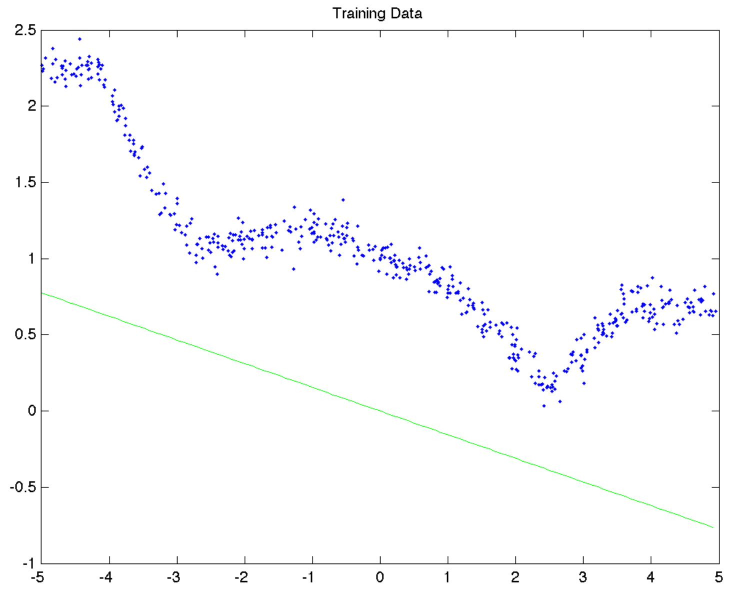
Let u be the maximum length of the first (sorted) list and p be the maximum length of the second list. What is the worst-case cost of making an item recommendation in terms of u and p?

Answer:
To compute norms, we can actually just count the length of the user list, so this is $O(1)$. To compute inner products, we can go sequentially through the lists for both products and count the number of users they share. This would cost $O(u)$ instead of $O(n)$. Further, instead of computing the cosine similarity to all $d-1$ other objects, we only need to compare it for up to p products with non-zero cosine similarity. This gives a total cost of $O(up)$. This will be much smaller than $O(nd)$, provided that we don't have both a user that has bought everything and a product that has non-zero similarity with all other products.
(If we want to answer queries even faster, for each product we can maintain a list of the top-k most similar products. This has extra building/maintenance/storage costs, but allows us to answer queries in $O(k)$. In

cases where we can't afford to build this data structure, then region-based pruning is often employed to do it exactly or approximately.)

3 Linear Regression and Change of Basis

The script *example_basis* loads a one-dimensional regression dataset and displays the result of applying a simple linear regression model. Unfortunately, this is an awful model of the data:



3.1 Linear Regression with a Bias Variable

Write a new function, *simpleLeastSquares*, that has the same input/model/predict format as the *leastSquares* function, but that includes a *bias* variable w_0, and makes predictions using the model

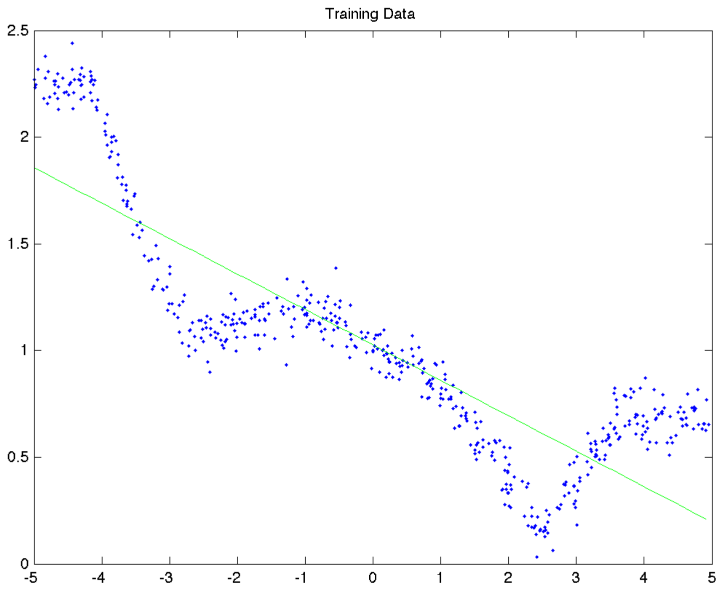
$$y_i = wx_i + w_0.$$

Hand in your new function and the updated plot.

Answer:
One way to implement the centeredLeastSquares function would be:

```
function [model] = simpleLeastSquares(X,y)

% Add bias variable
[N,D] = size(X);
X = [ones(N,1) X];

% Solve least squares problem
w = (X'*X)\X'*y;

model.w = w;
model.predict = @predict;

end

function [yhat] = predict(model,Xtest)
[T,D] = size(Xtest);
w = model.w;
Xtest = [ones(T,1) Xtest];
yhat = Xtest*w;
end
```

The plot when using this function now looks better:



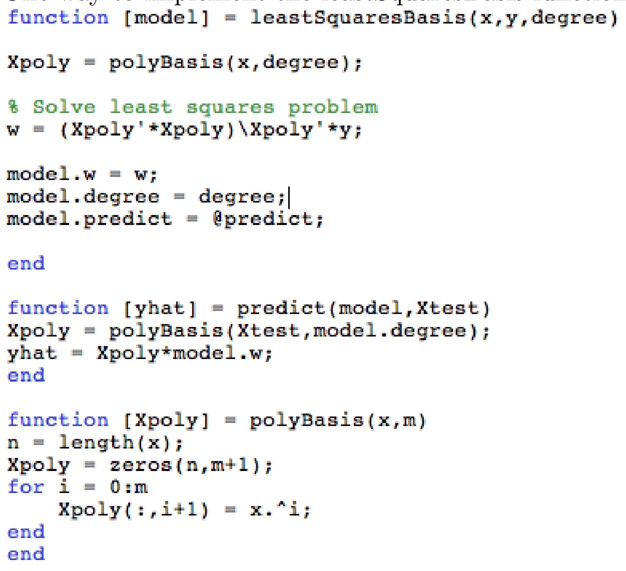
3.2 Polynomial Basis

Centering the target variables y_i improves the prediction substantially, but the model is still problematic because the target seems to be is a non-linear function of the input. Write a new function, *leastSquares-Basis(x,y,degree)*, that takes a data vector x (i.e., assuming we only have one feature) and the polynomial order *degree*. The function should perform a least squares fit based on a matrix *Xpoly* where each of its rows contains the values $(X_i)^j$ for $j = 0$ up to *degree*. E.g., *leastSquaresBasis(x,y,3)* should form the matrix

$$Xpoly = \begin{bmatrix} 1 & x_1 & (x_1)^2 & (x_1)^3 \\ 1 & x_2 & (x_2)^2 & (x_2)^3 \\ \vdots & & & \\ 1 & x_n & (x_n)^2 & (x_N)^3 \end{bmatrix},$$

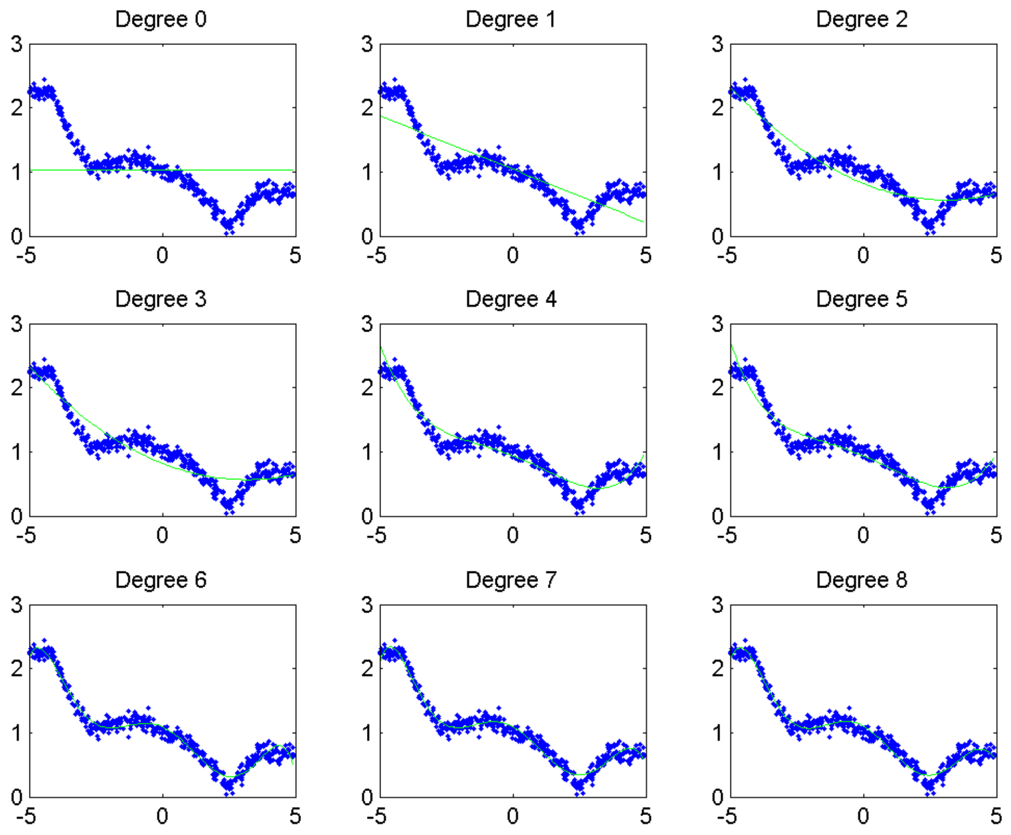
and fit a least squares model based on it. Hand in the new function and a 3 by 3 plot showing the fit for $degree = 0$ up to $degree = 8$.

Hints: You can use the *subplot* command to construct a figure containing multiple plots. Don't forget that you need to do the same transformation to the test data. You may want to write a new function *polyBasis* that you can use for both the training and testing data. Answer:
One way to implement the leastSquaresBasis function would be:



```
function [model] = leastSquaresBasis(x,y,degree)

Xpoly = polyBasis(x,degree);

% Solve least squares problem
w = (Xpoly'*Xpoly)\Xpoly'*y;

model.w = w;
model.degree = degree;
model.predict = @predict;

end

function [yhat] = predict(model,Xtest)
Xpoly = polyBasis(Xtest,model.degree);
yhat = Xpoly*model.w;
end

function [Xpoly] = polyBasis(x,m)
n = length(x);
Xpoly = zeros(n,m+1);
for i = 0:m
    Xpoly(:,i+1) = x.^i;
end
end
```

The plot should roughly look like this:



3.3 Choosing the Basis

Using the first 250 examples as a training set and the remaining 250 examples as a validation set, report the training and validation errors for models with degrees 0 through 20. Use the *averaged squared error* as the performance measure. How does the degree of the polynomial affect the fundamental trade-off in machine learning?

Hint: use a 'for degree = 0:20' loop, and use an 'fprintf' statement to output the training and testing error for each degree.

Answer:
I got the following values:
(Note that the exact values for the higher degress might vary a bit; they depend on the particular version of Matlab and how the underlying matrix operations are implemented in the hardware.) Degree 0: training error = 0.3008, testing error = 0.3114
Degree 1: training error = 0.0783, testing error = 0.0805
Degree 2: training error = 0.0365, testing error = 0.0440
Degree 3: training error = 0.0365, testing error = 0.0440
Degree 4: training error = 0.0253, testing error = 0.0323
Degree 5: training error = 0.0244, testing error = 0.0337
Degree 6: training error = 0.0096, testing error = 0.0101

Degree 7: training error = 0.0082, testing error = 0.0110
Degree 8: training error = 0.0082, testing error = 0.0106
Degree 9: training error = 0.0078, testing error = 0.0118
Degree 10: training error = 0.0062, testing error = 0.0068
Degree 11: training error = 0.0055, testing error = 0.0076
Degree 12: training error = 0.0051, testing error = 0.0058
Degree 13: training error = 0.0049, testing error = 0.0065
Degree 14: training error = 0.0049, testing error = 0.0066
Degree 15: training error = 0.0049, testing error = 0.0055
Degree 16: training error = 0.0049, testing error = 0.0054
Degree 17: training error = 0.0049, testing error = 0.0057
Degree 18: training error = 0.0048, testing error = 0.0065
Degree 19: training error = 0.0047, testing error = 0.0320
Degree 20: training error = 0.0046, testing error = 0.0571
As the degree increases, the training error gets smaller. However, the training error becomes a worse approximation of the testing error.

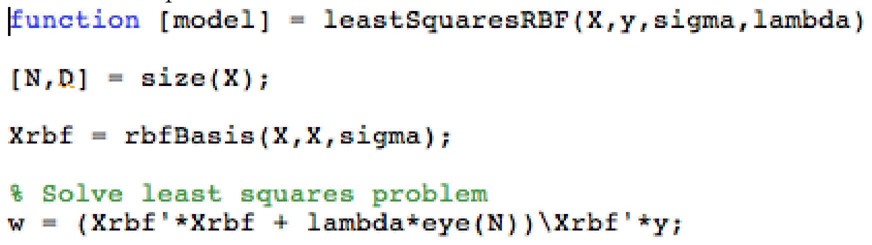
4 Radial Basis Functions and Regularization

The function *example_rbf* loads and displays a training data set $\{X, y\}$ and a corresponding test data set $\{Xtest, ytest\}$. Subsequently, it displays the performance of least squares using non-parametric radial basis function (RBFs). The performance of the model becomes better as the RBF parameter *sigma* is decreased, but the becomes substantially worse for low values.

4.1 Regularization

Using an RBF kernel leads to a much more complicated model, so we might expect to do better through the use of regularization. Modify the function *leastSquaresRBF* to take an extra parameter *lambda*, and use an L2-regularized estimate of w. Explore whether you can achieve a lower test error by exploring different values of λ. Hand in your modified code.

Answer:
The modified part of the code should look like this:



```
function [model] = leastSquaresRBF(X,y,sigma,lambda)

[N,D] = size(X);

Xrbf = rbfBasis(X,X,sigma);

% Solve least squares problem
w = (Xrbf'*Xrbf + lambda*eye(N))\Xrbf'*y;
```

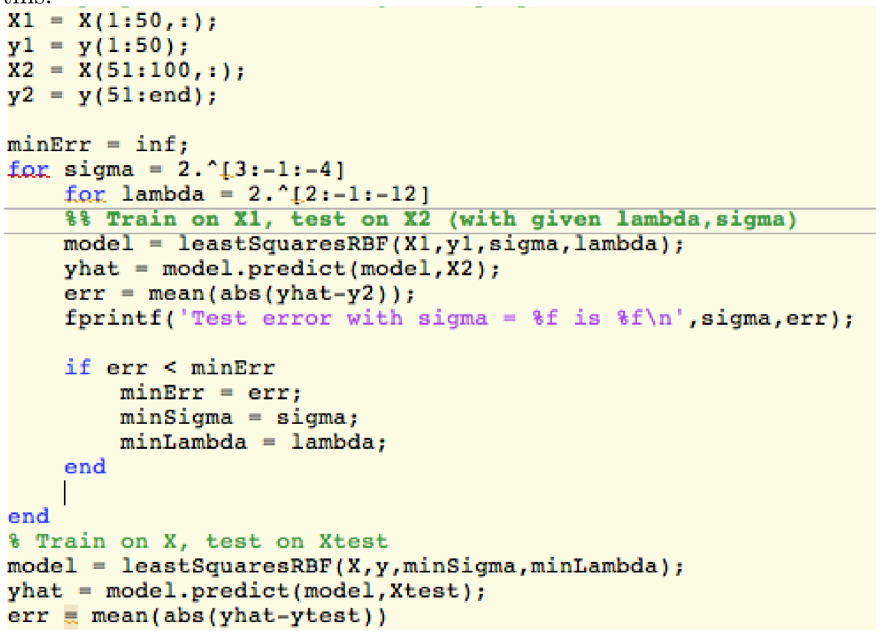
4.2 Proper Training/Validation/Testing

Unfortunately, this demo and exploring whether we can achieve a better test error by trying out different values of λ is violating the golden rule of machine learning, by looking at the test set multiple times. Make the following modifications to the demo:

1. Instead of training on the full training set and testing on the test set. Train on the first half of the training data and test on the second half of the training data (the 'validation' set).
2. Modify the demo to search over the 'hyper-parameters' σ and λ, and find the one that performs the best on the validation set. Measure performance based on the average absolute error. A reasonable range of λ values to search is $\{2^{-12}, 2^{-11}, 2^{-10}, \dots, 2^{2}\}$.
3. Once you have the best values of the hyper-parameters σ and λ, train on the full training set and compute the average absolute error on the test set.

Hand in your code, report the best values of σ and λ, and report the final test error estimate from this procedure.

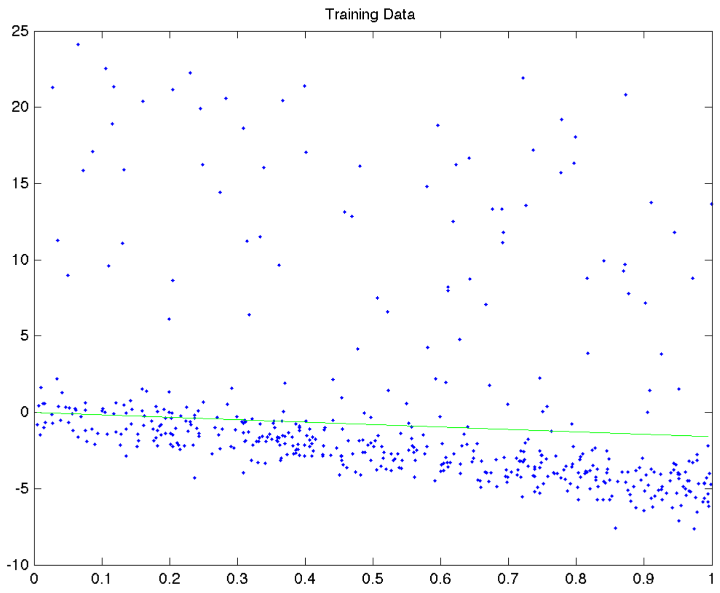
Answer:
The best value of σ is 1/2 and the best value of λ is 2^{-10}. If you train on the full data set with these values, the test error is 0.0577 (which is lower than the best unregularized error). The code could look roughly like this:



```
X1 = X(1:50,:);
y1 = y(1:50);
X2 = X(51:100,:);
y2 = y(51:end);

minErr = inf;
for sigma = 2.^[3:-1:-4]
    for lambda = 2.^[2:-1:-12]
    %% Train on X1, test on X2 (with given lambda,sigma)
    model = leastSquaresRBF(X1,y1,sigma,lambda);
    yhat = model.predict(model,X2);
    err = mean(abs(yhat-y2));
    fprintf('Test error with sigma = %f is %f\n',sigma,err);

    if err < minErr
        minErr = err;
        minSigma = sigma;
        minLambda = lambda;
    end

end
% Train on X, test on Xtest
model = leastSquaresRBF(X,y,minSigma,minLambda);
yhat = model.predict(model,Xtest);
err = mean(abs(yhat-ytest))
```

5 Least Squares with Outliers

The script *example_outliers* loads a one-dimensional regression dataset that has a non-trivial number of 'outlier' data points. These points do not fit the general trend of the rest of the data, and pull the least squares model away from the main downward trend that most data points exhibit:



5.1 Weighted Least Squares in One Dimension

One of the most common variations on least squares is *weighted* least squares. In this formulation, we have a weight z_i for every training example. To fit the model, we minimize the weighted squared error,

$$\operatorname*{arg\,min}_{w \in \mathbb{R}^d} \frac{1}{2} \sum_{i=1}^{n} z_i (y_i - w^T x_i)^2.$$

In this formulation, the model focuses on making the error small for examples i where z_i is high. Similarly, if z_i is low then the model allows a larger error. By taking the derivative and equating it with zero, solve for the the solution w to one-dimensional weighted least squares problems:

$$\operatorname*{arg\,min}_{w \in \mathbb{R}} f(w) = \frac{1}{2} \sum_{i=1}^{n} z_i (y_i - w x_i)^2.$$

Answer:
Let's define

$$f(w) = \frac{1}{2} \sum_{i=1}^{n} z_i (y_i - w x_i)^2,$$

remembering that we are focusing on the one-dimensional case. Taking the derivative we get

$$f'(w) = \sum_{i=1}^{n} z_i (y_i - w x_i) x_i,$$

and equating this to zero we have

$$\sum_{i=1}^{n} z_i y_i x_i = w \sum_{i=1}^{n} z_i x_i^2.$$

Solving for w gives

$$w = \frac{\sum_{i=1}^{n} z_i y_i x_i}{\sum_{i=1}^{n} z_i x_i^2}.$$

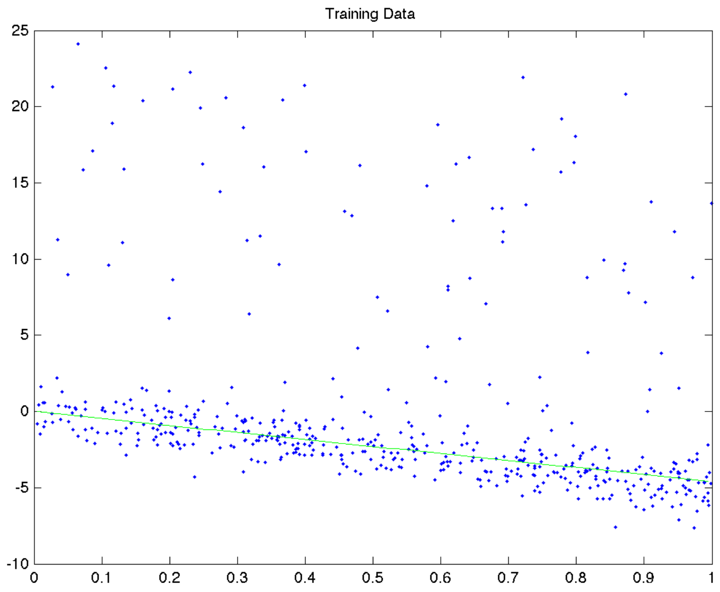
5.2 Weighted Least Squares Fitting

Write a model function, *weightedLeastSquares(x,y,z)*, that implements the model from the previous question. Apply this model to the data containing outliers, setting $z = 1$ for the first 400 data points and $z = 0.1$ for the last 100 data points (which are the outliers). Hand in your function and the updated plot.

Answer:
You only need to change the calculation of w in the leastSquares function to implement weighted least squares. In one dimension, it can be calculated using:

```
% Solve weighted least squares problem
w = sum(z.*x.*y)/sum(z.*x.^2);
```

The figure, when weighting the data points, now looks like this:



It now models the overall trend in the non-outlier points.

5.3 Smooth Approximation to the L1-Norm

Unfortunately, we typically do not know the identities of the outliers. In situations where we suspect that there are outliers, but we do not know which examples are outliers, it makes sense to use a loss function that is more robust to outliers. In class, we discussed using the sum of absolute values objective,

$$\operatorname*{arg\,min}_{w \in \mathbb{R}^d} \sum_{i=1}^{n} |y_i - w^T x_i|.$$

This is less sensitive to outliers than least squares, but it is non-differentiable and harder to optimize. Nevertheless, there are various smooth approximations to the absolute value function that are easy to optimize. One possible approximation is to use

$$|r| \approx \sqrt{r^2 + \epsilon},$$

for some small ϵ. This approximation becomes exact as ϵ goes to zero, but for any fixed ϵ the function will be differentiable. Using this approximation, we obtain an objective of the form

$$\operatorname*{arg\,min}_{w \in \mathbb{R}^d} \sum_{i=1}^{n} \sqrt{(y_i - w^T x_i)^2 + \epsilon},$$

which is smooth but less sensitive to outliers than the squared error. If we define f by

$$f(w) = \sum_{i=1}^{n} \sqrt{(y_i - w^T x_i)^2 + \epsilon},$$

derive the gradient ∇f of this function with respect to w. You should show your work but you do not have to express the final result in matrix notation.

Answer:
Let's first take the derivative of the approximation,

$$\frac{d}{dr}[\sqrt{r^2 + \epsilon}] = \frac{2r}{2\sqrt{r^2 + \epsilon}} = \frac{r}{\sqrt{r^2 + \epsilon}},$$

which is a reasonable approximation to the sign of r, $r/|r|$. An individual partial derivative will have the form

$$\frac{\partial f}{\partial j} = -\sum_{i=1}^{n} \frac{(y_i - w^T x_i) x_{ij}}{\sqrt{(y_i - w^T x_i)^2 + \epsilon}}.$$

The gradient will be the vector formed from these elements.
(If you wanted to express it in matrix notation, we could define a vector v with elements

$$v_i = -\frac{y_i - w^T x_i}{\sqrt{(y_i - w^T x_i)^2 + \epsilon}},$$

and with this notation we have

$$\nabla f(w) = X^T v,$$

which is similar to the gradient for least squares but where we've replaced the residuals $(Xw - y)$ with an approximation of the signs of the residuals.)

5.4 Robust Regression

The function *example_gradient* is the same as *example_outlier*, except that it fits the least squares model using a *gradient* method. One advantage of this strategy is that it only costs $O(nd)$ for an iteration of the gradient method, which is faster than forming $X^T X$ which costs $O(nd^2)$. Of course, we need to know the *number* of gradient iterations in order to precisely compare these two strategies, but for now we will assume that the number of gradient iterations is typically much less than d.

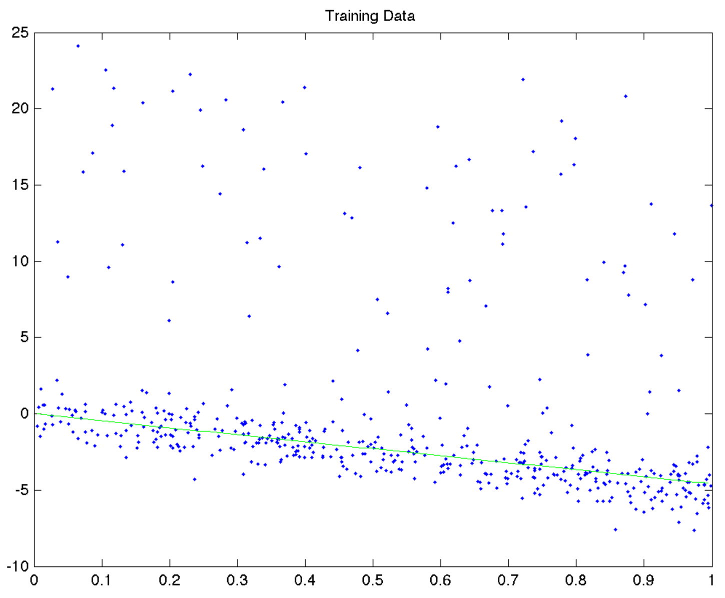
The usual input to a gradient method is a function that, given w, returns $f(w)$ and $\nabla f(w)$. See *funObj* in the *leastSquaresGradient* function for an example. Note that *leastSquaresGradient* also has a numerical check that the gradient code is approximately correct, since implementing gradients is often error-prone.

A second advantage of gradient-based strategies is that they are able to solve problems that do not have closed-form solutions, such as the formulation from the previous section. The function *robustRegression* has most of the implementation of a gradient-based strategy for fitting the robust regression model under the $\sqrt{r^2+\epsilon}$ approximation. The only part missing is the function and gradient calculation inside the *funObj* code. Modify this function to implement the objective function and gradient based on the smooth approximation to the absolute value function (from the previous section). Hand in your code, as well as the plot when we set $\epsilon = 0.1$.

Answer:
A particularly-elegant way to implement the function/gradient value would be something like this:

```
function [f,g] = funObj(w,X,y,epsilon)

% Compute residual
r = X*w - y;

% Compute objective function
f = sum(sqrt(r.^2 + epsilon));

% Compute sign-of-residual approximation
v = r./(sqrt(r.^2 + epsilon));

% Compute gradient
g = X'*v;
end
```

Using $\epsilon = 0.1$, we obtain similar results to the weighted least squares model:



However, in this case we didn't need to know which points were the outliers.