Stat 511 Exam 2

April 7, 2008
Prof. Vardeman

I have neither given nor received unauthorized assistance on this exam.

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Name

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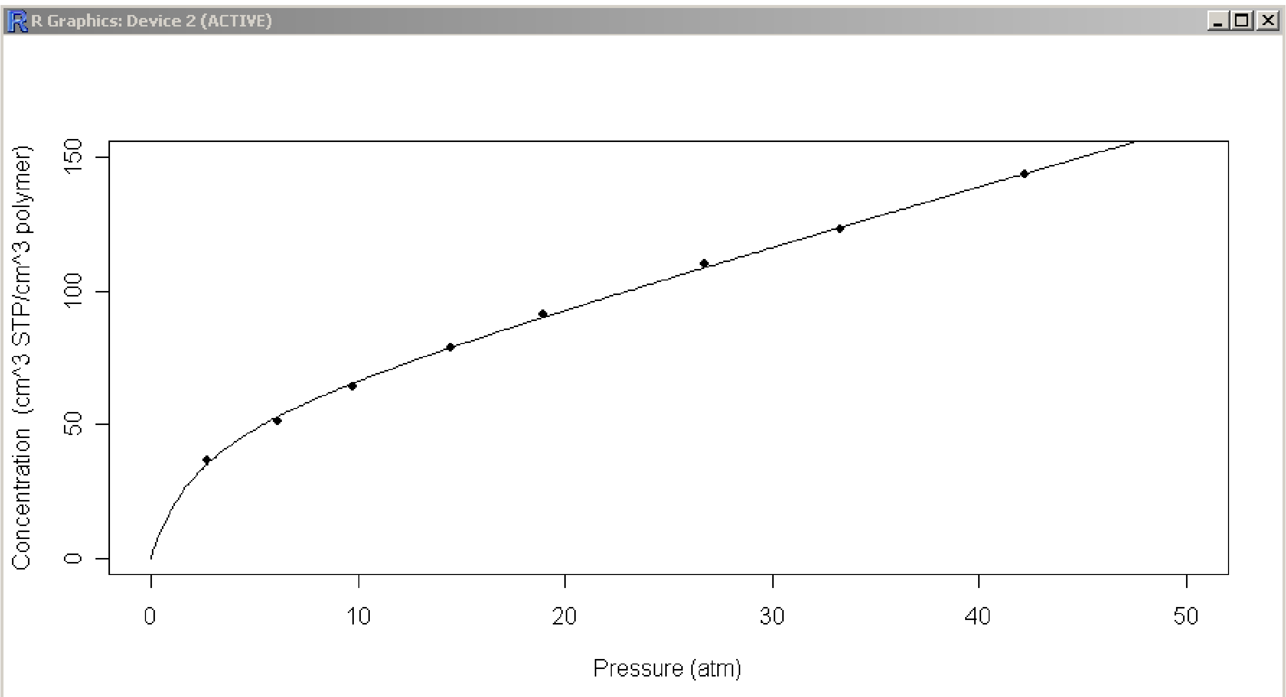
1. An experimental data set in a set of slides due to S.A. Jenekhe found on the University of Washington Chemistry Department web site of Prof. Lawrence Ricker concerns CO_2 solubility in a glassy polymer. Given are the pressures, p, and corresponding concentrations, c, of CO_2 below.

Pressure, p (atm)	2.74	6.10	9.76	14.45	18.92	26.74	33.28	42.23
Concentration, c (cm^3 (STP)/cm^3 polymer)	36.6	51.4	64.3	78.7	91.5	110.3	122.9	143.7

A standard deterministic model for gas solubility in a polymer is

$$c = Hp + L_c\left(\frac{L_a p}{1+L_a p}\right)$$

for constants H (the Henry's law constant), L_c (the Langmuir capacity constant), and L_a (the Langmuir affinity constant). Below is a plot of these data and a fitted concentration versus pressure curve. Note that for large pressure this (fitted) curve is nearly linear with slope H and intercept L_c, while the derivative of concentration with respect to pressure at 0 pressure is $H + L_c \cdot L_a$.



There is an R printout at the end of this exam from the session in which this plot was generated. Use it to answer the following questions about a nonlinear regression analysis of this situation based on a model

$$c_i = Hp_i + L_c\left(\frac{L_a p_i}{1+L_a p_i}\right) + \varepsilon_i \qquad (*)$$

for iid $N(0,\sigma^2)$ errors ε_i, $i = 1,2,\ldots,8$.

a) What are approximate 95% confidence limits for the standard deviation of concentration at any fixed pressure according to the model (*)? (If you need some percentage point(s) of a distribution that you don't have, say very carefully/completely exactly what you need.) Plug into any formula you provide.

b) Under what conditions on the parameters of model (*) is the mean concentration a simple multiple of pressure? Is there definitive evidence in these data that such a ("single mode") model is too simple and so the full complexity of model (*) is justified? Explain in terms of some measures of statistical significance.

c) What are approximate 95% confidence limits for the derivative of mean concentration with respect to pressure at 0 pressure? (Plug into an appropriate formula. You don't need to do arithmetic, but you must plug in, and if you don't have necessary percentage points of a distribution, say very carefully/completely exactly what you need.)

2. In a typical industrial "gauge R&R study," each of I different parts from some process is measured m times by each of J different operators, as a way of studying the consistency of measurement using a single gauge. We will here consider a case where the operators are "fixed" (being the only ones a company will ever use to do such measuring) while parts are "random" (representing ongoing production of such parts) and for

$$y_{ijk} = \text{the } k\text{th measurement obtained on part } i \text{ by operator } j$$

model as

$$y_{ijk} = \mu + \alpha_i + \beta_j + \alpha\beta_{ij} + \varepsilon_{ijk} \qquad (**)$$

where μ and the β_j are unknown constants and the $\alpha_i, \alpha\beta_{ij}$, and ε_{ijk} are independent random variables, with $\alpha_i \sim \text{iid N}\left(0, \sigma_\alpha^2\right)$, $\alpha\beta_{ij} \sim \text{iid N}\left(0, \sigma_{\alpha\beta}^2\right)$, and $\varepsilon_{ijk} \sim \text{iid N}\left(0, \sigma^2\right)$. (Here the β_j might be thought of as consistent operator biases and the $\alpha\beta_{ij}$ might be thought of as so-called operator "nonlinearities of measurement.")

To begin, first consider a small/toy case where $I = J = m = 2$ (there are 2 parts, 2 operators, and each part is measured 2 times by each operator).

a) For 8 observations written down in dictionary order, show how to write out model (**) in mixed linear model matrix form (by providing the elements of $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\varepsilon}$ indicated below).

$$\mathbf{Y} = \begin{pmatrix} y_{111} \\ y_{112} \\ y_{121} \\ y_{122} \\ y_{211} \\ y_{212} \\ y_{221} \\ y_{222} \end{pmatrix} \quad \mathbf{X} = \qquad \boldsymbol{\beta} = \qquad \mathbf{Z} = \qquad \mathbf{u} =$$

b) Write out the following in terms of model (**) parameters.

$\text{Var}\, y_{111} =$ ____________________ $\text{Cov}(y_{111}, y_{112}) =$ ____________________

$\text{Cov}(y_{111}, y_{121}) =$ ____________________ $\text{Cov}(y_{111}, y_{211}) =$ ____________________

At the end of this exam, there is an `R` printout for an analysis based on model (**) of a modification of a real data set from an R&R study based on $I = 4$ parts, $J = 3$ operators, and $m = 2$ measurements per part. (These are measured heights of some steel punches in 10^{-3} inch.) Use it to answer the next two questions.

c) Based on the results on the printout

- do you find clear evidence of differences in operator measurement "biases," and
- do operator "nonlinearities" appear to play a large role in measurement of these punch heights?

(Return to the parenthetical remark following model statement (**) for use of these terms.) Explain using appropriate values from the printout.

d) What are approximate BLUPs for

- $\mu + \alpha_1 + \beta_1 + \alpha\beta_{11}$ (a long-run average of measurements of part 1 by operator 1) (give a numerical value)

- $\mu + \alpha_5 + \beta_1 + \alpha\beta_{51} + \varepsilon_{511}$ (a measurement on a new punch by operator #1) Here, give both the BLUP AND an appropriate standard error (give numerical values).

3. Suppose that for $i = 1,2$ and $j = 1,2$, $y_{ij} = \mu + \alpha_i + \varepsilon_{ij}$ for independent variables $\alpha_i \sim$ iid $\mathrm{N}\left(0,\sigma_\alpha^2\right)$ and $\varepsilon_{ij} \sim$ iid $\mathrm{N}\left(0,\sigma^2\right)$. Take $\mathbf{W} = \mathbf{BY}$ for $\mathbf{Y} = \left(y_{11}, y_{12}, y_{21}, y_{22}\right)'$ and

$$\mathbf{B} = \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}.$$

a) Argue that REML estimation of σ_α^2 and σ^2 can be based on $\mathbf{W}$ and write out explicitly the function of $w_1, w_2, w_3, \sigma_\alpha^2,$ and σ^2 that can be maximized as a function of σ_α^2 and σ^2 to produce REML estimates.

b) The restricted loglikelihood from a) can be written as a function of log-variances $\gamma_1 = \log \sigma^2$ and $\gamma_2 = \log \sigma_\alpha^2$. For a particular $\mathbf{W}$, this is maximized at $\hat{\gamma}_1 = .6931$ and $\hat{\gamma}_2 = 1.3863$. The Hessian (matrix of second partial derivatives) of this function at its maximizer is $\begin{pmatrix} -1.5 & -1 \\ -1 & -2 \end{pmatrix}$. Find approximate 95% confidence limits for σ_α based on this information. (Plug in and evaluate.)

4. Suppose that for $i = 1, 2, 3$ independent observations $y_{ij} \sim$ iid $\mathrm{N}\left(\mu_i, \sigma_i^2\right)$ for $j = 1, \ldots, n_i$ (that is, we have independent samples of sizes n_i from three different normal distributions). For constants $c_1, c_2,$ and c_3, the random variable $c_1\bar{y}_1 + c_2\bar{y}_2 + c_3\bar{y}_3$ has variance

$$V = \frac{c_1^2}{n_1}\sigma_1^2 + \frac{c_2^2}{n_2}\sigma_2^2 + \frac{c_3^2}{n_3}\sigma_3^2$$

Based on variances for the 3 samples ($s_1^2, s_2^2,$ and s_3^2) use the Cochran-Satterthwaite approximation to identify approximate 95% confidence limits for V. (Say explicitly what percentage point(s) of exactly what distribution will be needed.)

For Problem #1

```
> pressure<-c(2.74,6.10,9.76,14.45,18.92,26.74,33.28,42.23)
> conc<-c(36.6,51.4,64.3,78.7,91.5,110.3,122.9,143.7)

> nlrfit<-
nls(formula=conc~H*pressure+LC*((LA*pressure)/(1+LA*pressure)),start=c(H=
2,LC=50,LA=.5),trace=T)
446.4045 :   2.0 50.0  0.5
11.02893 :   2.1865348 54.6735257  0.4116493
10.34221 :   2.1785177 55.0649938  0.4177164
10.34211 :   2.1789683 55.0447196  0.4182403
10.34211 :   2.1790082 55.0429003  0.4182864
10.34211 :   2.1790117 55.0427404  0.4182904

> summary(nlrfit)

Formula: conc ~ H * pressure + ((LC * LA)/(1 + LA * pressure)) * pressure

Parameters:
   Estimate Std. Error t value Pr(>|t|)
H   2.17901    0.08574  25.414 1.76e-06 ***
LC 55.04274    3.49365  15.755 1.87e-05 ***
LA  0.41829    0.08051   5.195  0.00348 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.438 on 5 degrees of freedom

Number of iterations to convergence: 5
Achieved convergence tolerance: 1.959e-06

> confint(nlrfit)
Waiting for profiling to be done...
51.67906 :  55.0427404  0.4182904
13.45704 :  58.8543577  0.3425121

:
:
:

47.62486 :   2.455613 43.357777
64.20141 :   2.523317 40.680263
61.44185 :   2.497246 41.751108
79.19115 :   2.562831 39.220090
76.03984 :   2.53446 40.34596
94.31986 :   2.598318 37.934771
90.55775 :   2.566830 39.146689
         2.5%      97.5%
H   1.9317119  2.3913757
LC 46.7938116 65.8979832
LA  0.2616633  0.7487824

> vcov(nlrfit)
              H         LC           LA
H   0.007351596 -0.2862178  0.005690264
LC -0.286217844 12.2056221 -0.259450579
LA  0.005690264 -0.2594506  0.006482498
```

For Problem #2

```
> height
 [1] 500 500 500 502 500 501 499 498 498 496 497 499 498 498 496 497
495 497 498 498 496 496 498 497
> Part
 [1] 1 1 1 1 1 1 2 2 2 2 2 2 3 3 3 3 3 3 4 4 4 4 4 4
Levels: 1 2 3 4
> Operator
 [1] 1 1 2 2 3 3 1 1 2 2 3 3 1 1 2 2 3 3 1 1 2 2 3 3
Levels: 1 2 3
> PartbyOperator
 [1] 1 1 2 2 3 3 1 1 2 2 3 3 1 1 2 2 3 3 1 1 2 2 3 3
Levels: 1 2 3

> lmeRandR<-lme(height~1+Operator,random=~1|Part/PartbyOperator)

> summary(lmeRandR)
Linear mixed-effects model fit by REML
 Data: NULL
       AIC     BIC    logLik
  85.73936 92.0065 -36.86968

Random effects:
 Formula: ~1 | Part
        (Intercept)
StdDev:    1.596437

 Formula: ~1 | PartbyOperator %in% Part
        (Intercept)  Residual
StdDev:   0.4930067 0.9128709

Fixed effects: height ~ 1 + Operator
              Value Std.Error DF  t-value p-value
(Intercept) 498.625 0.8955912 12 556.7552  0.0000
Operator2    -1.000 0.5743354  6  -1.7411  0.1323
Operator3    -0.625 0.5743354  6  -1.0882  0.3183
 Correlation:
          (Intr) Oprtr2
Operator2 -0.321
Operator3 -0.321  0.500

Standardized Within-Group Residuals:
        Min          Q1         Med          Q3         Max
-1.68303446 -0.54044333 -0.07409349  0.57924966  1.89128663

Number of Observations: 24
Number of Groups:
                    Part PartbyOperator %in% Part
                       4                       12


> fixed.effects(lmeRandR)
(Intercept)   Operator2   Operator3
    498.625      -1.000      -0.625


> vcov(lmeRandR)
            (Intercept)  Operator2  Operator3
(Intercept)   0.8020835 -0.1649306 -0.1649306
Operator2    -0.1649306  0.3298611  0.1649306
Operator3    -0.1649306  0.1649306  0.3298611


> intervals(lmeRandR)
```

```
Approximate 95% confidence intervals

 Fixed effects:
                 lower    est.      upper
(Intercept) 496.673675 498.625 500.576325
Operator2    -2.405348  -1.000   0.405348
Operator3    -2.030348  -0.625   0.780348
attr(,"label")
[1] "Fixed effects:"

 Random Effects:
  Level: Part
                    lower     est.    upper
sd((Intercept)) 0.6722698 1.596437 3.791055
  Level: PartbyOperator
                     lower      est.    upper
sd((Intercept)) 0.09020527 0.4930067 2.694472

 Within-group standard error:
    lower      est.     upper
0.5976521 0.9128709 1.3943452


> random.effects(lmeRandR)
Level: Part
  (Intercept)
1   2.2247074
2  -0.2301421
3  -1.1507107
4  -0.8438545

Level: PartbyOperator %in% Part
     (Intercept)
1/1 -0.313050149
1/2  0.423792081
1/3  0.101423605
2/1  0.038736586
2/2 -0.145473971
2/3  0.084789226
3/1  0.193682932
3/2  0.009472374
3/3 -0.312896102
4/1  0.080630631
4/2 -0.287790484
4/3  0.126683270

> predict(lmeRandR,level=0:2)
   Part PartbyOperator predict.fixed predict.Part predict.PartbyOperator
1     1            1/1       498.625     500.8497               500.5367
2     1            1/1       498.625     500.8497               500.5367
3     1            1/2       497.625     499.8497               500.2735
4     1            1/2       497.625     499.8497               500.2735
5     1            1/3       498.000     500.2247               500.3261
6     1            1/3       498.000     500.2247               500.3261
7     2            2/1       498.625     498.3949               498.4336
8     2            2/1       498.625     498.3949               498.4336
9     2            2/2       497.625     497.3949               497.2494
10    2            2/2       497.625     497.3949               497.2494
11    2            2/3       498.000     497.7699               497.8546
12    2            2/3       498.000     497.7699               497.8546
13    3            3/1       498.625     497.4743               497.6680
14    3            3/1       498.625     497.4743               497.6680
15    3            3/2       497.625     496.4743               496.4838
```

16	3	3/2	497.625	496.4743	496.4838
17	3	3/3	498.000	496.8493	496.5364
18	3	3/3	498.000	496.8493	496.5364
19	4	4/1	498.625	497.7811	497.8618
20	4	4/1	498.625	497.7811	497.8618
21	4	4/2	497.625	496.7811	496.4934
22	4	4/2	497.625	496.7811	496.4934
23	4	4/3	498.000	497.1561	497.2828
24	4	4/3	498.000	497.1561	497.2828