

1. In the calibration of a scientific instrument, “true” values x are known and produce experimental readings y on the instrument. Suppose that we are willing to assume that the mean value of y is proportional to x , so that

$$y_i = x_i \mathbf{b} + \mathbf{e}_i$$

where for $\mathbf{e} = (\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n)'$, $E \mathbf{e} = \mathbf{0}$. A particular calibration experiment produces $n = 4$ data points as per

x	3	4	5	6
y	3	6	11	14

Initially suppose that $\text{Var } \mathbf{e} = \mathbf{s}^2 \mathbf{I}$.

a) Find a matrix \mathbf{P}_X so that $\hat{\mathbf{Y}} = \mathbf{P}_X \mathbf{Y}$.

b) By the criterion of “size of the hats, h_{ii} ” which of the 4 observations is “most influential” in the fitting of the linear model here?

c) Give 90% two-sided confidence limits for \mathbf{s} in the normal version of this model. (No need to simplify.)

d) Give 90% two-sided prediction limits for a new y for $x = 10$. (No need to simplify.)

Now suppose that it is plausible that not only is the mean value of y is proportional to x , but that so too is the standard deviation of y . That is, suppose that $\text{Var } e = \mathbf{s}^2 \text{diag}(9,16,25,36)$.

e) Give a matrix \mathbf{T} such that \mathbf{TY} follows a Gauss-Markov model. What is the model matrix for \mathbf{TY} ?

\mathbf{T} :

Model Matrix:

f) Evaluate an appropriate point estimate of \mathbf{b} under these model assumptions.

g) Give a standard error (an estimated standard deviation) for your estimate of \mathbf{b} in part f) under these heteroscedastic model assumptions.

2. So-called “mixture experiments” are run to investigate how the composition of a substance (as measured by fractions of it that are of "pure component" types $i = 1, 2, \dots, r$) affect some physical property y . For example, y might be an octane rating for a gasoline blended from r “pure” components like butane, alkylate, cat cracked, etc. Notice that in a mixture study

$$x_1 + x_2 + \dots + x_r = 1$$

In this problem, we consider an $r = 4$ component mixture problem. Consider the linear model

$$\mathbf{Y} = \mathbf{X}\mathbf{B} + \mathbf{e}$$

for

$$\mathbf{X} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & .5 & .5 & 0 & 0 \\ 1 & .5 & 0 & .5 & 0 \\ 1 & .5 & 0 & 0 & .5 \\ 1 & 0 & .5 & .5 & 0 \\ 1 & 0 & .5 & 0 & .5 \\ 1 & 0 & 0 & .5 & .5 \\ 1 & .33 & .33 & .33 & 0 \\ 1 & .33 & .33 & 0 & .33 \\ 1 & .33 & 0 & .33 & .33 \\ 1 & 0 & .33 & .33 & .33 \\ 1 & .25 & .25 & .25 & .25 \end{pmatrix} = (\mathbf{1} \mid \mathbf{x}_1 \mid \mathbf{x}_2 \mid \mathbf{x}_3 \mid \mathbf{x}_4) \text{ and } \mathbf{B} = \begin{pmatrix} \mathbf{b}_0 \\ \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \\ \mathbf{b}_4 \end{pmatrix}$$

a) For an arbitrary composition vector (x_1, x_2, x_3, x_4) (with each $x_i \geq 0$ and $\sum x_i = 1$) argue carefully that the corresponding mean response $\mathbf{b}_0 + \sum_i \mathbf{b}_i x_i$ is estimable.

b) The parameter \mathbf{b}_0 is not estimable in this model. Argue this point carefully.

Now consider a full rank restricted version of the original mixture model of the form

$$\mathbf{Y} = \mathbf{X}^* \boldsymbol{\beta} = (\mathbf{x}_1 | \mathbf{x}_2 | \mathbf{x}_3 | \mathbf{x}_4) \boldsymbol{\beta} + \mathbf{e} \quad \text{for } \boldsymbol{\beta} = \begin{pmatrix} \boldsymbol{g}_1 \\ \boldsymbol{g}_2 \\ \boldsymbol{g}_3 \\ \boldsymbol{g}_4 \end{pmatrix}$$

c) In this restricted model and the mixture context, what is the interpretation of the parameter \boldsymbol{g}_1 ? What is $\boldsymbol{g}_1 - \boldsymbol{g}_2$?

\boldsymbol{g}_1 : $\boldsymbol{g}_1 - \boldsymbol{g}_2$:

d) Give a matrix \mathbf{C} and a vector \mathbf{d} so that the hypothesis that “pure component #1 has mean response 3 and simultaneously an ‘equal parts mixture of components’ has mean response 12” in the form $H_0 : \mathbf{C}\boldsymbol{\beta} = \mathbf{d}$.

\mathbf{C} : \mathbf{d} :

e) Is the hypothesis in d) testable? Explain.

There is some R output attached to this exam. The first part of it concerns this mixture problem. Use it to help you answer the following questions.

f) For which of the (x_1, x_2, x_3, x_4) mixtures in the data set is the mean of y most precisely estimated? Say why your answer agrees with intuition.

g) Give 90% two sided confidence limits for $\mathbf{g}_1 - \mathbf{g}_2$. (Plug in, but you need not simplify.)

h) Notice in this model that if $H_0: \mathbf{g}_1 = \mathbf{g}_2 = \mathbf{g}_3 = \mathbf{g}_4$ is true, then the fact that in the mixture context $\sum x_i = 1$ implies that $E \mathbf{Y} = \mathbf{g} \mathbf{1}$ for some \mathbf{g} , that is, the mean response is constant. Give the value of and degrees of freedom for an F statistic for testing this hypothesis.

$F =$ _____

$df =$ _____ , _____

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> X
      [,1]      [,2]      [,3]      [,4]
[1,] 1.0000000 0.0000000 0.0000000 0.0000000
[2,] 0.0000000 1.0000000 0.0000000 0.0000000
[3,] 0.0000000 0.0000000 1.0000000 0.0000000
[4,] 0.0000000 0.0000000 0.0000000 1.0000000
[5,] 0.5000000 0.5000000 0.0000000 0.0000000
[6,] 0.5000000 0.0000000 0.5000000 0.0000000
[7,] 0.5000000 0.0000000 0.0000000 0.5000000
[8,] 0.0000000 0.5000000 0.5000000 0.0000000
[9,] 0.0000000 0.5000000 0.0000000 0.5000000
[10,] 0.0000000 0.0000000 0.5000000 0.5000000
[11,] 0.3333333 0.3333333 0.3333333 0.0000000
[12,] 0.3333333 0.3333333 0.0000000 0.3333333
[13,] 0.3333333 0.0000000 0.3333333 0.3333333
[14,] 0.0000000 0.3333333 0.3333333 0.3333333
[15,] 0.2500000 0.2500000 0.2500000 0.2500000
> V<-ginv(t(X)%*%X)
> V
      [,1]      [,2]      [,3]      [,4]
[1,] 0.53218391 -0.08850575 -0.08850575 -0.08850575
[2,] -0.08850575 0.53218391 -0.08850575 -0.08850575
[3,] -0.08850575 -0.08850575 0.53218391 -0.08850575
[4,] -0.08850575 -0.08850575 -0.08850575 0.53218391
> H<-X%*%V%*%t(X)
> H
      [,1]      [,2]      [,3]      [,4]      [,5]      [,6]
[1,] 0.53218391 -0.08850575 -0.08850575 -0.08850575 0.22183908 0.22183908
[2,] -0.08850575 0.53218391 -0.08850575 -0.08850575 0.22183908 -0.08850575
[3,] -0.08850575 -0.08850575 0.53218391 -0.08850575 -0.08850575 0.22183908
[4,] -0.08850575 -0.08850575 -0.08850575 0.53218391 -0.08850575 -0.08850575
[5,] 0.22183908 0.22183908 -0.08850575 -0.08850575 0.22183908 0.06666667
[6,] 0.22183908 -0.08850575 0.22183908 -0.08850575 0.06666667 0.22183908
[7,] 0.22183908 -0.08850575 -0.08850575 0.22183908 0.06666667 0.06666667
[8,] -0.08850575 0.22183908 0.22183908 -0.08850575 0.06666667 0.06666667
[9,] -0.08850575 0.22183908 -0.08850575 0.22183908 0.06666667 -0.08850575
[10,] -0.08850575 -0.08850575 0.22183908 0.22183908 -0.08850575 0.06666667
[11,] 0.11839080 0.11839080 0.11839080 -0.08850575 0.11839080 0.11839080
[12,] 0.11839080 0.11839080 -0.08850575 0.11839080 0.11839080 0.01494253
[13,] 0.11839080 -0.08850575 0.11839080 0.11839080 0.01494253 0.11839080
[14,] -0.08850575 0.11839080 0.11839080 0.11839080 0.01494253 0.01494253
[15,] 0.06666667 0.06666667 0.06666667 0.06666667 0.06666667 0.06666667
      [,7]      [,8]      [,9]      [,10]      [,11]      [,12]
[1,] 0.22183908 -0.08850575 -0.08850575 -0.08850575 0.11839080 0.11839080
[2,] -0.08850575 0.22183908 0.22183908 -0.08850575 0.11839080 0.11839080
[3,] -0.08850575 0.22183908 -0.08850575 0.22183908 0.11839080 -0.08850575
[4,] 0.22183908 -0.08850575 0.22183908 0.22183908 -0.08850575 0.11839080
[5,] 0.06666667 0.06666667 0.06666667 -0.08850575 0.11839080 0.11839080
[6,] 0.06666667 0.06666667 -0.08850575 0.06666667 0.11839080 0.01494253
[7,] 0.22183908 -0.08850575 0.06666667 0.06666667 0.01494253 0.11839080
[8,] -0.08850575 0.22183908 0.06666667 0.06666667 0.11839080 0.01494253
[9,] 0.06666667 0.06666667 0.22183908 0.06666667 0.01494253 0.11839080
[10,] 0.06666667 0.06666667 0.06666667 0.22183908 0.01494253 0.01494253
[11,] 0.01494253 0.11839080 0.01494253 0.01494253 0.11839080 0.04942529
[12,] 0.11839080 0.01494253 0.11839080 0.01494253 0.04942529 0.11839080
[13,] 0.11839080 0.01494253 0.01494253 0.11839080 0.04942529 0.04942529
[14,] 0.01494253 0.11839080 0.11839080 0.11839080 0.04942529 0.04942529
[15,] 0.06666667 0.06666667 0.06666667 0.06666667 0.06666667 0.06666667

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      [,13]      [,14]      [,15]
[1,]  0.11839080 -0.08850575  0.06666667
[2,] -0.08850575  0.11839080  0.06666667
[3,]  0.11839080  0.11839080  0.06666667
[4,]  0.11839080  0.11839080  0.06666667
[5,]  0.01494253  0.01494253  0.06666667
[6,]  0.11839080  0.01494253  0.06666667
[7,]  0.11839080  0.01494253  0.06666667
[8,]  0.01494253  0.11839080  0.06666667
[9,]  0.01494253  0.11839080  0.06666667
[10,] 0.11839080  0.11839080  0.06666667
[11,] 0.04942529  0.04942529  0.06666667
[12,] 0.04942529  0.04942529  0.06666667
[13,] 0.11839080  0.04942529  0.06666667
[14,] 0.04942529  0.11839080  0.06666667
[15,] 0.06666667  0.06666667  0.06666667
> Y
      [,1]
[1,] 11.5
[2,] 12.5
[3,]  4.7
[4,] 16.5
[5,] 11.3
[6,]  6.6
[7,] 13.0
[8,]  6.4
[9,] 13.3
[10,] 10.4
[11,] 10.2
[12,] 12.4
[13,] 11.4
[14,] 13.4
[15,]  9.6
> t(Y)%%(diag(rep(1,15))-H)%%Y
      [,1]
[1,] 16.47676
> V%%t(X)%%Y
      [,1]
[1,] 10.807586
[2,] 11.873103
[3,]  4.466207
[4,] 16.373103
> C<-matrix(c(1,-1,0,0,1,0,-1,0,1,0,0,-1),3,byrow=T)
> C
      [,1] [,2] [,3] [,4]
[1,]  1  -1   0   0
[2,]  1   0  -1   0
[3,]  1   0   0  -1
> t(C%%V%%t(X)%%Y)%%ginv(C%%V%%t(C))%%(C%%V%%t(X)%%Y)
      [,1]
[1,] 116.4872
> t(Y)%%(H-(1/15)*matrix(c(rep(1,225)),15))%%Y
      [,1]
[1,] 116.4872

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