Stats 315a: Statistical Learning
Problem Set 1

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Problem 1

(a)

MATLAB is used for this homework instead of R; I already asked professor if we can use MATLAB, and he said it's okay. My teammates are Jin Chen, and Wenqiong Guo. Basically, the code will generate a training sample of size 100 for each class, as well as a test sample of 5,000 per class. Then, we use linear regression and K-nearest neighbour (trained with training sample) to do the classification on test sample.

Problem 2 (ESL 2.4)

The squared distance from any sample point to the origin has a χ^2_p distribution with mean p; therefore, since a prediction point x_0 is drawn from this distribution, it will have a expected squared distance p from the origin.

Because $z_i = a^T x_i$, and a is independent from x_i, we can conclude that $z_i \sim N$, normal distribution. Now, let's calculate the expectation value of z_i. We know that for a p dimensional vector a

$$E(z) = E(a^T x) = a^T E(x) = 0 \tag{1}$$

The co-variant can be given by

$$Cov(a^T x) = a^T a = 1 \tag{2}$$

As a result, we get $z_i \sim N(0, 1)$, and the expected squared distance will be $E(z^2) = 1$.

Problem 3 (ESL 2.7)

(a)

For linear regression, the exact solution can be given by

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \tag{3}$$

therefore, the predicted value for a given input will be

$$\hat{f}(x_0) = x_0^T \hat{\beta} \tag{4}$$

Compare with the desired form of the estimator,

$$\hat{f}(x_0) = \sum_{i=1}^{N} l_i(x_0; \mathbf{X}) y_i \tag{5}$$

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it's found that

$$l_i(x_0;\mathbf{X}) = x_0^T(\mathbf{X}^T\mathbf{X})^{-1}x_i^T \tag{6}$$

Therefore, linear regression is the member of this class of estimators.

For k-nearest-neighbour regression, the estimator is

$$\hat{f}(x_0) = \frac{1}{k}\sum_{x_i\in N_k(x_0)} y_i \tag{7}$$

where $N_k(x_0)$ is the neighbourhood of x_0 defined by the k closest points x_i in the training sample. Now, compare with the desired estimator form, it's found that

$$l_i(x_0;\mathbf{X}) = \begin{cases} 0 & x_i \notin N_k(x_0) \\ \frac{1}{k} & x_i \in N_k(x_0) \end{cases} \tag{8}$$

Therefore, k-nearest-neighbour regression is the member of this class of estimators.

(b)

Using Eq. (2.25) in the textbook, the conditional mean squared error can be rewritten as

$$\begin{aligned} E_{\mathbf{y}|\mathbf{x}}(f(x_0)-\hat{f}(x_0))^2 &= E_{\mathbf{y}|\mathbf{x}}(\hat{f}(x_0)-E_{\mathbf{y}|\mathbf{x}}\hat{f}(x_0))^2 + (E_{\mathbf{y}|\mathbf{x}}\hat{f}(x_0)-f(x_0))^2 \\ &= Var_{\mathbf{y}|\mathbf{x}}(\hat{f}(x_0)) + Bias^2_{\mathbf{y}|\mathbf{x}}(\hat{f}(x_0)) \end{aligned} \tag{9}$$

Substitute Eq. (5) into Eq. (9), we have

$$\begin{aligned} Var_{\mathbf{y}|\mathbf{x}}(\hat{f}(x_0)) &= Var_{\mathbf{y}|\mathbf{x}}\left(\sum_{i=1}^N l_i(x_0;\mathbf{X})y_i\right) \\ &= \sum_{i=1}^N l_i(x_0;\mathbf{X})Var_{\mathbf{y}|\mathbf{x}}(y_i) \\ &= \sum_{i=1}^N l_i(x_0;\mathbf{X})\sigma^2 \end{aligned} \tag{10}$$

and

$$\begin{aligned} Bias_{\mathbf{y}|\mathbf{x}}(\hat{f}(x_0)) &= Bias_{\mathbf{y}|\mathbf{x}}\left(\sum_{i=1}^N l_i(x_0;\mathbf{X})y_i\right) \\ &= E_{\mathbf{y}|\mathbf{x}}\sum_{i=1}^N l_i(x_0;\mathbf{X})y_i - f(x_0) \\ &= \sum_{i=1}^N l_i(x_0;\mathbf{X})f(x_i) - f(x_0) \end{aligned} \tag{11}$$

(c)

For the unconditional mean squared error, we have

$$E_{\mathbf{y},\mathbf{x}}(f(x_0)-\hat{f}(x_0))^2 = Var_{\mathbf{y},\mathbf{x}}(\hat{f}(x_0)) + Bias^2_{\mathbf{y},\mathbf{x}}(\hat{f}(x_0)) \tag{12}$$

Therefore, the variance will be

$$
\begin{aligned}
Var_{\mathbf{y},\mathbf{x}}(\hat{f}(x_0)) &= E_{\mathbf{y},\mathbf{x}}(\hat{f}(x_0) - E_{\mathbf{y},\mathbf{x}}\hat{f}(x_0))^2 \\
&= E_x E_{\mathbf{y}|\mathbf{x}}(\hat{f}(x_0) - E_x E_{\mathbf{y}|\mathbf{x}}\hat{f}(x_0))^2 \\
&= E_x E_{\mathbf{y}|\mathbf{x}} \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) y_i - E_x \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) \right) \right)^2 \\
&= E_x \left[E_{\mathbf{y}|\mathbf{x}} \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) y_i \right)^2 - 2E_{\mathbf{y}|\mathbf{x}} \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) y_i \right) \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) \right) \right. \\
&\quad \left. + E_x \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) \right) \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) \right) \right] \\
&= E_x E_{y|x} \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) y_i - \sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) \right)^2 + E_x \left(E_x(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i)) - \sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) \right)^2 \\
&= E_x Var_{y|x}(\hat{f}(x_0)) + Var_x \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) \right) \\
&= E_x \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) \sigma^2 \right) + Var_x \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) \right)
\end{aligned} \tag{13}
$$

The Bias will be

$$
\begin{aligned}
Bias_{y,x}(\hat{f}(x_0) &= E_{\mathbf{y},\mathbf{x}}\hat{f}(x_0) - E_x f(x_0) \\
&= E_x(E_{y|x}\hat{f}(x_0) - f(x_0)) \\
&= E_x(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) - f(x_0)) \\
&= E_x Bias_{y|x}(\hat{f}(x_0))
\end{aligned} \tag{14}
$$

(d)

Compare the result in (b), and (c), we find that the unconditional squared bias is the expected value respected to X of conditional squared bias. $E_x Bias_{y|x}(\hat{f}(x_0)) = Bias_{x,y}(\hat{f}(x_0))$

The unconditional variance will be the expected value respected to X of conditional variance with extra variance term.

$$
Var_{y,x}(\hat{f}(x_0)) = E_x Var_{y|x}(\hat{f}(x_0)) + Var_x \left(\sum_{i=1}^{N} l_i(x_0;\mathbf{X}) f(x_i) \right)
$$

Problem 4

(a)

Let $\hat{\beta}$ be the least squares estimation over a set of training data $(x_1, y_1), ..., (x_n, y_n)$ using

$$
R_{tr}(\hat{\beta}) = \frac{1}{N} \sum_{1}^{N} (y_i - \hat{\beta}^T x_i)^2 \tag{15}
$$

, while $\tilde{\beta}$ is the least squares estimation over another set of training data $(\tilde{x}_1, \tilde{y}_1), ..., (\tilde{x}_n, \tilde{y}_n)$ drawn at random from the same population as the first training data using

$$R_{te}(\tilde{\beta}) = \frac{1}{M}\sum_{1}^{M}(\tilde{y}_i - \tilde{\beta}^T\tilde{x}_i)^2 \tag{16}$$

Since both training data are drawn from the same population, if they are randomly picked up, we can say

$$E[R_{tr}(\hat{\beta})] = E[R_{te}(\tilde{\beta})] \tag{17}$$

, which can be formally proven by

$$\begin{aligned}
E[R_{tr}(\hat{\beta})] &= E[\frac{1}{N}\sum_{1}^{N}(y_i - \hat{\beta}^T x_i)^2] \\
&= \frac{1}{N}E[\sum_{1}^{N}(y_i - \hat{\beta}^T x_i)^2] \\
&= \frac{1}{M}E[\sum_{1}^{M}(y_i - \hat{\beta}^T x_i)^2] \\
&= \frac{1}{M}E[\sum_{1}^{M}(\tilde{y}_i - \tilde{\beta}^T \tilde{x}_i)^2] \\
&= E[R_{te}(\tilde{\beta})]
\end{aligned} \tag{18}$$

Also, $\tilde{\beta}$ is the least squares estimation over $(\tilde{x}_1, \tilde{y}_1), ..., (\tilde{x}_n, \tilde{y}_n)$, so

$$\begin{gathered}
\frac{1}{M}\sum_{1}^{M}(\tilde{y}_i - \tilde{\beta}^T\tilde{x}_i)^2 \leq \frac{1}{M}\sum_{1}^{M}(\tilde{y}_i - \hat{\beta}^T\tilde{x}_i)^2 \\
\Rightarrow R_{te}(\tilde{\beta}) \leq R_{te}(\hat{\beta}) \\
\therefore E[R_{te}(\tilde{\beta})] \leq E[R_{te}(\hat{\beta})]
\end{gathered} \tag{19}$$

With Eq. (17) and Eq. (20), we get

$$\therefore E[R_{tr}(\hat{\beta})] \leq E[R_{te}(\hat{\beta})] \tag{20}$$

Problem 5 (ESL 3.2)

Method 1

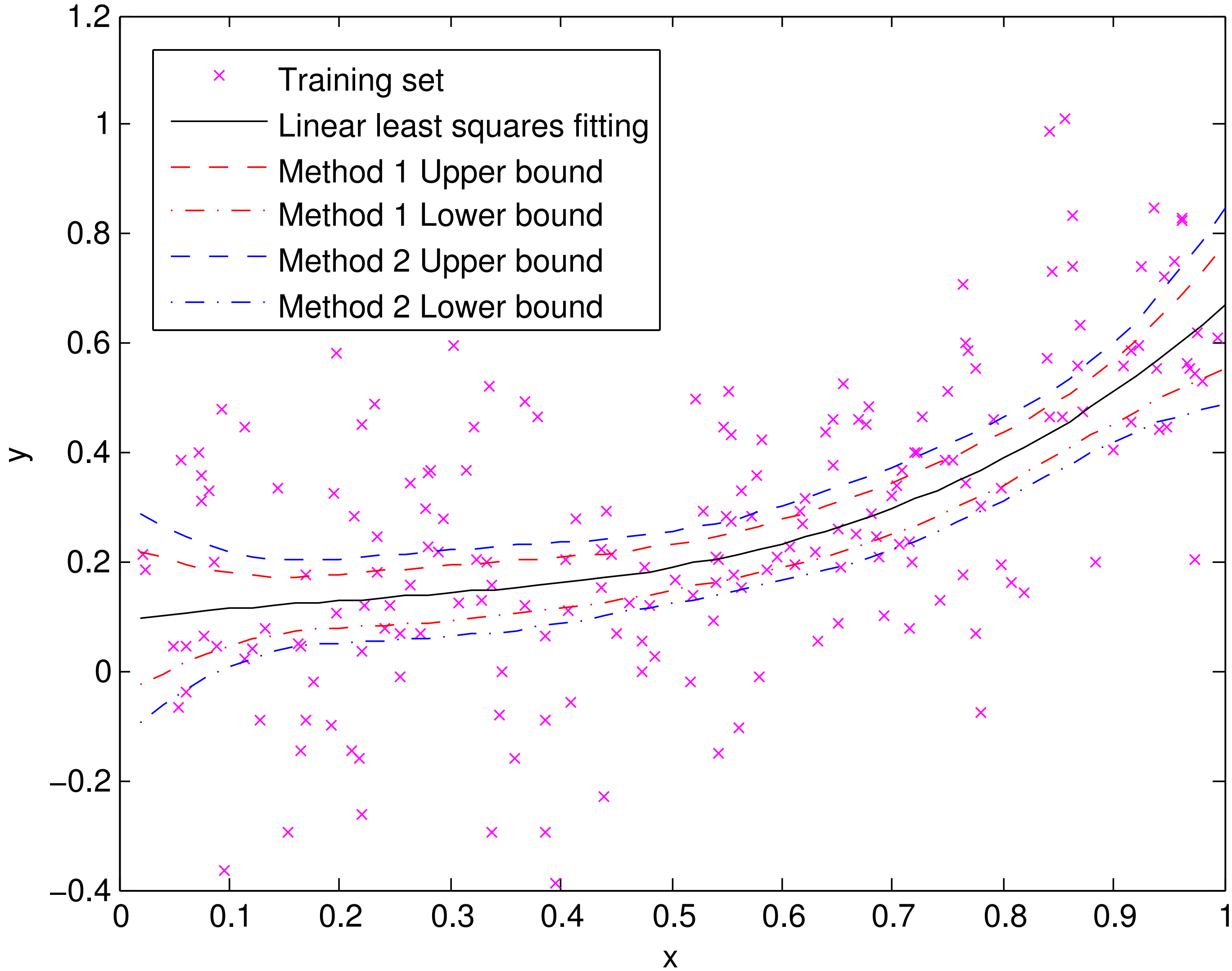
For each point x_0, forming a 95% confidence interval implies that we need to know the confidence interval for $\hat{\beta}$, and using linear function $a^T\hat{\beta}$ to construct the 95% confidence band. Since $\hat{\beta} \sim N(\beta, (\mathbf{X}^T\mathbf{X})^{-1}\sigma^2))$, we can obtain the $1 - 2\alpha$ confidence interval for β as

$$\left(\hat{\beta} - z^{(1-\alpha)}\sqrt{(\mathbf{X}^T\mathbf{X})^{-1}}\sigma, \hat{\beta} + z^{(1-\alpha)}\sqrt{(\mathbf{X}^T\mathbf{X})^{-1}}\sigma\right) \tag{21}$$

where $z^{(1-\alpha)}$ is the $1 - \alpha$ percentile of the normal distribution. (Note that if we replace the α to known value $\hat{\alpha}$, the distribution will become t distribution, and it normally become negligible as the sample increases; therefore, we typically use the normal quartiles.) As a result, the confidence interval from each input point x_0 will be

$$\left(a^T\hat{\beta} - z^{(1-\alpha)}\sqrt{a^T(\mathbf{X}^T\mathbf{X})^{-1}a}\sigma, \hat{\beta} + z^{(1-\alpha)}\sqrt{a^T(\mathbf{X}^T\mathbf{X})^{-1}a}\sigma\right) \tag{22}$$

where $y_0 = a^T\hat{\beta} = \sum_{j=0}^{3}\hat{\beta}_j x_0^j$. For 95%, α is 0.025.



Method 2

From Eq. (3.15) from textbook, the confidence set for β can be given by

$$C_\beta = \left\{\beta | (\hat{\beta} - \beta)^T \mathbf{X}^T \mathbf{X} (\hat{\beta} - \beta) \leq \sigma^2 \chi_4^{2^{(1-2\alpha)}} \right\} \tag{23}$$

Therefore, the 95%confidence band from each input point x_0 will be

$$\left(a^T \hat{\beta} - \sqrt{a^T (\mathbf{X}^T \mathbf{X})^{-1} a \chi_4^{2^{(1-2\alpha)}}} \sigma, \hat{\beta} + \sqrt{a^T (\mathbf{X}^T \mathbf{X})^{-1} a \chi_4^{2^{(1-2\alpha)}}} \sigma \right) \tag{24}$$

where α is 0.025, and $\chi_l^{2^{(1-\alpha)}}$ is the chi-squared distribution on l degrees of freedom. (Similar to the discussion in method 1, if we don't know the α, but we know $\hat{\alpha}$ which can be calculated from training set, the chi-squared distribution will be replaced by $F_{p_1 - p_0, M - p_1 - 1}$ distribution.)

According to simulation result shown in the figure, it's observed that Method 2 has wider confidence band.

```
% HW1, Q5 (ESL3.2)
% Dong-Bang Tsai
clear all;

N = 200;             % N of training set
```

```
alpha = (1-0.95)/2; % 95% confidence interval
sigma = 0.2;        % Gaussian random noise

% The training set
beta = randn(4,1);
x_points = rand(N,1);
X = [ones(N,1),x_points,x_points.^2,x_points.^3];
y = X*beta + normrnd(0,sigma,N,1);
% Learned hypothesis
hat_beta = ((X'*X))\X'*y;

% Plot array
N_plot = 50;
x_plot_points = [1/N_plot:1/N_plot:1]';
a = [ones(N_plot,1),x_plot_points,x_plot_points.^2,x_plot_points.^3];

% Compute the confidence band
hat_sigma = sqrt( 1/(N-4)*sum( (X*beta-y).^2 ) );
delta1 = norminv(1-alpha)*sqrt(diag(a*((X'*X)\a')))*hat_sigma;
delta2 = sqrt(diag(a*((X'*X)\a'))*chi2inv(1-2*alpha,4))*hat_sigma;

plot(x_points,y(:,1),'mx');
hold on;
plot(x_plot_points,a*beta,'k-');
plot(x_plot_points,a*beta + delta1,'r--');
plot(x_plot_points,a*beta - delta1,'r-.');
plot(x_plot_points,a*beta + delta2,'b--');
plot(x_plot_points,a*beta - delta2,'b-.');
xlabel('x'); ylabel('y');
legend('Training set','Linear least squares fitting','Method 1 Upper bound', 'Method 1 Lower bound', 'Metho
hold off;
```

Problem 6

(a)

When $p \gg N$, the columns of X are not lineraly independent which implies X isn't of full rank. Therefore, the solution of least squares given by $\hat{\beta} = (X^TX)^{-1}X^Ty$ will not be uniquely defined since X^TX is singular, and the residuals of the solution will be 0. The solution is unique only if X has a full column rank, and X^TX is positive definite.

(b)

In the ridge regression approach, the equation we are trying to solve is

$$(X^TX + \lambda I)\beta = X^Ty \tag{25}$$

The solution can be given by $\hat{\beta}_\lambda = (X^TX + \lambda I)^{-1}X^Ty$. We add positive constant to diagonal of X^TX; therefore, $(X^TX + \lambda I)^{-1}$ is non-singular, even if X^TX is not of full rank. As a result, the solution always exists, and is unique.

(c)

As we show that the solution of ridge regression is $\hat{\beta}_\lambda = (X^TX + \lambda I)^{-1}X^Ty$, if we try to get the λ smaller, it will eventually become least squares solution which is $\hat{\beta}_\lambda = (X^TX)^{-1}X^Ty$.

(d)

Using $X = UDV^T$

$$
\begin{aligned}
\hat{\beta}_\lambda &= (X^T X + \lambda I)^{-1} X^T y \\
&= \left(V D^T U^T U D V^T + \lambda I\right) V D U^T y \\
&= V \left(D^2 + \lambda I\right) V^T D U^T y \\
&= V \left(D^2 + \lambda I\right) D U^T y
\end{aligned}
\tag{26}
$$