Chapter 2 Supplemental Text Material

S2.1. Models for the Data and the *t*-Test

The model presented in the text, equation (2.23) is more properly called a *means* model. Since the mean is a *location parameter*, this type of model is also sometimes called a *location model*. There are other ways to write the model for a *t*-test. One possibility is

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij} \begin{cases} i = 1,2 \\ j = 1,2,\cdots,n_i \end{cases}$$

where μ is a parameter that is common to all observed responses (an overall mean) and τ_i is a parameter that is unique to the *i*th factor level. Sometimes we call τ_i the *i*th treatment effect. This model is usually called the *effects* model.

Since the means model is

$$y_{ij} = \mu_i + \varepsilon_{ij} \begin{cases} i = 1,2 \\ j = 1,2,\cdots,n_i \end{cases}$$

we see that the *i*th treatment or factor level mean is $\mu_i = \mu + \tau_i$; that is, the mean response at factor level *i* is equal to an overall mean plus the effect of the *i*th factor. We will use both types of models to represent data from designed experiments. Most of the time we will work with effects models, because it's the "traditional" way to present much of this material. However, there are situations where the means model is useful, and even more natural.

S2.2. Estimating the Model Parameters

Because models arise naturally in examining data from designed experiments, we frequently need to estimate the model parameters. We often use **the method of least squares** for parameter estimation. This procedure chooses values for the model parameters that minimize the sum of the squares of the errors ε_{ij}. We will illustrate this procedure for the means model. For simplicity, assume that the sample sizes for the two factor levels are equal; that is $n_1 = n_2 = n$. The least squares function that must be minimized is

$$\begin{aligned} L &= \sum_{i=1}^{2}\sum_{j=1}^{n}\varepsilon_{ij}^2 \\ &= \sum_{i=1}^{2}\sum_{j=1}^{n}(y_{ij} - \mu_i)^2 \end{aligned}$$

Now $\dfrac{\partial L}{\partial \mu_1} = 2\sum_{j=1}^{n}(y_{1j} - \mu_1)$ and $\dfrac{\partial L}{\partial \mu_2} = 2\sum_{j=1}^{n}(y_{2j} - \mu_2)$ and equating these partial derivatives to zero yields the **least squares normal equations**

$$n\hat{\mu}_1 = \sum_{i=1}^{n} y_{1j}$$

$$n\hat{\mu}_2 = \sum_{i=1}^{n} y_{2j}$$

The solution to these equations gives the least squares estimators of the factor level means. The solution is $\hat{\mu}_1 = \bar{y}_1$ and $\hat{\mu}_2 = \bar{y}_2$; that is, the sample averages at leach factor level are the estimators of the factor level means.

This result should be intuitive, as we learn early on in basic statistics courses that the sample average usually provides a reasonable estimate of the population mean. However, as we have just seen, this result can be derived easily from a simple location model using least squares. It also turns out that if we assume that the model errors are normally and independently distributed, the sample averages are the **maximum likelihood estimators** of the factor level means. That is, if the observations are normally distributed, least squares and maximum likelihood produce exactly the same estimators of the factor level means. Maximum likelihood is a more general method of parameter estimation that usually produces parameter estimates that have excellent statistical properties.

We can also apply the method of least squares to the effects model. Assuming equal sample sizes, the least squares function is

$$\begin{aligned} L &= \sum_{i=1}^{2}\sum_{j=1}^{n} \varepsilon_{ij}^2 \\ &= \sum_{i=1}^{2}\sum_{j=1}^{n} (y_{ij} - \mu - \tau_i)^2 \end{aligned}$$

and the partial derivatives of L with respect to the parameters are

$$\frac{\partial L}{\partial \mu} = 2\sum_{i=1}^{2}\sum_{j=1}^{n}(y_{ij} - \mu - \tau_i),\ \ \frac{\partial L}{\partial \tau_1} = 2\sum_{j=1}^{n}(y_{1j} - \mu - \tau_1), \text{and } \frac{\partial L}{\partial \tau_2} = 2\sum_{j=1}^{n}(y_{2j} - \mu - \tau_2)$$

Equating these partial derivatives to zero results in the following least squares normal equations:

$$\begin{aligned} 2n\hat{\mu} + n\hat{\tau}_1 + n\hat{\tau}_2 &= \sum_{i=1}^{2}\sum_{j=1}^{n} y_{ij} \\ n\hat{\mu} + n\hat{\tau}_1 \qquad\quad &= \sum_{j=1}^{n} y_{1j} \\ n\hat{\mu} \qquad\quad + n\hat{\tau}_2 &= \sum_{j=1}^{n} y_{2j} \end{aligned}$$

Notice that if we add the last two of these normal equations we obtain the first one. That is, the normal equations are not linearly independent and so they do not have a unique solution. This has occurred because the effects model is **overparameterized**. This situation occurs frequently; that is, the effects model for an experiment will always be an overparameterized model.

One way to deal with this problem is to add another linearly independent equation to the normal equations. The most common way to do this is to use the equation $\hat{\tau}_1 + \hat{\tau}_2 = 0$. This is, in a sense, an intuitive choice as it essentially defines the factor effects as deviations from the overall mean μ. If we impose this constraint, the solution to the normal equations is

$$\begin{aligned} &\hat{\mu} = \bar{y} \\ &\hat{\tau}_i = \bar{y}_i - \bar{y}, i = 1,2 \end{aligned}$$

That is, the overall mean is estimated by the average of all 2*n* sample observation, while each individual factor effect is estimated by the difference between the sample average for that factor level and the average of all observations.

This is not the only possible choice for a linearly independent "constraint" for solving the normal equations. Another possibility is to simply set the overall mean equal to a constant, such as for example $\hat{\mu} = 0$. This results in the solution

$$\begin{aligned} &\hat{\mu} = 0 \\ &\hat{\tau}_i = \bar{y}_i, i = 1,2 \end{aligned}$$

Yet another possibility is $\hat{\tau}_2 = 0$, producing the solution

$$\begin{aligned} &\hat{\mu} = \bar{y}_2 \\ &\hat{\tau}_1 = \bar{y}_1 - \bar{y}_2 \\ &\hat{\tau}_2 = 0 \end{aligned}$$

There are an infinite number of possible constraints that could be used to solve the normal equations. An obvious question is "which solution should we use?" It turns out that it really doesn't matter. For each of the three solutions above (indeed for *any* solution to the normal equations) we have

$$\hat{\mu}_i = \hat{\mu} + \hat{\tau}_i = \bar{y}_i, i = 1,2$$

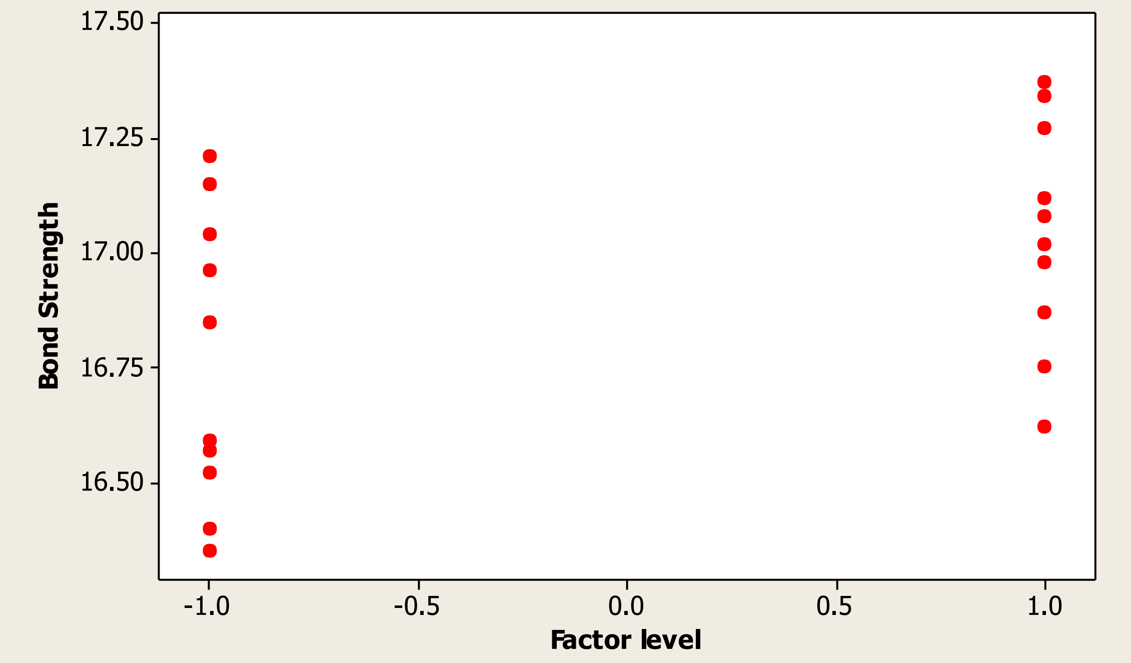
That is, the least squares estimator of the mean of the *i*th factor level will always be the sample average of the observations at that factor level. So even if we cannot obtain unique estimates for the parameters in the effects model we *can* obtain unique estimators of a *function* of these parameters that we are interested in. We say that the mean of the *i*th factor level is *estimable*. Any function of the model parameters that can be uniquely estimated regardless of the constraint selected to solve the normal equations is called an **estimable function**. This is discussed in more detail in Chapter 3.

S2.3. A Regression Model Approach to the *t*-Test

The two-sample *t*-test can be presented from the viewpoint of a simple linear regression model. This is a very instructive way to think about the *t*-test, as it fits in nicely with the general notion of a factorial experiment with factors at two levels, such as the golf experiment described in Chapter 1. This type of experiment is very important in practice, and is discussed extensively in subsequent chapters.

In the *t*-test scenario, we have a factor *x* with two levels, which we can arbitrarily call "low" and "high". We will use *x* = -1 to denote the low level of this factor and *x* = +1 to denote the high level of this factor. The figure below is a scatter plot (from Minitab) of the Portland cement mortar tension bond strength data in Table 2.1 of Chapter 2.

Figure 2-3.1 Scatter plot of bond strength



We will a simple linear regression model to this data, say

$$y_{ij} = \beta_0 + \beta_1 x_{ij} + \varepsilon_{ij}$$

where β_0 and β_1 are the intercept and slope, respectively, of the regression line and the regressor or predictor variable is $x_{1j} = -1$ and $x_{2j} = +1$. The method of least squares can be used to estimate the slope and intercept in this model. Assuming that we have equal sample sizes *n* for each factor level the least squares normal equations are:

$$2n\hat{\beta}_0 = \sum_{i=1}^{2}\sum_{j=1}^{n} y_{ij}$$

$$2n\hat{\beta}_1 = \sum_{j=1}^{n} y_{2j} - \sum_{j=1}^{n} y_{1j}$$

The solution to these equations is

$$\hat{\beta}_0 = \bar{y}$$

$$\hat{\beta}_1 = \frac{1}{2}(\bar{y}_2 - \bar{y}_1)$$

Note that the least squares estimator of the intercept is the average of all the observations from both samples, while the estimator of the slope is one-half of the difference between the sample averages at the “high” and “low’ levels of the factor *x*. Below is the output from the linear regression procedure in Minitab for the tension bond strength data.

Regression Analysis: Bond Strength versus Factor level

```
The regression equation is
Bond Strength = 16.9 + 0.139 Factor level


Predictor        Coef  SE Coef       T      P
Constant      16.9030   0.0636  265.93  0.000
Factor level  0.13900  0.06356    2.19  0.042


S = 0.284253   R-Sq = 21.0%   R-Sq(adj) = 16.6%


Analysis of Variance

Source          DF       SS       MS     F      P
Regression       1  0.38642  0.38642  4.78  0.042
Residual Error  18  1.45440  0.08080
Total           19  1.84082
```

Notice that the estimate of the slope (given in the column labeled “Coef” and the row labeled “Factor level” above) is 0.139 $= \frac{1}{2}(\bar{y}_2 - \bar{y}_1) = \frac{1}{2}(17.0420 - 16.7640)$ and the estimate of the intercept is 16.9030. Furthermore, notice that the *t*-statistic associated with the slope is equal to 2.19, exactly the same value (apart from sign) that we gave in the Minitab two-sample t-test output in Table 2.2 in the text. Now in simple linear regression, the *t*-test on the slope is actually testing the hypotheses

$$H_0\colon \beta_1 = 0$$
$$H_0\colon \beta_1 \neq 0$$

and this is equivalent to testing $H_0\colon \mu_1 = \mu_2$.

It is easy to show that the *t*-test statistic used for testing that the slope equals zero in simple linear regression is identical to the usual two-sample *t*-test. Recall that to test the above hypotheses in simple linear regression the *t*-statistic is

$$t_0 = \frac{\hat{\beta}_1}{\sqrt{\dfrac{\hat{\sigma}^2}{S_{xx}}}}$$

where $S_{xx} = \sum_{i=1}^{2}\sum_{j=1}^{n}(x_{ij} - \bar{x})^2$ is the "corrected" sum of squares of the *x*'s. Now in our specific problem, $\bar{x} = 0, x_{1j} = -1$ and $x_{2j} = +1,$ so $S_{xx} = 2n.$ Therefore, since we have already observed that the estimate of σ is just S_p,

$$t_0 = \frac{\hat{\beta}_1}{\sqrt{\dfrac{\hat{\sigma}^2}{S_{xx}}}} = \frac{\dfrac{1}{2}(\bar{y}_2 - \bar{y}_1)}{S_p\sqrt{\dfrac{1}{2n}}} = \frac{\bar{y}_2 - \bar{y}_1}{S_p\sqrt{\dfrac{2}{n}}}$$

This is the usual two-sample *t*-test statistic for the case of equal sample sizes.

S2.4. Constructing Normal Probability Plots

While we usually generate normal probability plots using a computer software program, occasionally we have to construct them by hand. Fortunately, it's relatively easy to do, since specialized **normal probability plotting paper** is widely available. This is just graph paper with the vertical (or probability) scale arranged so that if we plot the cumulative normal probabilities $(j - 0.5)/n$ on that scale versus the rank-ordered observations $y_{(j)}$ a graph equivalent to the computer-generated normal probability plot will result. The table below shows the calculations for the unmodified portland cement mortar bond strength data.

j	$y_{(j)}$	$(j - 0.5)/10$	$z_{(j)}$
1	16.62	0.05	-1.64
2	16.75	0.15	-1.04
3	16.87	0.25	-0.67
4	16.98	0.35	-0.39
5	17.02	0.45	-0.13
6	17.08	0.55	0.13
7	17.12	0.65	0.39
8	17.27	0.75	0.67
9	17.34	0.85	1.04
10	17.37	0.95	1.64

Now if we plot the cumulative probabilities from the next-to-last column of this table versus the rank-ordered observations from the second column on normal probability paper, we will produce a graph that is identical to the results for the unmodified mortar formulation that is shown in Figure 2.11 in the text.

A normal probability plot can also be constructed on ordinary graph paper by plotting the standardized normal *z*-scores $z_{(j)}$ against the ranked observations, where the standardized normal *z*-scores are obtained from

$$P(Z \le z_j) = \Phi(z_j) = \frac{j - 0.5}{n}$$

where $\Phi(\bullet)$ denotes the standard normal cumulative distribution. For example, if $(j - 0.5)/n = 0.05$, then $\Phi(z_j) = 0.05$ implies that $z_j = -1.64$. The last column of the above table displays the values of the normal *z*-scores. Plotting these values against the ranked observations on ordinary graph paper will produce a normal probability plot equivalent to the unmodified mortar results in Figure 2.11. As noted in the text, many statistics computer packages present the normal probability plot this way.

S2.5. More About Checking Assumptions in the *t*-Test

We noted in the text that a normal probability plot of the observations was an excellent way to check the normality assumption in the *t*-test. Instead of plotting the observations, an alternative is to plot the *residuals* from the statistical model.

Recall that the means model is

$$y_{ij} = \mu_i + \varepsilon_{ij} \begin{cases} i = 1,2 \\ j = 1,2,\cdots,n_i \end{cases}$$

and that the estimates of the parameters (the factor level means) in this model are the sample averages. Therefore, we could say that the *fitted* model is

$$\hat{y}_{ij} = \bar{y}_i, i = 1,2 \text{ and } j = 1,2,\cdots,n_i$$

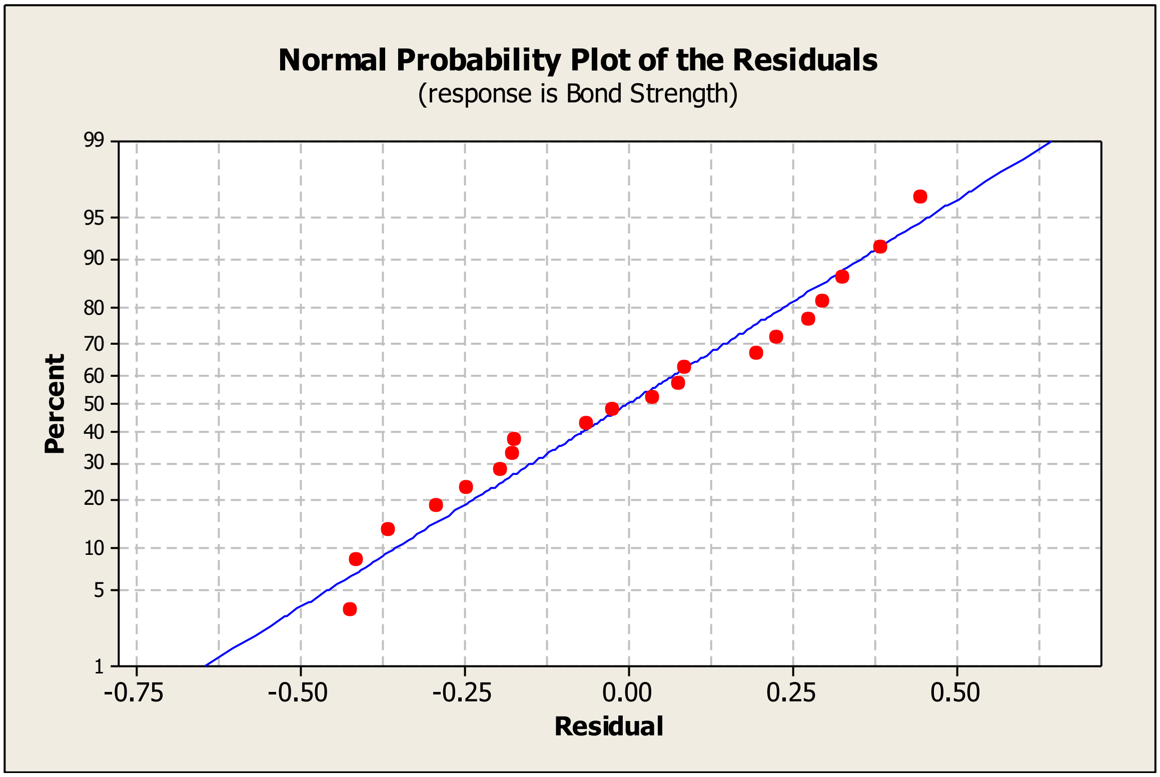
That is, an estimate of the *ij*th observation is just the average of the observations in the *i*th factor level. The difference between the observed value of the response and the predicted (or fitted) value is called a **residual**, say

$$e_{ij} = y_{ij} - \hat{y}_i, i = 1,2 .$$

The table below computes the values of the residuals from the portland cement mortar tension bond strength data.

Observation j	y_{1j}	$e_{1j} = y_{1j} - \bar{y}_1$ $= y_{1j} - 16.76$	y_{2j}	$e_{2j} = y_{2j} - \bar{y}_2$ $= y_{2j} - 17.04$
1	16.85	0.09	16.62	-0.42
2	16.40	-0.36	16.75	-0.29
3	17.21	0.45	17.37	0.33
4	16.35	-0.41	17.12	0.08
5	16.52	-0.24	16.98	-0.06
6	17.04	0.28	16.87	-0.17
7	16.96	0.20	17.34	0.30
8	17.15	0.39	17.02	-0.02
9	16.59	-0.17	17.08	0.04
10	16.57	-0.19	17.27	0.23

The figure below is a normal probability plot of these residuals from Minitab.



As noted in section S2.3 above we can compute the *t*-test statistic using a simple linear regression model approach. Most regression software packages will also compute a table or listing of the residuals from the model. The residuals from the Minitab regression model fit obtained previously are as follows:

```
     Factor      Bond
Obs   level  Strength      Fit  SE Fit  Residual  St Resid
  1   -1.00   16.8500  16.7640  0.0899    0.0860      0.32
  2   -1.00   16.4000  16.7640  0.0899   -0.3640     -1.35
  3   -1.00   17.2100  16.7640  0.0899    0.4460      1.65
  4   -1.00   16.3500  16.7640  0.0899   -0.4140     -1.54
  5   -1.00   16.5200  16.7640  0.0899   -0.2440     -0.90
  6   -1.00   17.0400  16.7640  0.0899    0.2760      1.02
  7   -1.00   16.9600  16.7640  0.0899    0.1960      0.73
  8   -1.00   17.1500  16.7640  0.0899    0.3860      1.43
  9   -1.00   16.5900  16.7640  0.0899   -0.1740     -0.65
 10   -1.00   16.5700  16.7640  0.0899   -0.1940     -0.72
 11    1.00   16.6200  17.0420  0.0899   -0.4220     -1.56
 12    1.00   16.7500  17.0420  0.0899   -0.2920     -1.08
 13    1.00   17.3700  17.0420  0.0899    0.3280      1.22
 14    1.00   17.1200  17.0420  0.0899    0.0780      0.29
 15    1.00   16.9800  17.0420  0.0899   -0.0620     -0.23
 16    1.00   16.8700  17.0420  0.0899   -0.1720     -0.64
 17    1.00   17.3400  17.0420  0.0899    0.2980      1.11
 18    1.00   17.0200  17.0420  0.0899   -0.0220     -0.08
 19    1.00   17.0800  17.0420  0.0899    0.0380      0.14
 20    1.00   17.2700  17.0420  0.0899    0.2280      0.85
```

The column labeled "Fit" contains the averages of the two samples, computed to four decimal places. The residuals in the sixth column of this table are the same (apart from rounding) as we computed manually.

S2.6. Some More Information about the Paired *t*-Test

The paired *t*-test examines the difference between two variables and test whether the mean of those differences differs from zero. In the text we show that the mean of the differences μ_d is identical to the difference of the means in two independent samples, $\mu_1 - \mu_2$. However the variance of the differences is not the same as would be observed if there were two independent samples. Let $\bar{d}$ be the sample average of the differences. Then

$$\begin{aligned} V(\bar{d}) &= V(\bar{y}_1 - \bar{y}_2) \\ &= V(\bar{y}_1) + V(\bar{y}_2) - 2Cov(\bar{y}_1, \bar{y}_2) \\ &= \frac{2\sigma^2(1-\rho)}{n} \end{aligned}$$

assuming that both populations have the same variance σ^2 and that ρ is the correlation between the two random variables y_1 and y_2. The quantity S_d^2 / n estimates the variance of the average difference $\bar{d}$. In many paired experiments a strong positive correlation is expected to exist between y_1 and y_2 because both factor levels have been applied to the *same* experimental unit. When there is positive correlation within the pairs, the denominator for the paired *t*-test will be smaller than the denominator for the two-sample or *independent t*-test. If the two-sample test is applied incorrectly to paired samples, the procedure will generally understate the significance of the data.

Note also that while for convenience we have assumed that both populations have the same variance, the assumption is really unnecessary. The paired *t*-test is valid when the variances of the two populations are different.