CSCI 567 HW#2

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October 3, 2016

Sol. 1.1 The negative of log likelihood can be written as:

$$\mathcal{L}(\mathbf{w}) = -log\Bigg(\prod_{i=1}^{N} P(Y = y_i|\mathbf{X} = x_i)\Bigg)$$

$$\mathcal{L}(\mathbf{w}) = \begin{cases} y_n = 1 & -\sum_{i=0}^{N} log(\sigma(b + \mathbf{w}^T\mathbf{x}_n)) \\ y_n = 0 & -\sum_{i=0}^{N} log(1 - \sigma(b + \mathbf{w}^T\mathbf{x}_n)) \end{cases}$$

combining the two parts, we get

$$\mathcal{L}(\mathbf{w}) = -\sum_{i=0}^{N} y_n[log(\sigma(b + \mathbf{w}^T\mathbf{x}_n))] + (1 - y_n)[log(1 - \sigma(b + \mathbf{w}^T\mathbf{x}_n))] \quad (1)$$

Sol. 1.2 First we will transform the eq(1) above by appending 1 to $\mathbf{x}$ and b to $\mathbf{w}$ i.e.

$$\mathbf{x} = [1 \quad x_i \quad x_2 \quad x_3 \quad ... \quad x_D]$$

$$\mathbf{w} = [b \quad w_1 \quad w_2 \quad w_3 \quad ... \quad w_D]$$

$\therefore$ the eq(1) can be written as

$$\mathcal{L}(\mathbf{w}) = -\sum_{i=0}^{N} y_n[log(\sigma(\mathbf{w}^T\mathbf{x}_n))] + (1 - y_n)[log(1 - \sigma(\mathbf{w}^T\mathbf{x}_n))] \quad (2)$$

Now, we know that the derivative of $\sigma(a)$ is given as

$$\frac{d\,\sigma(a)}{d\,a} = \frac{1}{1 + e^{-a}}\Bigg(1 - \frac{1}{1 + e^{-a}}\Bigg)$$

$$= \sigma(a)[1 - \sigma(a)]$$

similarly we can write the derivative of $log(\sigma(a))$ w.r.t a

$$\frac{d\,log(\sigma(a))}{d\,\sigma(a)} = 1 - \sigma(a)$$

Now, using the above definitions and we can write the derivative of the loss function i eq(2) as

$$\frac{\partial\mathcal{L}(\mathbf{w})}{\partial\mathbf{w}} = -\sum_{i=0}^{N} y_n(1 - \sigma(\mathbf{w}^T\mathbf{x}_n))\mathbf{x}_n + (1 - y_n)\sigma(\mathbf{w}^T\mathbf{x}_n)\mathbf{x}_n$$

$$\frac{\partial\mathcal{L}(\mathbf{w})}{\partial\mathbf{w}} = \sum_{i=0}^{N}\{\sigma(\mathbf{w}^T\mathbf{x}_n) - y_n\}\mathbf{x}_n \quad (3)$$

from eq(3) we get the error as

$$e_n = \sigma(\mathbf{w}^T\mathbf{x}_n) - y_n$$

and the stationary point as

$$\sum_{i=0}^{N} \sigma(\mathbf{w}^T \mathbf{x}_n)\mathbf{x}_n = \sum_{i=0}^{N} \mathbf{x}_n y_n$$

Now, let η be the step size, then we can write the update rule for $\mathbf{w}$ as

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \sum_{i=0}^{N} \{\sigma(\mathbf{w}^T \mathbf{x}_n) - y_n\} x_n \tag{4}$$

Yes, it would converge to a global minimum. Since, the curve is linear and the local minimum would be the global minimum itself, which we can reach through gradient descent while following along the curve.

Sol. 1.3 For multi-class classification we are given the posterior probability as

$$P(Y = k|\mathbf{X} = \mathbf{x}) = \frac{exp(\mathbf{w}_k^T \mathbf{x})}{1 + \sum_{t=1}^{K-1} exp(\mathbf{w}_t^T \mathbf{x})} \quad for \quad k = 1, ... K - 1 \tag{5}$$

$$P(Y = k|\mathbf{X} = \mathbf{x}) = \frac{1}{1 + \sum_{t=1}^{K-1} exp(\mathbf{w}_t^T \mathbf{x})} \quad for \quad k = K \tag{6}$$

since, $\mathbf{w}_K = 0$, we can simply write

$$P(Y = k|\mathbf{X} = \mathbf{x}) = \frac{exp(\mathbf{w}_k^T \mathbf{x})}{1 + \sum_{1}^{K-1} exp(\mathbf{w}_t^T \mathbf{x})} \tag{7}$$

Now, using eq(7) we can write the negative log-likelihood as

$$\mathcal{L}(\mathbf{w}_1 ... \mathbf{w}_K) = -\sum_n log(P(y_n|\mathbf{x}_n = \mathbf{x})) = -\sum_n log(\prod_k [P(y = k|\mathbf{x}_n)])$$

$$\mathcal{L}(\mathbf{w}_1 ... \mathbf{w}_K) = -\sum_n \sum_k log\, P(y = k|\mathbf{x}_n))$$

using, eq(7), we can write the negative log-likelihood function as

$$\mathcal{L}(\mathbf{w}_1 ... \mathbf{w}_K) = -\sum_n \sum_k \left[\mathbf{w}_k^T \mathbf{x}_n - log(1 + \sum_{k=1}^{K-1} exp(\mathbf{w}_t^T \mathbf{x}_n))\right] \tag{8}$$

So. 1.4 To find the maximum log-likelihood, we use eq(8) and take partial derivative w.r.t $\mathbf{w}_i$, we get

$$\frac{\partial \mathcal{L}(\mathbf{w}_1 ... \mathbf{w}_K)}{\partial \mathbf{w}_i} = -\sum_n [\mathbf{x}_i - \frac{exp(\mathbf{w}_i^T \mathbf{x}_i)\mathbf{x}_i}{1 + \sum_{k=1}^{K-1} exp(\mathbf{w}_t^T \mathbf{x}_n)}]$$

$$= -\sum_n [1 - \frac{exp(\mathbf{w}_i^T \mathbf{x}_i)}{1 + \sum_{k=1}^{K-1} exp(\mathbf{w}_t^T \mathbf{x}_n)}]\mathbf{x}_i$$

$$= -\sum_n \big[1 - P(y = i|\mathbf{x}_i)\big]\mathbf{x}_i$$

$\therefore$ we can define the error as

$$e_i = 1 - P(y = i|\mathbf{x}_i)$$

let η be the step function, then we can write the update rule as

$$\mathbf{w}_{(i+1)} = \mathbf{w}_{(i)} - \eta \sum_n \big[1 - P(y = i|\mathbf{x}_i)\big]\mathbf{x}_i$$

Sol. 2.1 From the definition of $p(x_n, y_n)$ we can write the log-likelihood as

$$\mathcal{L}(D) = \sum_{n=1, y_n=1}^{N} log(p_1 \frac{1}{\sqrt{2\pi}\sigma_1} exp(-\frac{(x_n - \mu_1)^2}{2\sigma_1^2}))$$

$$+ \sum_{n=1, y_n=2}^{N} log(p_2 \frac{1}{\sqrt{2\pi}\sigma_2} exp(-\frac{(x_n - \mu_2)^2}{2\sigma_2^2}))$$

$$\mathcal{L}(D) = \sum_{n=1, y_n=1}^{N} log(p_1) - log(\sqrt{2\pi}\sigma_1) - \frac{(x_n - \mu_1)^2}{2\sigma_1^2}$$

$$+ \sum_{n=1, y_n=2}^{N} log(p_2) - log(\sqrt{2\pi}\sigma_2) - \frac{(x_n - \mu_2)^2}{2\sigma_2^2}$$

Now, we know that $p_1 + p_2 = 1$. Let, $N_1 =$ no. of samples where $y_n = 1$ and $N_2 =$ no. of samples where $y_n = 2$ we'll first find the estimate of p_1 that minimizes $-\mathcal{L}(D)$

$$\mathcal{L}(D) = \sum_{n=1, y_n=1}^{N} log(p_1) - log(\sqrt{2\pi}\sigma_1) - \frac{(x_n - \mu_1)^2}{2\sigma_1^2}$$

$$+ \sum_{n=1, y_n=2}^{N} log(1 - p_1) - log(\sqrt{2\pi}\sigma_2) - \frac{(x_n - \mu_2)^2}{2\sigma_2^2}$$

taking partial derivative w.r.t. p_1, we get

$$\frac{\partial \mathcal{L}(D)}{\partial p_1} = \sum_{n=1, y_n=1}^{N} \frac{1}{p_1} - \sum_{n=1, y_n=2}^{N} \frac{1}{1 - p_1}$$

from definition of N_1 and N_2, we get

$$\frac{\partial \mathcal{L}(D)}{\partial p_1} = 0 = \frac{N_1}{p_1} + \frac{N_2}{1 - p_1}$$

$$\hat{p_1} = \frac{N_1}{N_1 + N_2}$$

similarly, $\hat{p_2}$ will be

$$\hat{p_2} = \frac{N_2}{N_1 + N_2}$$

To, estimate μ_1, we take the partial derivative of $\mathcal{L}(D)$ w.r.t μ_1, we get

$$\frac{\partial \mathcal{L}(D)}{\partial \mu_1} = \sum_{n=1, y_n=1}^{N} (x_n - \mu_1) = 0$$

$$\hat{\mu_1} = \frac{1}{N_1} \sum_{n=1, y_n=1}^{N} x_n$$

similarly, estimate of μ_2 will be

$$\hat{\mu_2} = \frac{1}{N_2} \sum_{n=1, y_n=2}^{N} x_n$$

To, estimate σ_1, we take the partial derivative of $\mathcal{L}(D)$ w.r.t σ_1, we get

$$\frac{\partial \mathcal{L}(D)}{\partial \sigma_1} = \sum_{n=1, y_n=1}^{N} -\frac{1}{\sigma_1} + \frac{(x_n - \mu_1)^2}{\sigma_i^3} = 0$$

which gives us

$$\hat{\sigma_1^2} = \frac{\sum_{n=1, y_n=1}^{N} (x_n - \mu_1)^2}{N_1}$$

similarly, estimate of σ_2^2 will be

$$\hat{\sigma_2^2} = \frac{\sum_{n=1, y_n=2}^{N} (x_n - \mu_2)^2}{N_2}$$

Sol. 2.2 From Baye's formula we can write that

$$P(y = k|x) = \frac{P(x|y = k)\, P(y = k)}{\sum_k P(x|y = k)\, P(y = k)}$$

Now, since $P(y = 1) + P(y = 2) = 1$, then let $P(y = 1) = \pi$, $\therefore P(y = 2) = 1 - \pi$. We'll first find the probability $P(y = 1|x)$

$$\begin{aligned} P(y = 1|x) &= \frac{P(x|y = 1)\, P(y = 1)}{[P(x|y = 1)\, P(y = 1)] + [P(x|y = 2)\, P(y = 2)]} \\ &= \frac{\pi \mathcal{N}(\mu_1, \Sigma)}{\pi \mathcal{N}(\mu_1, \Sigma) + (1 - \pi)\pi \mathcal{N}(\mu_2, \Sigma)} \end{aligned}$$

$$= \frac{1}{1 + \frac{(1-\pi)\mathcal{N}(\mu_2,\Sigma)}{\pi\mathcal{N}(\mu_1,\Sigma)}}$$

Now,

$$\frac{(1-\pi)\mathcal{N}(\mu_2,\Sigma)}{\pi\mathcal{N}(\mu_1,\Sigma)} = exp(log(\frac{(1-\pi)\mathcal{N}(\mu_2,\Sigma)}{\pi\mathcal{N}(\mu_1,\Sigma)}))$$

Solving for $log(\frac{(1-\pi)\mathcal{N}(\mu_2,\Sigma)}{\pi\mathcal{N}(\mu_1,\Sigma)})$

$$log(\frac{(1-\pi)\mathcal{N}(\mu_2,\Sigma)}{\pi\mathcal{N}(\mu_1,\Sigma)}) =$$

$$= -log(\frac{\pi}{1-\pi}) + log(\frac{\mathcal{N}(\mu_2,\Sigma)}{\mathcal{N}(\mu_1,\Sigma)})$$

$$= -log(\frac{\pi}{1-\pi}) - \frac{1}{2}(x-\mu_2)^T\Sigma^{-1}(x-\mu_2) + \frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)$$

$$= -log(\frac{\pi}{1-\pi}) - \frac{1}{2}x^T\Sigma^{-1}x + \mu_2^T\Sigma^{-1}x - \frac{1}{2}\mu_2^T\Sigma^{-1}\mu_2 + \frac{1}{2}x^T\Sigma^{-1}x - \mu_1^T\Sigma^{-1}x + \frac{1}{2}\mu_1^T\Sigma^{-1}\mu_1$$

$$= (\mu_2-\mu_1)^T\Sigma^{-1}x - \frac{1}{2}\mu_2^T\Sigma^{-1}\mu_2 + \frac{1}{2}\mu_1^T\Sigma^{-1}\mu_1 - log(\frac{\pi}{1-\pi})$$

$$= -\boldsymbol{\theta}^T\mathbf{x} + b$$

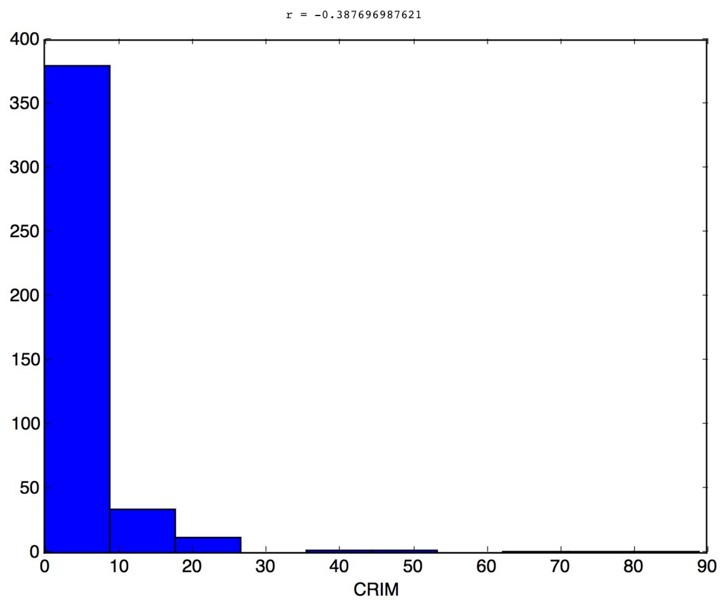
where,

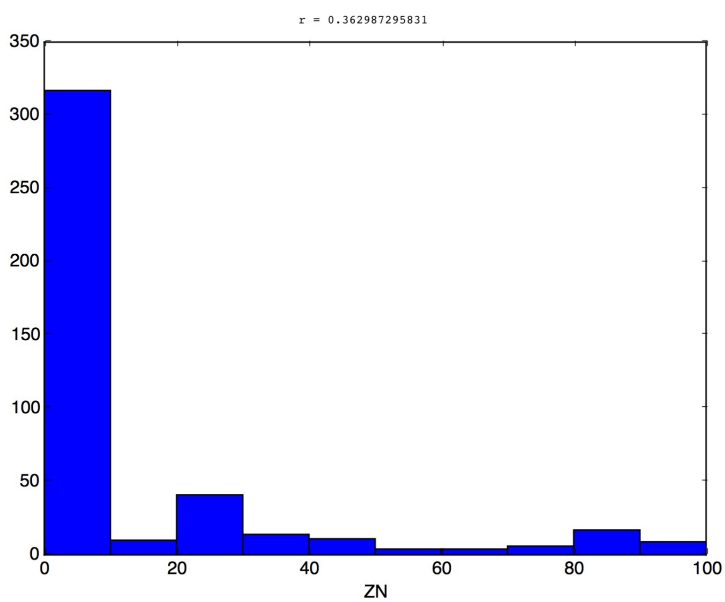
$$\theta = \Sigma^{-1}(\mu_1 - \mu_2)$$

and

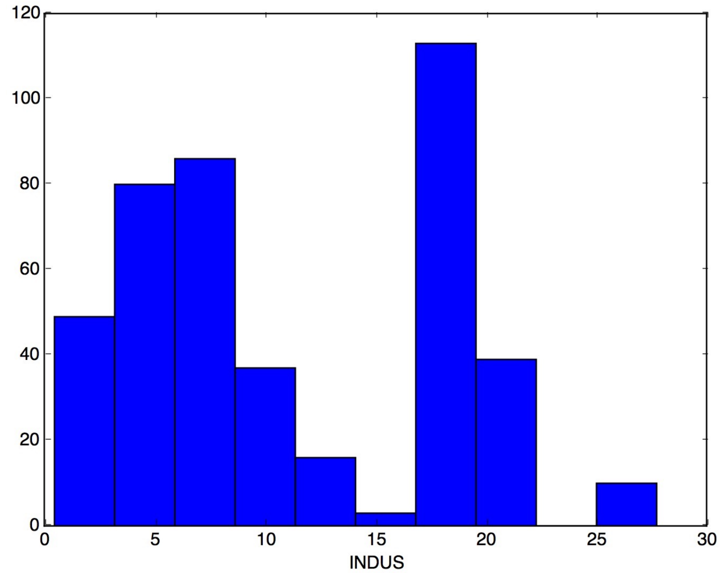
$$b = -\frac{1}{2}\mu_2^T\Sigma^{-1}\mu_2 + \frac{1}{2}\mu_1^T\Sigma^{-1}\mu_1 - log\frac{\pi}{1-\pi}$$

Sol. 3.1 Data Analysis

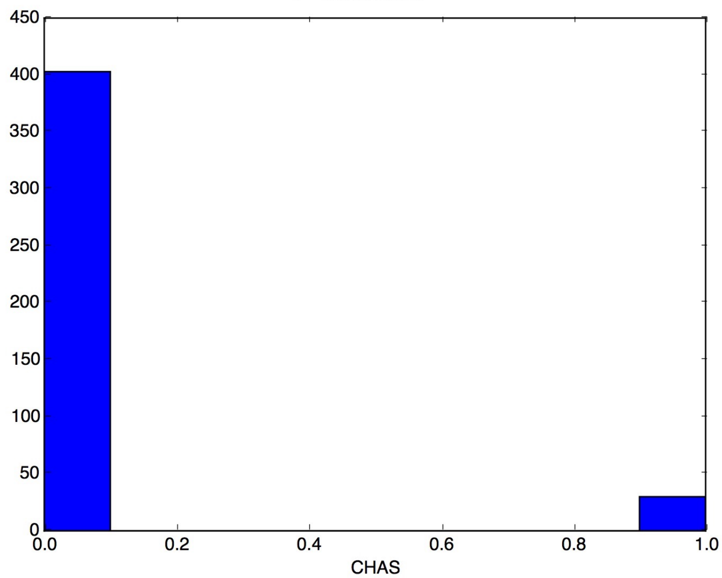

r = -0.387696987621
400
350
300
250
200
150
100
50
0
0
10
20
30
40
50
60
70
80
90
CRIM

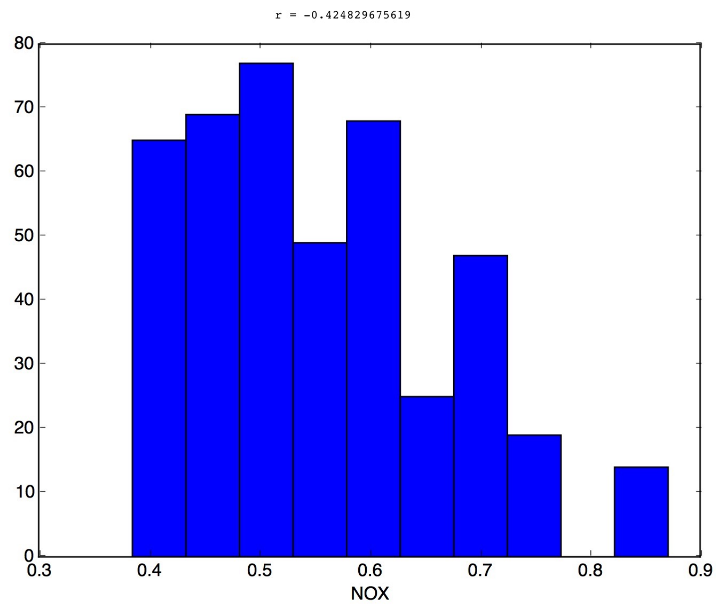

r = 0.362987295831
350
300
250
200
150
100
50
0
0
20
40
60
80
100
ZN

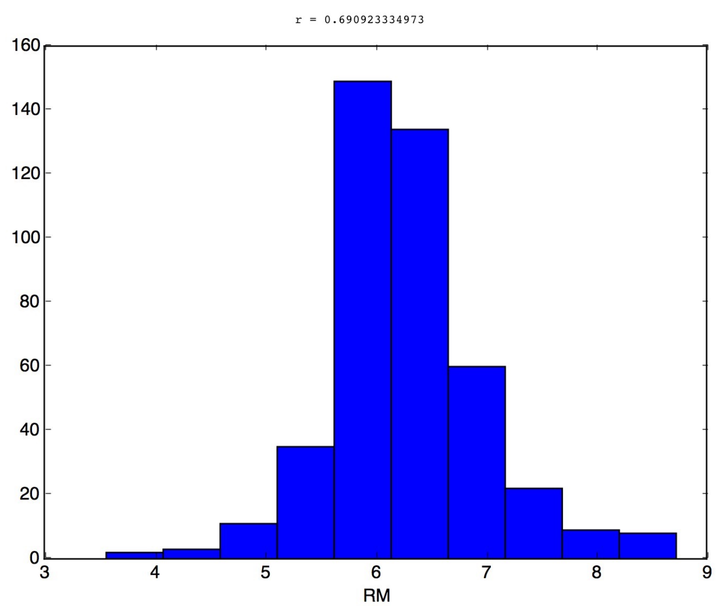
r = -0.483067421758

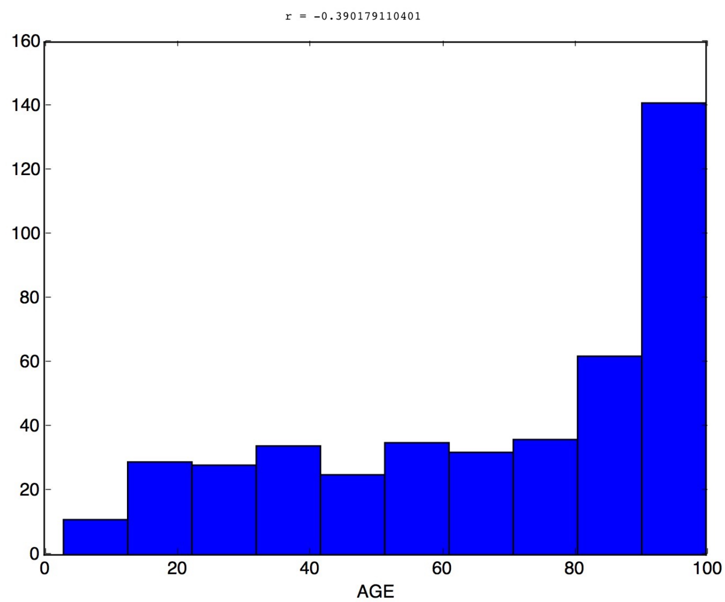


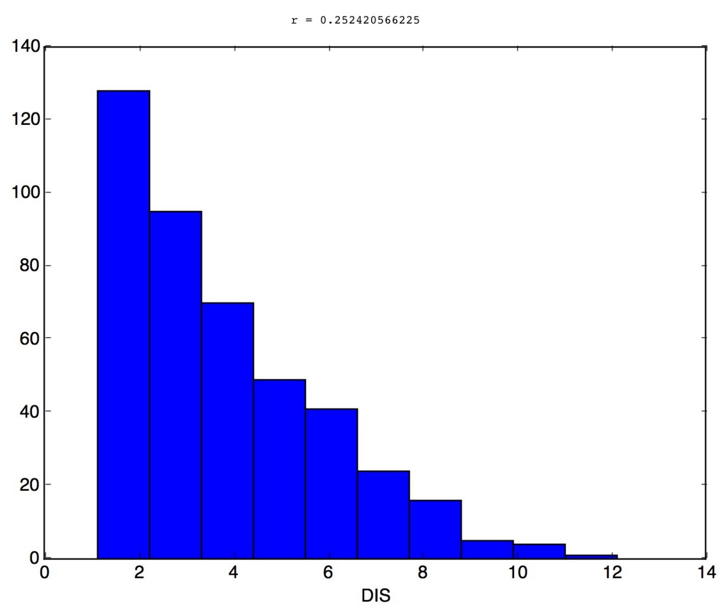
r = 0.203600144696

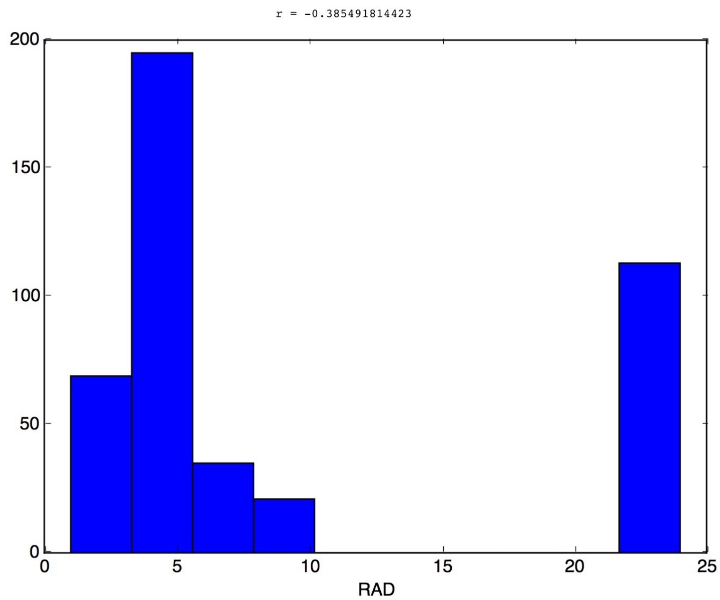


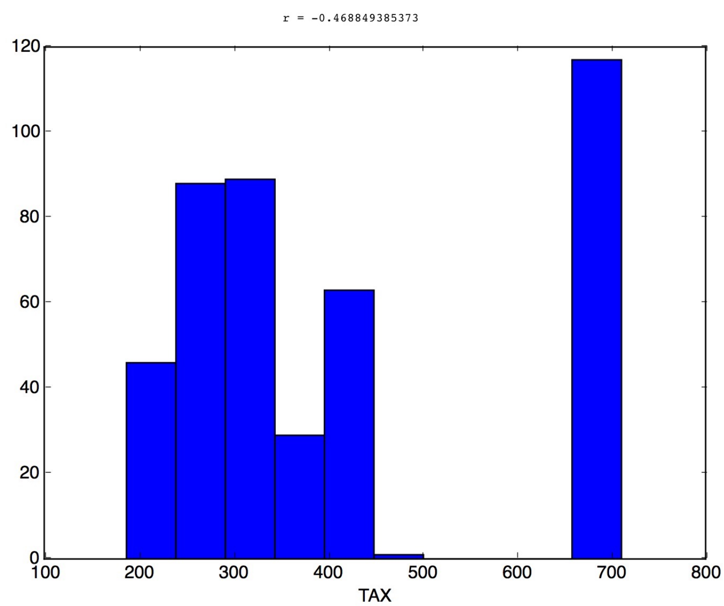

r = −0.424829675619
0
10
20
30
40
50
60
70
80
0.3
0.4
0.5
0.6
0.7
0.8
0.9
NOX


r = 0.690923334973
0
20
40
60
80
100
120
140
160
3
4
5
6
7
8
9
RM

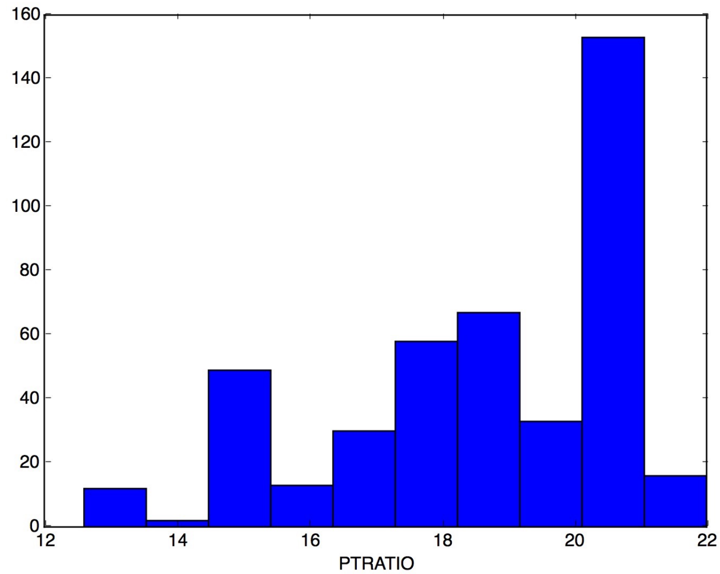

r = -0.390179110401
AGE


r = 0.252420566225
DIS

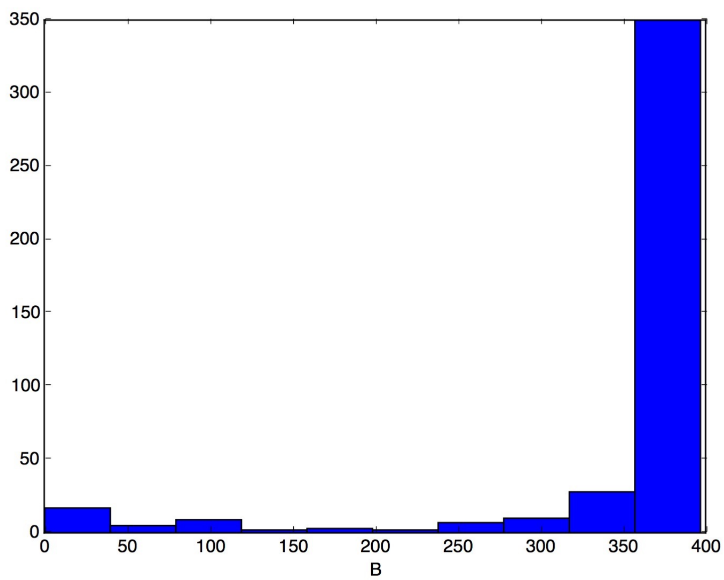

r = −0.385491814423
200
150
100
50
0
0
5
10
15
20
25
RAD

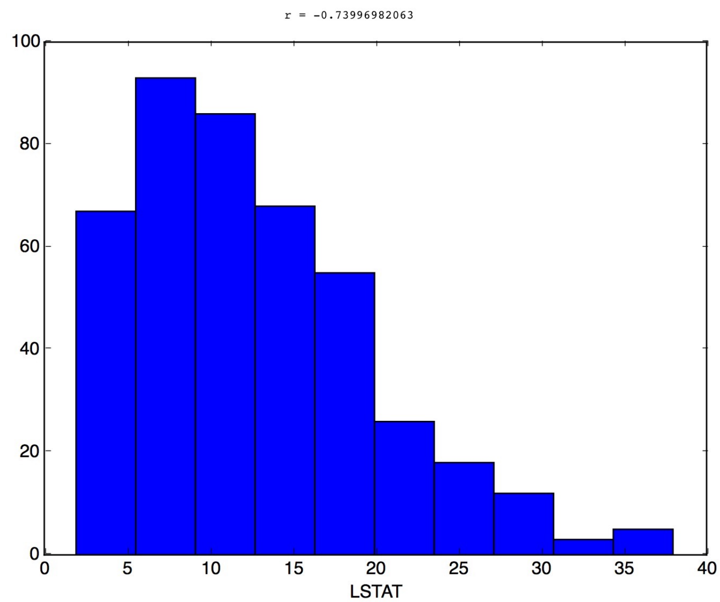

r = −0.468849385373
120
100
80
60
40
20
0
100
200
300
400
500
600
700
800
TAX

r = -0.505270756892



r = 0.343434137151





Sol. 3.2 The after applying Linear Regression to the training set, we get the results

Test Data	MSE
test_data	28.4644
training_data	20.9512

After applying Ridge regression for different λ we get the following results

λ	Test Data	MSE
0.01	test_data	28.4183
0.01	train_data	20.9501
0.1	test_data	28.4217
0.1	train_data	20.9502
1	test_data	28.4574
1	train_data	20.9539

λ	CVE
0.001	9.99383
0.01	9.99273
0.02	9.9915
0.1	9.98177
0.1	9.98177
1	9.8773
2	9.77169
3	9.67664
4	9.59175
5	9.51671
6	9.45125
7	9.39513
8	9.34814
9	9.31007
10	9.28075

As we see that the cross-validation error is minimum for $\lambda = 10$, therefore we choose $\lambda = 10$ for out MSE calculation. For **Test Data set we get MSE = 28.98456207** and for **Training Data set we get MSE = 21.28681485**.

Sol. 3.3.a First, we will calculate the Pearson's Coefficient for each attribute with target values and we get

Feature	abs(r)
CRIM	0.387697
ZN	0.362987
INDUS	0.483067
CHAS	0.2036
NOX	0.42483
RM	0.690923
AGE	0.390179
DIS	0.252421
RAD	0.385492
TAX	0.468849
PTRATIO	0.505271
B	0.343434
LSTAT	0.73997

We see that the attributes with highest Pearson's Coefficients are INDUS, PTRATIO, RM, LSTAT.

Now, applying **Linear Regression**

Test Data	MSE
test_data	31.4962
train_data	26.4066

Now, applying Ridge Regression for different λ we get

λ	Test Data	MSE
0.01	test_data	31.496
0.01	train_data	26.4066
0.1	test_data	31.4944
0.1	train_data	26.4066
1	test_data	31.4806
1	train_data	26.4094

For K-Fold Ridge Regression we get the following values of CVE

λ	CVE
0.001	8.3003
0.01	8.2992
0.1	8.2885
1	8.1855
2	8.0791
3	7.9811
4	7.8915
5	7.8099
6	7.7363
7	7.67
8	7.6125
9	7.562
10	7.5189

Choosing $\lambda = 10$, we get the MSE as

λ	Test Data	MSE
10	test_data	31.5937
10	train_data	26.6775

Sol. 3.3.b From the previous exercise we know that the feature with the highest correlation coefficient with the target is LSTAT.

Now, calculating residue and correlation coefficient of the rest of the attributes with the residue we get

Feature	abs(r(residue, attr_vals)
CRIM	0.426588158091
ZN	0.398133315751
INDUS	0.537842703653
CHAS	0.175073939283
NOX	0.491958859016
RM	0.702473672384
AGE	0.469369575525
DIS	0.331853691887
RAD	0.436013562838
TAX	0.514184631153
PTRATIO	0.496710217811
B	0.374589793897

We get RM as the next feature with highest correlation coefficient.

After updating the residue, we get the correlation coeff. as

Feature	abs(r(residue, attr_vals)
CRIM	0.129554112358
ZN	0.0461901567406
INDUS	0.0561934824677
CHAS	0.249301273706
NOX	0.0109129511978
AGE	0.0159396362859
DIS	0.134713549718
RAD	0.087477994304
TAX	0.13681944445
PTRATIO	0.297604744231
B	0.156620202695

We get PTRATIO as the next feature with highest correlation coefficient.

Again,

Feature	abs(r(residue, attr_vals)
CRIM	0.0889293951571
ZN	0.0323063735902
INDUS	0.00214795182009
CHAS	0.2195949638
NOX	0.0198942311859
AGE	0.0435891823287
DIS	0.170389023828
RAD	0.0210281033187
TAX	0.0440426778355
B	0.144133379832

Finally, we select the feature CHAS.

So, finally our selected features (in-order) are LSTAT, RM, PTRATIO, CHAS.

Now, calculating MSE from previously fitted data, we get

Input Data	MSE
test_data	34.5988
train_data	25.106

Brute Force: The best combination is B, RM, LSTAT, PTRATIO with $MSE = 30.09226$ with test data set.

Sol. 3.4 The result after calculating the MSE using Linear Regression with the augmented data is

Input Data	MSE
test_data	14.5553
train_data	5.05978