Prediction of a new observation : note that this is a single observation, not the regression line.

First, the variance of a generic linear combination (from Chapter 1:1.27a & b)

$$T = aW + bX + cZ$$

$$E(T) = aE(W) + bE(X) + cE(Z)$$

$$Var(T) = a^{2}Var(W) + b^{2}Var(X) + c^{2}Var(Z) + 2(Covariances)$$

$$Var(T) = a^{2}Var(W) + b^{2}Var(X) + c^{2}Var(Z)$$

$$abCov(W,X) + bcCov(X,Z) + acCov(X,Z)$$

If we are able to assume that the three terms are stochastically independent, then the covariances are equal to zero.

We have already seen a series of Linear Combinations

1) First we saw,

$$b_1 = \frac{\Sigma(X_i - \overline{X})Y_i}{\Sigma(X_i - X)^2} = \sum_{i=1}^n k_i Y_i$$
so, $Var(b_1) = k_1^2 Var(Y_1) + k_2^2 Var(Y_2) + k_3^2 Var(Y_3) + \dots$

since all Y_i at all values of X_i have the same variance (homogeneous), then

$$= \sum_{i=1}^{n} k_i^2 \operatorname{Var}(\mathbf{Y}_i)$$

and recall that $\sum_{i=1}^{n} k_i^2 = \frac{1}{\Sigma(X_i - \overline{X})^2}$

and that $Var(Y_i)$ is estimated by the MSE, then

$$\operatorname{Var}(\mathbf{b}_1) = \frac{\operatorname{MSE}}{\Sigma(\mathbf{X}_i - \overline{\mathbf{X}})^2}$$

1) Show that b_1 is a linear combination of $k_i \left(= \frac{(X_i - \bar{X})}{\Sigma(X_i - \bar{X})^2} \right)$

a)
$$b_1 = \frac{\Sigma(X_i - \overline{X})(Y_i - \overline{Y})}{\Sigma(X_i - \overline{X})^2}$$

where
b) $\Sigma(X_i - \overline{X})(Y_i - \overline{Y}) = \Sigma(X_iY_i - \overline{X}Y_i - X_i\overline{Y} + \overline{X}\overline{Y})$
 $= \Sigma(X_i - \overline{X})Y_i - \Sigma(X_i - \overline{X})\overline{Y}$
 $= \Sigma(X_i - \overline{X})Y_i - \overline{Y}\Sigma(X_i - \overline{X})$

and since

then

$$\Sigma(X_i - \overline{X}) = 0$$

$$\Sigma(X_i - \overline{X})(Y_i - \overline{Y}) = \Sigma(X_i - \overline{X})Y_i$$

as a result,

d)
$$\mathbf{b}_1 = \frac{\Sigma(\mathbf{X}_i - \overline{\mathbf{X}})(\mathbf{Y}_i - \overline{\mathbf{Y}})}{\Sigma(\mathbf{X}_i - \overline{\mathbf{X}})^2} = \frac{\Sigma(\mathbf{X}_i - \overline{\mathbf{X}})\mathbf{Y}_i}{\Sigma(\mathbf{X}_i - \overline{\mathbf{X}})^2} = \frac{\Sigma(\mathbf{X}_i - \overline{\mathbf{X}})}{\Sigma(\mathbf{X}_i - \overline{\mathbf{X}})^2} \mathbf{Y}_i = \sum_{i=1}^n \mathbf{k}_i \mathbf{Y}_i$$

where

e)
$$\Sigma \mathbf{k}_i = \sum_{i=1}^n \frac{(\mathbf{X}_i - \overline{\mathbf{X}})}{\Sigma (\mathbf{X}_i - \overline{\mathbf{X}})^2} = \frac{\Sigma (\mathbf{X}_i - \overline{\mathbf{X}})}{\Sigma (\mathbf{X}_i - \mathbf{X})^2}$$

note that $\Sigma \mathbf{k}_i = 0$ since $\Sigma (\mathbf{X}_i - \overline{\mathbf{X}}) = 0$

now prove that $\sum_{i=1}^{n} k_i^2 = \frac{1}{\Sigma(X_i - \overline{X})^2}$

f)
$$\Sigma k_i^2 = \sum_{i=1}^n \left[\frac{(X_i - \overline{X})}{\Sigma (X_i - \overline{X})^2} \right]^2 = \sum_{i=1}^n \frac{(X_i - \overline{X})^2}{[\Sigma (X_i - \overline{X})^2]^2}$$

$$= \frac{1}{[\Sigma (X_i - \overline{X})^2]^2} \Sigma (X_i - \overline{X})^2 = \frac{1}{\Sigma (X_i - \overline{X})^2}$$

2) Then we say that $\hat{\mathbf{Y}}_i = \mathbf{b}_0 + \mathbf{b}_1 \mathbf{X}_i$, also a linear combination.

$$Var(\hat{Y}_i) = 1*Var(b_0) + X_i*Var(b_1) + 2*1*X_i*Cov(b_0,b_1)$$

note that we do NOT assume that b_0 and b_1 are independent.

The covariance is included, not equal to zero.

Using previous definitions of $Var(b_0)$ and $Var(b_1)$, and the Gaussian multipliers from the $(X'X)^{-1}$ matrix for the covariance

$$\operatorname{Var}(\hat{\mathbf{Y}}_{i}) = \sigma^{2} * 1^{2} \left[\frac{1}{n} + \frac{\overline{\mathbf{X}}^{2}}{\Sigma(\overline{\mathbf{X}_{i}} - \overline{\mathbf{X}})^{2}} \right] + \sigma^{2} * X_{i}^{2} \left[\frac{1}{\Sigma(\overline{\mathbf{X}_{i}} - \overline{\mathbf{X}})^{2}} \right] + 2 * 1 * X_{i} \sigma^{2} \left[\frac{-\Sigma X_{i}}{n\Sigma(\overline{\mathbf{X}_{i}} - \overline{\mathbf{X}})^{2}} \right]$$
$$\operatorname{Var}(\hat{\mathbf{Y}}_{i}) = \sigma^{2} \left[\frac{1}{n} + \frac{\overline{\mathbf{X}}^{2}}{\Sigma(\overline{\mathbf{X}_{i}} - \overline{\mathbf{X}})^{2}} + \frac{X_{i}^{2}}{\Sigma(\overline{\mathbf{X}_{i}} - \overline{\mathbf{X}})^{2}} - \frac{2X_{i}\overline{\mathbf{X}}}{\Sigma(\overline{\mathbf{X}_{i}} - \overline{\mathbf{X}})^{2}} \right]$$
$$\operatorname{Var}(\hat{\mathbf{Y}}_{i}) = \sigma^{2} \left[\frac{1}{n} + \frac{(X_{i} - \overline{\mathbf{X}})^{2}}{\Sigma(\overline{\mathbf{X}_{i}} - \overline{\mathbf{X}})^{2}} \right]$$

3) Now we want a confidence interval for a single (new) observation.

The equation for that observation is

or

$$\mathbf{Y}_i = \mathbf{\hat{Y}}_i + \epsilon_i$$

 $\mathbf{Y}_i = \mathbf{b}_0 + \mathbf{b}_1 \mathbf{X}_i + \mathbf{\epsilon}_i$

We assumed independence once before (each Y_i independent of others). We are now going to assume independence again. We assume that the residuals are independent of the model (ie. assume that ϵ_i are independent of \hat{Y}_i).

So the variance of single observations will be

$$\operatorname{Var}(\mathbf{Y}_{i}) = \operatorname{Var}(\hat{\mathbf{Y}}_{i}) + \operatorname{Var}(\epsilon_{i}) + \left[2^{*}\operatorname{Cov}(\hat{\mathbf{Y}}_{i},\epsilon_{i}) = 0\right]$$

We know from previous work that

$$\operatorname{Var}(\mathbf{\hat{Y}}_{i}) = \sigma^{2} \left[\frac{1}{n} + \frac{(X_{i} - \overline{X})^{2}}{\Sigma(X_{i} - \overline{X})^{2}} \right]$$

$$Var(\epsilon_i) = \sigma^2$$

therefore

$$\operatorname{Var}(\mathbf{Y}_i) = \sigma^2 \left[\frac{1}{n} + \frac{(\mathbf{X}_i - \bar{\mathbf{X}})^2}{\Sigma(\mathbf{X}_i - \mathbf{X})^2} \right] + \sigma^2$$

or

$$\operatorname{Var}(\mathbf{Y}_i) = \sigma^2 \left[1 + \frac{1}{n} + \frac{(\mathbf{X}_i - \overline{\mathbf{X}})^2}{\Sigma(\mathbf{X}_i - \mathbf{X})^2} \right]$$

where the estimator of σ^2 is MSE

Note that both your textbook and I have been using σ^2 for both Var(Y_i) and for Var(ϵ_i). Each is "the variance", but they are variances of different things. A better notation perhaps is Var(ϵ_i) = σ_{ϵ}^2

There is another confidence interval of potential interest between

$$\operatorname{Var}(\hat{\mathbf{Y}}_{i}) = \sigma^{2} \left[\frac{1}{n} + \frac{(\mathbf{X}_{i} - \overline{\mathbf{X}})^{2}}{\Sigma(\mathbf{X}_{i} - \mathbf{X})^{2}} \right], \text{ the regression line}$$

and
$$\operatorname{Var}(\mathbf{Y}_{i}) = \sigma^{2} \left[1 + \frac{1}{n} + \frac{(\mathbf{X}_{i} - \overline{\mathbf{X}})^{2}}{\Sigma(\mathbf{X}_{i} - \mathbf{X})^{2}} \right], \text{ a new observation}$$

This is the confidence interval for the mean of a new sample taken at some

particular value of X_i , where m is the size of the new sample. This cannot be as narrow as the confidence interval for the regression, but should be narrower than the confidence interval for a single sample. This CI is given by,

$$\operatorname{Var}(\mathbf{Y}_i) = \sigma^2 \left[\frac{1}{m} + \frac{1}{n} + \frac{(\mathbf{X}_i - \overline{\mathbf{X}})^2}{\Sigma(\mathbf{X}_i - \mathbf{X})^2} \right], \, \overline{\mathbf{X}} \text{ for a new sample}$$

Example : From *vial breakage regressed on number of airline transfers* example Place a confidence interval on the breakage for 3 transfers for a single new

observation.

$$s_{Y_{i}}^{2} = MSE\left(1 + \frac{1}{n} + \frac{(X_{i} - \overline{X})^{2}}{\Sigma(X_{i} - \overline{X})^{2}}\right)$$
$$= 2.2\left(1 + \frac{1}{10} + \frac{(3 - 1)^{2}}{20 - \frac{10^{2}}{10}}\right) = 2.2\left(1 + \frac{1}{10} + \frac{4}{10}\right) = 2.2*1.5 = 3.3$$

we previously calculated the variance of the regression line at $s_{\hat{Y}_i}^2 = 1.1$. Note that the variance of a single point is $s_{\hat{Y}_i}^2 + s^2 = 1.1 + 2.2 = 3.3$

$$s_{Y_i} = \sqrt{3.3} = 1.816$$

since $t_{\frac{\alpha}{2}, 8 df} = 2.306$, then

$$P(\hat{Y}_{X=3} - t_{1-\frac{\alpha}{2}, n-2} s_{Y_i} \le E(\hat{Y}) \le \hat{Y}_{X=3} + t_{1-\frac{\alpha}{2}, n-2} s_{Y_i}) = 1-\alpha$$

$$P(22.2 - 2.306*1.816 \le E(\hat{Y}) \le 22.2 + 2.306*1.816) = 1-\alpha$$

$$P(18.011 \le E(\hat{Y}) \le 26.389) = 0.95$$

SAS will calculate confidence intervals for either the regression line (option CLM) or for individual points (option CLI). But not for a new sample.

Check this against the SAS output

$$s_{\overline{Y}_{i}}^{2} = MSE\left(\frac{1}{m} + \frac{1}{n} + \frac{(X_{i} - \overline{X})^{2}}{\Sigma(X_{i} - \overline{X})^{2}}\right) = 2.2\left(\frac{1}{4} + \frac{1}{10} + \frac{(3-1)^{2}}{20 - \frac{10^{2}}{10}}\right)$$
$$= 2.2\left(\frac{1}{4} + \frac{1}{10} + \frac{4}{10}\right) = 2.2*0.75 = 1.65$$

 $s_{\bar{Y}_i} \;=\; \sqrt{1.65} \;=\; 1.2845$

since $t_{\frac{\alpha}{2}, 8 df} = 2.306$, then

$$\begin{split} & \mathsf{P}(\bar{\mathsf{Y}}_{X=3} - \mathsf{t}_{1-\frac{\alpha}{2},n-2} \; \mathsf{s}_{\bar{\mathsf{Y}}_i} \; \le \; \mathsf{E}(\bar{\mathsf{Y}}) \; \le \; \bar{\mathsf{Y}}_{X=3} + \mathsf{t}_{1-\frac{\alpha}{2},n-2} \; \mathsf{s}_{\bar{\mathsf{Y}}_i} \;) \; = \; 1 \text{-}\alpha \\ & \mathsf{P}(22.2 - 2.306^* 1.2845 \leq \; \mathsf{E}(\bar{\mathsf{Y}}) \; \le \; 22.2 + 2.306^* 1.2845) \; = \; 1 \text{-}\alpha \\ & \mathsf{P}(19.238 \; \le \; \mathsf{E}(\bar{\mathsf{Y}}) \; \le \; 25.162) \; = \; 0.95 \end{split}$$

The MEAN of the 4 cases falls in this range.

The CI for the regression line is narrower The CI for individual points is higher