1. Linear and polynomial regression

For this exercise, you will experiment in Matlab with linear and polynomial regression on a given data set. The inputs are in the _le hw1x.dat and the desired outputs in hw1y.dat.

(a) [5 points] Load the data into memory and plot it (using the load and plot functions; use the help function if you do not know how to call them).

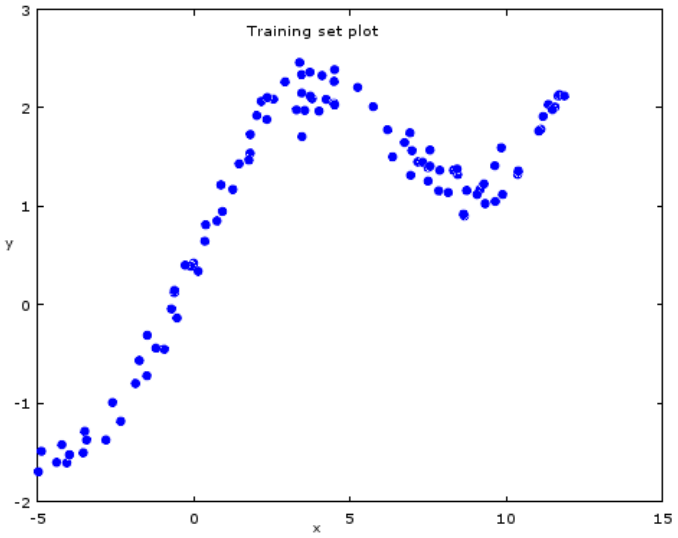


Fig 1. Training set plot

(b) [5 points] Add a column vector of 1s to the inputs, then use the linear regression formula discussed in class to obtain a weight vector w. Plot both the linear regression line and the data on the same graph. (Note: matrix formulas translate almost verbatim in Matlab)

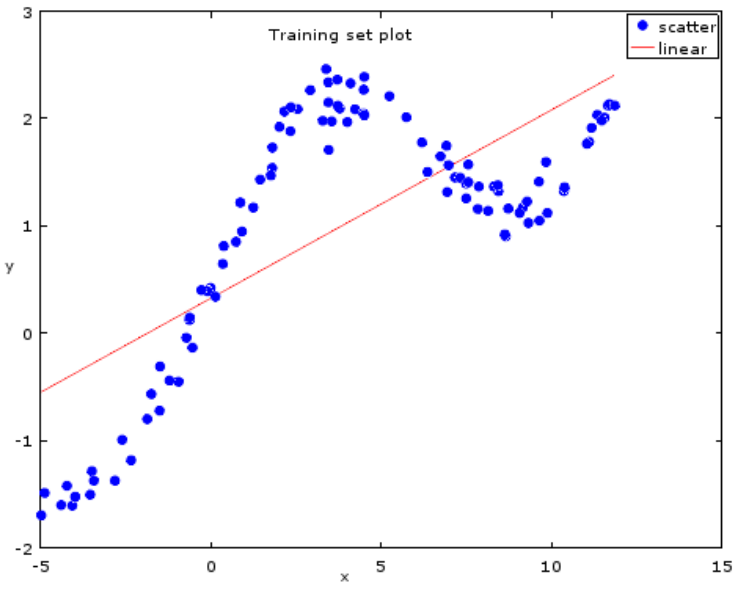


Fig 2. Linear Regression

(c) [5 points] Write a Matlab function that will evaluate the training error of the resulting fit, and report what this error is.

the error function is denoted as sum-of-square function:

$$J(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(h_{\mathbf{w}}(\mathbf{x}_i) - y_i)^2$$

After obtain the weight vector, and knowing X, and Y

W= 0.17531
0.32768

The training error is = 33.336

(d) [5 points] Write a Matlab function called PolyRegress(x,y,d) which adds the features x_2; x_3; :::x_d to the inputs and performs polynomial regression.

The implementation in in Q1.

(e) [5 points] Use your function to get a quadratic fit of the data. Plot the data and the fit. Report the training error. Is this a better fit?

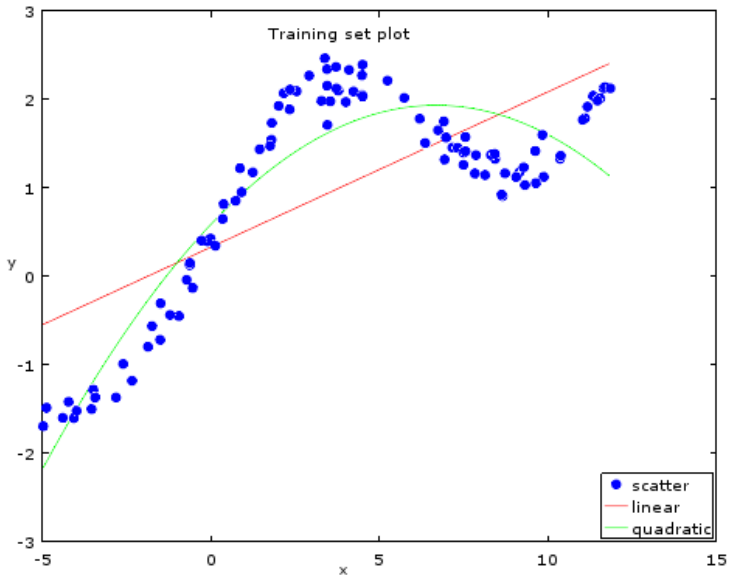


Fig 3. Quadratic regression

After obtain the weight vector, and knowing X, and Y

W= -0.030122
0.402405
0.585094

The training error is = 12.613

It is a better fit since the training error is smaller.

(f) [5 points] Repeat the previous exercise for a cubic fit.

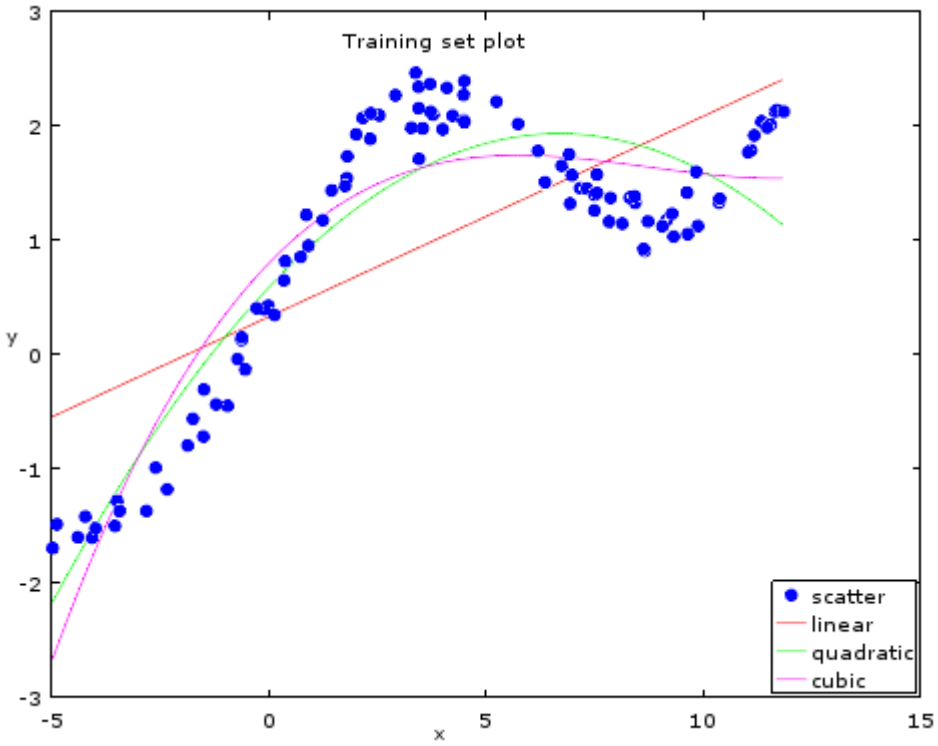


Fig 4. Cubic regression

After obtain the weight vector, and knowing X, and Y

$$W = \begin{matrix} 0.0019533 \\ -0.0510024 \\ 0.3927950 \\ 0.7954747 \end{matrix}$$

The training error is = 10.878

It is a better fit since the training error is smaller.

(g) [5 points] Suppose that the data were sorted in increasing value of the target variable y, and you simply partitioned it by putting the first m=k examples in the first fold, the next ones in the second fold, etc. Explain what would happen if you tried to perform cross-validation with these folds.

Perform kth fold cross-validation with these folds could estimate the true error of predicator, and find the best fit model to data set in terms of polynomial order.

By deciding the polynomial order of model, the training error is decreasing as the order increasing, the testing error decreases, then starts increasing again due to over fitting.

If the data sets are organized by increasing order, not equally distributed, the data set will not be independently, and identically distributed.

(h) [10 points]Write a procedure that performs five-fold cross-validation on your data. Use it to determine the best degree for polynomial regression. Show the data that supports your conclusion, and explain how you have come to this conclusion. For the best fit, plot the data and the polynomial obtained.

Five-fold cross validation

degree	Error_train	Error_valid
1	26.55568	6.92412
2	10.03406	2.65285
3	8.5881	2.47171
4	1.149	0.3334
5	1.1382	0.33771
6	0.85694	0.26229
7	0.85157	0.27419
8	14.91192	4.17644
9	35.88806	9.2989
10	49.34058	12.76735

Tab. 5 Cross Validation five-fold

From the result table we can see degree 6 has the minimum sum of average training error and average validation error. The result is by analyzing polynomial degree from 1 to 10 and by taking the average error of different combination of 5-fold data partition (1 out of 5 is validation set, 4 out of 5 is training set).

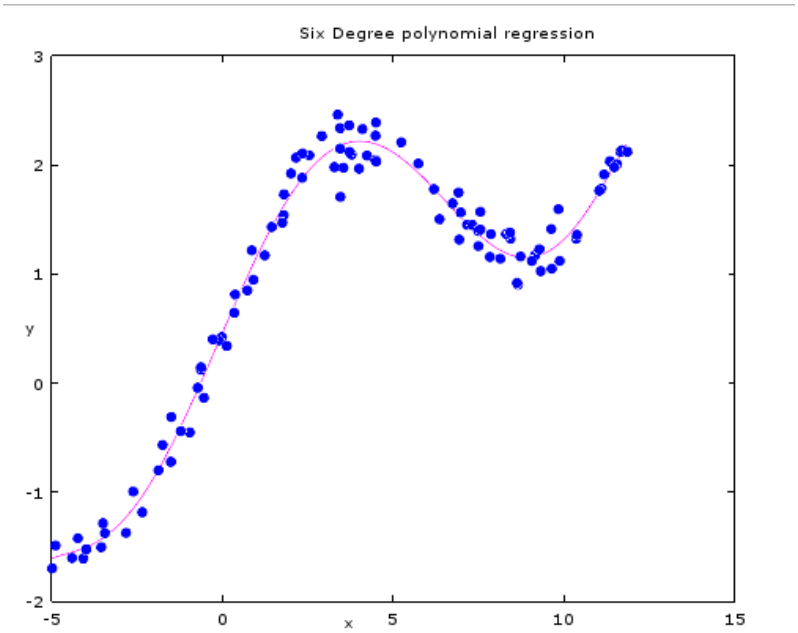


Fig. 6 six degree polynomial regression

The training error is = 1.0936.

Although by additional validation, we found that the 7 degree's polynomial training error of whole data model is = 1.0924

But the difference is too small, and we don't want to have any risk of over fitting. Hence 6 degree polynomial is our best fit.

(i) [10 points] Change the Matlab code such that you normalize the input data in each column by the maximum absolute value in that column. What is the best degree for polynomial regression now? Justify your answer.

Normalized Five-fold cross validation

degree	Error_train	Error_valid
1	26.55568	7.01619
2	10.03406	2.63169
3	8.5881	2.50249
4	1.149	0.42477
5	1.1382	0.42697
6	0.85694	0.35273
7	0.85157	0.3685
8	0.84869	0.37166
9	0.83419	0.37078
10	0.82882	0.36763

Table 7. Normalized Five-fold cross validation

From the result table we can see degree 6 has the minimum sum of average training error and average validation error.

The best fit is still 6 degree with no change.

The training error is 1.0936

(j) [10 points] As you witnessed, polynomial regression often causes the features to get extreme values, which may cause numerical problems. In such cases, it can be helpful to normalize the features, e.g. by dividing the value of each feature x_j by $\max_i jx_{i;j}j$; $i = 1; : : : ; m$; $j = 1; : : : ; d + 1$, like you did in the example above. Prove that this change results in a scaling of the output, but has no other e_ect on the approximator.

If we normalized the X by times the diagonal matrix X_{norm} , the expression of sum-of-square error function becomes:

$$J(w) = \frac{1}{2}\sum_{i=1}^{m}(h_w(x_i^{norm}) - y_i)^2$$

its gradient is

$$\nabla_w J = 2(XX_{norm})^T(XX_{norm})w - 2(XX_{norm})^T Y$$

gradient is 0 means:

$$2(XX_{norm})^T(XX_{norm})w - 2(XX_{norm})^T Y = 0$$

gives:

$$\mathrm{w}_{norm} = ((XX_{norm})^T(XX_{norm}))^{-1}(XX_{norm})^T Y$$

Diagonal constant matrix can be taken out from transpose. and can be reversed as constant

$$\mathrm{w}_{norm} = (X_{norm}\, X_{norm}\, X^T X)^{-1} X_{norm}\, X^T Y$$

$$\mathrm{w}_{norm} = X_{norm}^{-1}\,(X^T X)^{-1} X^T Y$$

$$\mathrm{w}_{norm} = X_{norm}^{-1}\; w$$

such normalization will scale up or down the weight factor, but no change.

$$J(w) = \frac{1}{2}\sum_{i=1}^{m}(h_w(x_i^{norm}) - y_i)^2$$

will become

$$J(w) = \frac{1}{2}\sum_{i=1}^{m}(XX_{norm}\, X_{norm}^{-1}\; w - Y)^2 \; = \frac{1}{2}\sum_{i=1}^{m}(h_w(x_i) - y_i)^2$$

Hence, error function result will not change，

2. [25 points] **Weighted linear regression**
Sometimes we might want to do linear regression but weight the different training examples differently. This is the case, for instance, if we believe that some examples are more important than others, or that some examples are less prone to noise. In particular, suppose we want to minimize the following error function:

$$J(\mathbf{w}) = \sum_{i=1}^{m} u_i(\mathbf{w}^T\mathbf{x_i} - y_i)^2$$

where $\mathbf{x_i} \in \mathbb{R}^n, u_i \in \mathbb{R}, i = 1, \ldots, m, \mathbf{w} \in \mathbb{R}^n$ are training samples, weights of training samples and model weights, respectively.

(a) [5 points] Show that this can be re-written in matrix form as:

$$J(\mathbf{w}) = (\mathbf{X}\mathbf{w} - \mathbf{y})^T\mathbf{U}(\mathbf{X}\mathbf{w} - \mathbf{y}).$$

Clearly state what $\mathbf{U}$ is.

a) when u is the model weight applies to each of i =1, 2, 3 ....m
then if

$$J(w) = \sum_{i=1}^{m} (w^T x_i - y_i)^2$$

can be rewritten in to

$$J(w) = (Xw - y)^T(Xw - y)$$

as vector multiplying.

the model weight, can be written as matrix form as

$$J(w) = (Xw - y)^T U(Xw - y)$$

U is the diagonal matrix

$$\mathrm{U} = \begin{bmatrix} u_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & u_m \end{bmatrix}$$

(b) [5 points] Compute $\nabla_{\mathbf{w}} J(\mathbf{w})$. Set this to 0 and solve for the parameter vector $\mathbf{w}$. You should obtain a generalization of the formula we derived in class, with $\mathbf{w}$ as a function of $\mathbf{X}, \mathbf{y}$ and $\mathbf{U}$. Check that for the case in which all weights are equal to 1, you get the same formula as for linear regression.

$$\nabla_w J = \nabla_w (Xw - Y)^T U(Xw - Y) = 0$$

expand

$$\nabla_w (w^T X^T UXw - Y^T UXw - w^T X^T UY + Y^T UY) = 0$$

$$\nabla_w (w^T X^T UXw - Y^T UXw - Y^T U(w^T X^T)^T + Y^T UY) = 0$$

take the gradient of w

$$2X^T UXw - Y^T UX - Y^T UX = 0$$

$$2X^T UXw = 2X^T UY$$

$$w = (X^T UX)^{-1} X^T UY$$

If all weight are equal to 1

$$w = (X^T IX)^{-1} X^T IY$$

$$w = (X^T X)^{-1} X^T Y$$

(c) [10 points] Implement weighted linear regression for the data set used in question 1. Weight all points equally, except the point with the largest input value. Gradually increase the weight of this point. Describe what happens, and why.

Linear regression W is 2*2 matrix, originally started with identity matrix. Then the weight of the largest input value from 1 to 50, by the step of 1.

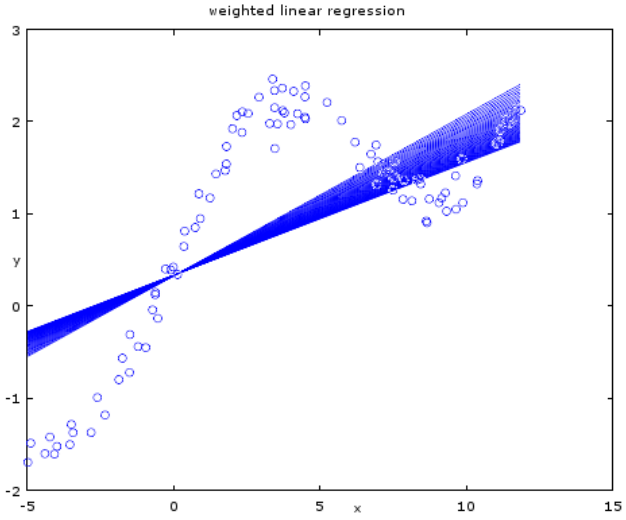
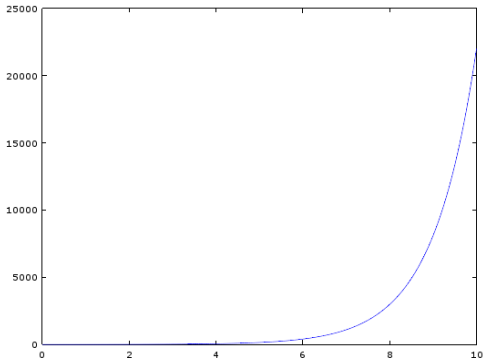


Fig 2.1 weighted linear regression

We can see the slope is increasing as the increase of weight. The larger weight of the largest input, the more influence of the term to the cost function.

(d) [5 points] Draw an example of a data set in which you would expect weighted linear regression to work a lot better than the unweighted version. Explain why you chose this data set.

if higher order term takes the majority of the weight, the weighted linear regression works better than unweighted.



such plot is the exponential function y = exp(x) , here if we weighted more on the higher order term of linear regression, it could give better description than unweighted.

3. [10 points] **Error criterion for exponential noise**
At the end of Lecture 2, we showed that one justification for minimizing the squared-error in a regression problem is probabilistic: we obtain the hypothesis under which the data has maximum likelihood if we assume that the target values are generated by a hypothesis from the same class, but perturbed by additive Gaussian noise. Now, suppose that the noise variables were not Gaussian but rather exponentially distributed. Recall that the exponential distribution has a single parameter, λ, and its density has the formula:

$$p_\lambda(t) = \begin{cases} \lambda e^{-\lambda t} & \text{if } t \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

Using a similar derivation to the one in class, show that under this assumption, the hypothesis that maximizes the likelihood of the data is no longer the one that minimizes the squared error. Derive the error criterion minimized in this case. Show your final result, as well as the derivation.

In order to find most probable hypothesis

We need to find out Maximum a posteriori (MAP) hypothesis

$$h_{map} = \arg\max_{h \in H} P(h|D)$$

Use Bayes Theorem we get

$$h_{map} = \arg\max_{h \in H} \frac{P(D|h)\,P(h)}{P(D)}$$ $P(D)$ is independent of h

$$= \arg\max_{h \in H} P(D|h)\,P(h)$$

If we assume $P(h_i) = P(h_j)$ (all hypotheses are equally likely a priori) the we can further simplify and choose the Maximum likelihood (ML) hypothesis.

$$h_{ML} = \arg\max_{h \in H} P(D|h) = \arg\max_{h \in H} \mathcal{L}(h)$$

this allow us to simplify $P(D|h)$

$$P(D|h) = \prod_{i=1}^{m} P((x_i, y_i)|h) = \prod_{i=1}^{m} P(y_i|x_i; h)\,P(x_i)$$

this is hard to simplify, then we maximize $\mathcal{L}(h)$

Apply log trick.

$$\log \mathcal{L}(h) = \prod_{i=1}^{m} \log P(y_i|x_i; h) + \prod_{i=1}^{m} \log P(x_i)$$

since 2nd term is not depends on h, it is ignored

Adop the assumption that $y_i = h_w(x_i) + \lambda_i$

where λ_i is exponential distribution $P_\lambda = \begin{cases} \lambda e^{-\lambda t} & t \geq 0 \\ 0 & \text{otherwise} \end{cases}$

Hence

$$\mathcal{L}(w) = \prod_{i=1}^{m} \lambda \cdot e^{-\lambda(y_i - h_w(x_i))}$$

Apply log trick

$$\log \mathcal{L}(w) = \sum_{i=1}^{m} (\log\lambda - \lambda(y_i - h_w(x_i)))$$

$$= \sum_{i=1}^{m} \log\lambda - \sum_{i=1}^{m} \lambda(y_i - h_w(x_i))$$

maximize RHS is same as minimize $\sum_{i=1}^{m} \lambda(y_i - h_w(x_i))$

the square term is gone

the maximum likelihood parameters w are those minimizing the sum error

$$w^* = \arg\min_{w} \sum_{i=1}^{m} (y_i - h_w(x_i))$$