COMPREHENSIVE WRITTEN EXAMINATION, PAPER III FRIDAY AUGUST 13, 2021 9:00 A.M.–1:00 P.M. STOR 664 Questions (100 points in total)

1. Consider the quadratic regression problem

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \epsilon_i, \ i = 1, \dots, n$$
 (1)

where β_0 , β_1 and β_2 are unknown parameters and $\epsilon_i \sim N[0, \sigma^2]$ are independent errors with common unknown variance σ^2 . Assume $\sum x_i = \sum x_i^3 = 0$.

(a) Show that the least squares estimator of β_0 is

$$\hat{\beta}_0 = \frac{\sum y_i \sum x_i^4 - \sum x_i^2 y_i \sum x_i^2}{\Delta}$$
(2)

where $\Delta = n \sum x_i^4 - (\sum x_i^2)^2$, and derive similar expressions for $\hat{\beta}_1$ and $\hat{\beta}_2$. [12 points] (b) With \bar{y} the usual sample mean, show that

$$\hat{\beta}_0 - \bar{y} = -\frac{\hat{\beta}_2 \sum x_i^2}{n}.$$
(3)

[6 points]

(c) Suppose we are interested in testing H_0 : $\beta_1 = \beta_2 = 0$ against the alternative H_1 where β_0 , β_1 and β_2 are all unrestricted. In standard linear models notation, let SSE_0 , SSE_1 be the error (residual) sums of squares under H_0 and H_1 respectively. Show that

$$SSE_0 - SSE_1 = C_1 \hat{\beta}_1^2 + C_2 \hat{\beta}_2^2 \tag{4}$$

and find explicit expressions for the constants C_1 and C_2 (they are functions of x_1, \ldots, x_n but not of y_1, \ldots, y_n). [10 points]

- (d) Using the formulas in parts (a), (b) and (c), write down the F test for testing H₀ against H₁. Your answer should include an explicit formula for the F statistic, a statement of its distribution when H₀ is true, and a formula for calculating the critical value of the test statistic for a significance test of prescribed level α. [You may express your answer in terms of the R function qf(p,m,n) for the p-quantile of an F_{m,n} distribution.] [10 points]
- (e) Show how to calculate the power of this test when β_1 and β_2 take given non-zero values. [Your answer may be expressed in terms of the R function pf(c,m,n,ncp=lambda) where c, m, n are the values of the F statistic and its degrees of freedom, and lambda (λ) is the noncentrality parameter; you should give explicit formulas for c, m, n and λ but you are not expected to evaluate any of these terms numerically. Note also that your formulas will depend on x_1, \ldots, x_n and σ^2 as well as β_1 and β_2 .] [12 points]

Question 2 on the next page

2. The Environmental Protection Agency (EPA) is conducting a study on the distribution of particulate matter (PM), a common air pollutant regulated by the EPA. They set up a network of 16 monitors to measure the long-term average atmospheric concentration of PM. Because not all the monitors are in action at the same times, there are different numbers of readings per monitor. Figure 1 shows a map of the monitor locations, where the numbers indicate the number of observations at each monitor. In total, there are 117 observations.

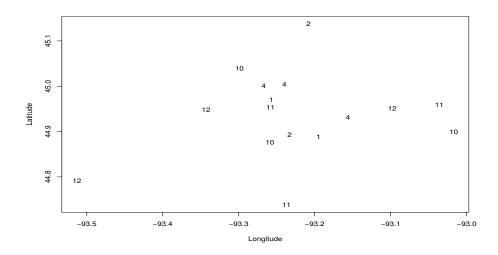


Figure 1. Map of monitor sites. The numbers indicate the number of observations at each monitor.

Based on these 117 observations and assuming the standard assumptions for a linear model, the EPA's statisticians have fitted the following five models:

- M0: Common mean for each monitor
- M1: Each monitor has a different mean with no predetermined relationship (unbalanced one-way ANOVA experiment)
- M2: The mean at each monitor is given by a linear function of latitude and longitude
- M3: The mean at each monitor is given by a quadratic function of latitude and longitude
- M4: The mean at each monitor is given by a cubic function of latitude and longitude

A table that shows the error sum of squares (ESS) for each model, the corresponding degrees of freedom (DF), the F statistic against the null model M0, and the associated p-value, is as follows:

Model	ESS	DF	F statistic	p-value
M0	90.983	116		
M1	28.369	101	???	2.6e-19
M2	84.489	114	4.381	???
M3	51.880	???	16.733	2.7e-12
M4	???	107	12.89	1e-13

The table entries marked by ??? are left blank for you to fill in (note that the F statistic and p-value in the first line are not defined because you cannot test a model against itself).

(a) Fill in the four blanks in this table. [You are not expected to provide numerical answers, but state explicitly the expressions that must be evaluated. For the p-value, your answer will be expressed as a tail probability of an F distribution.] [20 points]

For the model M4 (fitted in R by a command of the form $m4=lm(y\sim X,...)$), the command plot(m4) produces the plot in Figure 2. In addition, R produces the following output (the three-digit numbers represent the order of observations in the original dataset of which this is a subset):

> sort(rstandard(m4))									
112 224 222	219	116 168		121 154	161 141				
-2.935651346 -2.066516118 -2.009799803									
177 119 214	172	225 181		201 227	180 173				
-1.320739667 -1.312233868 -1.233646507			4 -1.037364310 -0.992198						
188 208 134	152	206 148		129 185	191 136				
-0.802464401 -0.797691097 -0.777072841 160 125 190		0889 -0.687459241 157 205		312 -0.525535117 -0 146 145	.512747757 -0.503267642 169 183				
-0.502645595 -0.495715084 -0.491301018			-0.368493577 -0.306625		.253398161 -0.241058072				
159 124 143	166	184 142		187 209	165 176				
-0.227490147 -0.205912242 -0.198733956					.063645971 -0.061282298				
216 175 113	167	156 217		202 194	195 147				
-0.003369503 0.008857137 0.025148754				972 0.116349036 0	.131846108 0.150940531				
130 155 115	158	226 117	7 170	174 204	137 197				
0.164323420 0.180745577 0.207236818	0.231765655 0.27137	0.271700427	0.282883962 0.297902	541 0.331812297 0	.333930686 0.338864088				
211 123 182	200	193 135	5 186	139 140	212 215				
0.347091705 0.382976906 0.439042147	0.440691124 0.46333				.540600650 0.601413973				
178 198 171	189	196 150		213 133	218 207				
0.604528526 0.611224134 0.621240772					.774530398 0.824451396				
132 199 153	122	162 138		114 210	120 221				
0.917177569 0.985922834 1.042116845	1.091438824 1.09494			576 1.360671980 1	.377898281 1.852082462				
220 192 118	151	128 111							
1.863846165 1.899568158 1.970913013	1.975139274 2.13996	3451 2.423544043	3 2.556352478						
> sort(rstudent(m4)) 112 224 222	219	116 168	3 149	121 154	161 141				
-3.047191105 -2.099153120 -2.039247688					.458549726 -1.415723952				
177 119 214	172	225 181		201 227	180 173				
-1.325401483 -1.316725586 -1.236694654					.868367892 -0.855569297				
188 208 134		206 148		129 185	191 136				
-0.801120060 -0.796326158 -0.775624807					.510974260 -0.501504308				
160 125 190	163	157 205	5 164	146 145	169 183				
-0.500882972 -0.493960755 -0.489552321	-0.392009939 -0.39185	3337 -0.376334114	4 -0.367000546 -0.305323	528 -0.280670099 -0	.252286988 -0.239994164				
159 124 143	166	184 142		187 209	165 176				
-0.226479390 -0.204988395 -0.197839629	-0.185526855 -0.15080				.063349061 -0.060996330				
216 175 113	167	156 217		202 194	195 147				
-0.003353721 0.008815655 0.025031035	0.028152914 0.04597				.131239220 0.150249542				
130 155 115	158	226 117		174 204	137 197				
0.163574391 0.179926459 0.206307556	0.230738020 0.27019	1822 0.270521153 193 135			.332539922 0.337458016 212 215				
211 120 102	200	100 100		100 110	212 210				
0.345660621 0.381444618 0.437379874 178 198 171	0.439025590 0.46162 189	3852 0.495571917 196 150		127 0.525738888 0 213 133	.538804871 0.599611340 218 207				
0.602727172 0.609426090 0.619449123	0.668279934 0.66905				.773072770 0.823208668				
132 199 153	122	162 138		114 0.702334300 0	120 221				
0.916491385 0.985792848 1.042539885					.383776172 1.873685530				
220 192 118	151	128 111							
1.885984493 1.923380018 1.998289515	2.002736439 2.17703	3564 2.481255588	3 2.625827182						
> sort(hatvalues(m4))									
122 132 143	156 167	179 190	199 207	216 22	3 111 169				
0.04100220 0.04100220 0.04100220 0.041			0.04100220 0.04100220 0						
181 141 154	165 177	126 136	149 161	173 18					
0.05336682 0.05778113 0.05778113 0.057									
211 218 225 0.05858191 0.05858191 0.05858191 0.058	116 128	138 151	118 121 0.07231535 0.08091843 0	131 14					
178 189 198 0.08091843 0.08091843 0.08091843 0.080	206 112 91843 0 08091843 0 082	114 124 3334 0.08273334	134 147 0 08273334 0 08273334 0	159 17 08273334 0 0827333					
201 209 217	224 119	129 139	152 163	175 18					
	73334 0.08332363 0.083			.08332363 0.0833236					
213 220 227	117 127	137 150	162 174	186 19					
0.08332363 0.08332363 0.08332363 0.086			0.08603352 0.08603352 0						
226 145 157	168 180	120 130	140 153	164 17	6 188 197				
0.08603352 0.08876747 0.08876747 0.088	76747 0.08876747 0.090	34161 0.09084161	0.09084161 0.09084161 0	.09084161 0.0908416	1 0.09084161 0.09084161				
205 215 222	144 113	123 133	146 158	170 18					
0.09084161 0.09084161 0.09084161 0.094									
208 125 135	148 160	172 184	193 202	210 11					
0.09856016 0.09980983 0.09980983 0.099	80983 0.09980983 0.099	0.09980983	0.09980983 0.09980983 0	.09980983 0.0998098	3 0.49731930 0.49731930				

> sort(cooks.distance(m4))										
216	175	167	113	156	165	203	176	209	217	187
4.854241e-08	7.130810e-07	3.420668e-06	6.915087e-06	9.122314e-06	2.484140e-05	3.595139e-05	3.752454e-05	4.284908e-05	4.866786e-05	8.003438e-05
194	202	144	195	143	142	147	184	130	155	166
8.423771e-05	1.130355e-04	1.257693e-04	1.636334e-04	1.688627e-04	1.919788e-04	2.054928e-04	2.544851e-04	2.698014e-04	2.876264e-04	3.058045e-04
169	124	159	115	183	158	226	117	211	145	174
3.619900e-04	3.824276e-04	4.667777e-04	4.761819e-04	5.241170e-04	5.873038e-04	6.932188e-04	6.948932e-04	7.496688e-04	7.740557e-04	8.353839e-04
170	204	146	190	137	197	164	163	205	157	136
8.749461e-04	1.000777e-03	1.027972e-03	1.032012e-03			1.356766e-03	1.407975e-03	1.426561e-03	1.507721e-03	1.576083e-03
123	185	182	200	193	139	186	129	125	135	212
1.603651e-03	1.718638e-03	2.107546e-03	2.123407e-03	2.380294e-03	2.390563e-03	2.448151e-03	2.609826e-03	2.724603e-03	2.742365e-03	2.751000e-03
140	160	191	207	178	198	171	132	215	218	189
2.780561e-03	2.801320e-03	2.874565e-03	2.906161e-03	3.217563e-03	3.289231e-03	3.481006e-03	3.596636e-03	3.614034e-03	3.732999e-03	3.952412e-03
196	131	199	206	173	150	122	213	148	127	152
4.090050e-03	4.116774e-03	4.155999e-03	4.380424e-03	4.566469e-03	4.774985e-03	5.093172e-03	5.145624e-03	5.240020e-03	5.316530e-03	5.323086e-03
134	133	188	126	181	208	180	179	227	225	201
5.446386e-03	6.380095e-03	6.434233e-03	6.696434e-03	6.899026e-03	6.957195e-03	7.362605e-03	7.444905e-03	7.706337e-03	8.000135e-03	8.879359e-03
177	153	162	141	138	161	154	149	119	114	172
1.069717e-02	1.085121e-02	1.128545e-02	1.217683e-02	1.300801e-02	1.310001e-02	1.314304e-02	1.555690e-02	1.565217e-02	1.577579e-02	1.672105e-02
120	121	210	116	111	223	118	151	220	168	192
1.897054e-02	1.964214e-02	2.052797e-02	2.344334e-02	2.680720e-02	2.794030e-02	3.028064e-02	3.041064e-02	3.157710e-02	3.176247e-02	3.254578e-02
128	219	224	222	112	214	221				
3.569792e-02	3.742004e-02	3.851789e-02	4.035997e-02	7.587564e-02	1.505652e-01	3.393624e-01				
>										

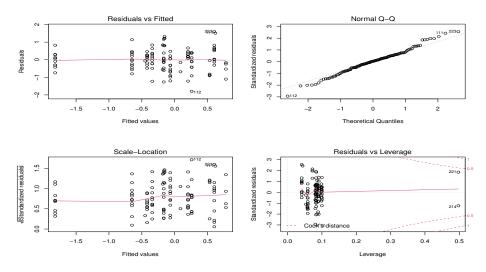


Figure 2: Results of the plot(m4) command for model M4.

- (b) What is the distinction between rstandard and rstudent? State which one would be more suitable for testing the presence of an outlier, and describe how to perform such a test. [6 points]
- (c) For the model M4, show how to interpret the above diagnostics with specific reference to (i) presence of outliers, (ii) suitability of the linear model, (iii) normal distribution of errors, (iv) constancy of variance, (v) points of high leverage, (vi) influential values. [As in earlier parts of the exam, you are not expected to make explicit numerical calculations, but if you refer to any calculated statistics or tests, you should state the appropriate formulas.] [24 points]

SOLUTIONS

1. (a) We write

$$X = \begin{pmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{pmatrix}, \ X^T X = \begin{pmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{pmatrix}.$$
 (5)

After substituting $\sum x_i = \sum x_i^3 = 0$, we note that $X^T X$ is effectively of block diagonal form where $\begin{pmatrix} n & \sum x_i^2 \\ \sum x_i^2 & \sum x_i^2 \end{pmatrix}^{-1} = \frac{1}{\Delta} \begin{pmatrix} \sum x_i^4 & -\sum x_i^2 \\ -\sum x_i^2 & n \end{pmatrix}$ and hence

$$(X^T X)^{-1} X^T \mathbf{y} = \begin{pmatrix} \frac{\sum x_i^4}{\Delta} & 0 & -\frac{\sum x_i^2}{\Delta} \\ 0 & \frac{1}{\sum x_i^2} & 0 \\ -\frac{\sum x_i^2}{\Delta} & 0 & \frac{n}{\Delta} \end{pmatrix} \begin{pmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{pmatrix}$$
(6)

from which we deduce the given expression for $\hat{\beta}_0$ and similarly

$$\hat{\beta}_1 = \frac{\sum x_i y_i}{\sum x_i^2}, \ \hat{\beta}_2 = \frac{-\sum y_i \sum x_i^2 + n \sum x_i^2 y_i}{\Delta}.$$
 (7)

 $\begin{bmatrix} Note added after the exam. An alternative solution is to write <math>X^T X \hat{\boldsymbol{\beta}} = X^T \mathbf{y}$ as three simultaneous linear equations and solve by elimination of variables; this avoids having to explicitly compute a matrix inverse. Also, the first (top row) equation in this sequence implies $n\hat{\beta}_0 + (\sum x_i^2)\hat{\beta}_2 = \sum y_i$ which gives directly the answer to (b) below.

(b) We have

$$\hat{\beta}_{0} - \bar{y} = \frac{\sum x_{i}^{4} \sum y_{i} - \sum x_{i}^{2} \sum x_{i}^{2} y_{i}}{\Delta} - \frac{\sum y_{i}}{n}$$

$$= \frac{n \sum x_{i}^{4} \sum y_{i} - n \sum x_{i}^{2} \sum x_{i}^{2} y_{i} - n \sum x_{i}^{4} \sum y_{i} + (\sum x_{i}^{2})^{2} \sum y_{i}}{n\Delta}$$

$$= \sum x_{i}^{2} \cdot \frac{-n \sum x_{i}^{2} y_{i} + (\sum x_{i}^{2}) \sum y_{i}}{n\Delta} = -\frac{(\sum x_{i}^{2}) \hat{\beta}_{2}}{n}$$

as required.

(c) By a standard formula (see, for example, page 127 of the Smith and Young course text),

$$SSE_{0} - SSE_{1} = \sum (\hat{y}_{i} - \bar{y})^{2}$$

=
$$\sum \left\{ (\hat{\beta}_{0} - \bar{y}) + \hat{\beta}_{1}x_{i} + \hat{\beta}_{2}x_{i}^{2} \right\}^{2}$$

=
$$n \sum (\hat{\beta}_{0} - \bar{y})^{2} + \hat{\beta}_{1}^{2} \sum x_{i}^{2} + \hat{\beta}_{2}^{2} \sum x_{i}^{4} + 2(\hat{\beta}_{0} - \bar{y})\hat{\beta}_{2} \sum x_{i}^{2}$$

(other cross - products are 0)

$$= \hat{\beta}_{1}^{2} \sum x_{i}^{2} + \hat{\beta}_{2}^{2} \left\{ \frac{(\sum x_{i}^{2})^{2}}{n} + \sum x_{i}^{4} - 2 \frac{(\sum x_{i}^{2})^{2}}{n} \right\}$$
(using the result of (b))
$$= \hat{\beta}_{1}^{2} \sum x_{i}^{2} + \frac{\hat{\beta}_{2}^{2} \Delta}{n}$$

which is of the desired form with $C_1 = \sum x_i^2$ and $C_2 = \frac{\Delta}{n}$.

- (d) The *F* statistic is $F = \frac{SSE_0 SSE_1}{2} \cdot \frac{n-3}{SSE_1}$ where $SSE_0 = \sum (y_i \bar{y})^2$ and $SSE_0 SSE_1$ is given by the formula in (c). When H_0 is true, the distribution of *F* is $F_{2,n-3}$. The critical value for a test of significance level α is expressed in R notation as qf(1-alpha,2,n-3).
- (e) The formula for λ is $\lambda \sigma^2 = \beta_1^2 \sum x_i^2 + \frac{\beta_2^2 \Delta}{n}$ (substitution rule). The answer will be given by the R formula 1-pf(c,2,n-3,ncp=lambda) where c is the critical value computed in (d).

 $\begin{bmatrix} \text{An alternative solution is as follows. We want to test } H_0: C\beta = \mathbf{h} \text{ where } \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix}$

and $C = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. Then

$$C(X^{T}X)^{-1}C^{T} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\sum x_{i}^{4}}{\Delta} & 0 & -\frac{\sum x_{i}^{2}}{\Delta} \\ 0 & \frac{1}{\sum x_{i}^{2}} & 0 \\ -\frac{\sum x_{i}^{2}}{\Delta} & 0 & \frac{n}{\Delta} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & -\frac{\sum x_{i}^{2}}{\Delta} \\ \frac{1}{\sum x_{i}^{2}} & 0 \\ 0 & \frac{n}{\Delta} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sum x_{i}^{2}} & 0 \\ 0 & \frac{n}{\Delta} \end{pmatrix}$$

so with $\mathbf{h} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$, $\mathbf{h}' = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}$, we find

$$(\mathbf{h}'-\mathbf{h})^T \left\{ C(X^T X)^{-1} C^T \right\}^{-1} (\mathbf{h}'-\mathbf{h}) = \begin{pmatrix} \beta_1 & \beta_2 \end{pmatrix} \begin{pmatrix} \sum x_i^2 & 0 \\ 0 & \frac{\Delta}{n} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = \beta_1^2 \sum x_i^2 + \beta_2^2 \frac{\Delta}{n}$$

From the theory of the F test, the last expression is $\lambda \sigma^2$ and the result then follows.

2. (a) In order from top to bottom: (i) the F statistic is $\frac{90.983-28.369}{15} \cdot \frac{101}{28.369} = 14.861$; (ii) pf(4.381,2,114,lower.tail=F)=0.01468693; (iii) n - p = 117 - 6 = 111 (the reason p = 6 is because we have an intercept, two coefficients of linear terms and three coefficients of quadratic terms); (iv) we must solve $\frac{90.983-x}{9} \cdot \frac{107}{x} = 12.89$; rearrange to give $x = 90.983 / \left(\frac{12.89 \times 9}{107} + 1\right) = 43.65356...$ The full table is:

Model	ESS	DF	F statistic	p-value
M0	90.983	116		
M1	28.369	101	14.861	2.6e-19
M2	84.489	114	4.381	0.015
M3	51.880	111	16.733	$2.7e{-}12$
M4	43.653	107	12.89	1e-13

- (b) Definitions: the standardized (rstandard) and studentized (rstudent) residual are given respectively by $e_i^* = \frac{e_i}{s\sqrt{1-h_{ii}}}$ and $d_i^* = \frac{e_i}{s_{(i)}\sqrt{1-h_{ii}}}$ where e_i is the uncorrected residual, s the sample standard deviation, h_{ii} the *i*th leverage value, and $s_{(i)}$ denotes the sample standard deviation omitting observation *i*; there are several equivalent algebraic formulas which would also be acceptable answers. For testing outliers, rstudent is preferable because the marginal distribution is exactly t_{n-p-1} which in this case (n = 117, p = 10) reduces to t_{106} . The most extreme value of rstudent is -3.047 for which the two-sided p-value is 2*pt(-3.047, 106) which is 0.0029. However, this is subject to multiple testing and a Bonferroni correction $(117 \times 0.0029 = 0.33)$ would lead you to the conclusion that there is no significant outlier. [Numerical calculations were not required but a precise description of the method would earn full credit.]
- (c) (i) Observations 111, 123 (at the upper end) and 112 (lower end) may be outliers as indicated by the residual and QQ plots; for formal testing, refer back to (b). (ii) There is no evidence of systematic trend in the residuals v. fitted values plot so this would indicate that the model is an adequate fit to the data (though you could refer back to the table of ESSs, it looks as though M1 is better). (iii) With the exception of the three possible outliers, the QQ plot shows a good fit to the normal distribution. (iv) The "Scale-Location" plot shows very slight increase in scale from left to right but overall the assumption of constant σ^2 is reasonable. (v) Only the largest two hat values (both 0.4973...) are large enough to be of concern and the fact that they are identical suggests that they come from the same monitor (which must therefore be the one at the top of the longitude–latitude plot, which has 2 observations). Note that the standard $\frac{2p}{n}$ criterion for high leverage comes to $\frac{2\times 20}{117} = 0.171$ which clarifies that the two observations with highest leverage are well over this level, but none of the others. (vi) Observations 214 and 221 have the largest values of Cook's D statistic as shown both by the table and by the bottom right plot (two observations at the right hand end of that plot). Since these are the same two observations as had large hat values in (v), these must have come from the same monitor in the top center of the longitude-latitude plot. These two values of D are considerably larger than those in the rest of the sample but they are still less than 0.5 — they are somewhat influential but still do not appear to be excessively so.

General comment on student solutions to 2(c). Several students gave good verbal descriptions of the methods but did not do such a good job of linking them to the data. With this type of question, there is no unique answer; for example, while I made the judgment that the data supported a normal distribution as characterized by the QQ plot, you could equally well have argued the opposite, and I would have accepted either conclusion so long as your answer was supported by relevant features of the data. (Some students also mentioned the existence of various tests, such as Shapiro-Wilk or Anderson-

Darling, that could settle the issue more definitively; however, I did not expect you to try to implement these methods and there is no practical way of doing so with the given information.) Despite these limitations, I did expect that students would justify their answers by making explicit references to the various tables and figures; not everyone did that.