IE 361 Module 7

Calibration Studies and Inference Based on Simple Linear Regression

Reading: Section 2.5 of Revised *SQAME*

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Calibration Studies

Calibration is an essential activity in the qualification and maintenance of measurement devices or systems. The basic idea is that one uses a measurement device to produce measurements on "standard" specimens with (relatively well-) "known" values of a measurand, and sees how the measurements compare to the measurand. In the event that there are systematic discrepancies between what is known to be true and what the device reads, the plan is then to invent some conversion scheme to (in future use of the device) adjust what is read to something that is hopefully closer to the (future) truth. A slight extension of "regression" analysis (curve fitting) from an elementary statistics course is the relevant statistical methodology in making this conversion.

Regression Analysis and Calibration

Calibration studies produce "true"/gold-standard-measurement values x and "local" measurements y and seek a "conversion" method from y to x. (Strictly speaking, y need not even be in the same units as x.) Regression analysis can provide both "point conversions" and measures of uncertainty (the latter through inversion of "prediction limits").

The simplest version of this is the case where

$$y \approx \beta_0 + \beta_1 x$$

This is "linear calibration." The standard statistical model for such a circumstance is

$$y = \beta_0 + \beta_1 x + \epsilon$$

for a normal error ϵ with mean 0 and standard deviation σ. (σ describes how much y's vary for a fixed x, and in the present context amounts to a "repeatability" standard deviation.) This can be pictured as follows.

Regression Analysis and Calibration

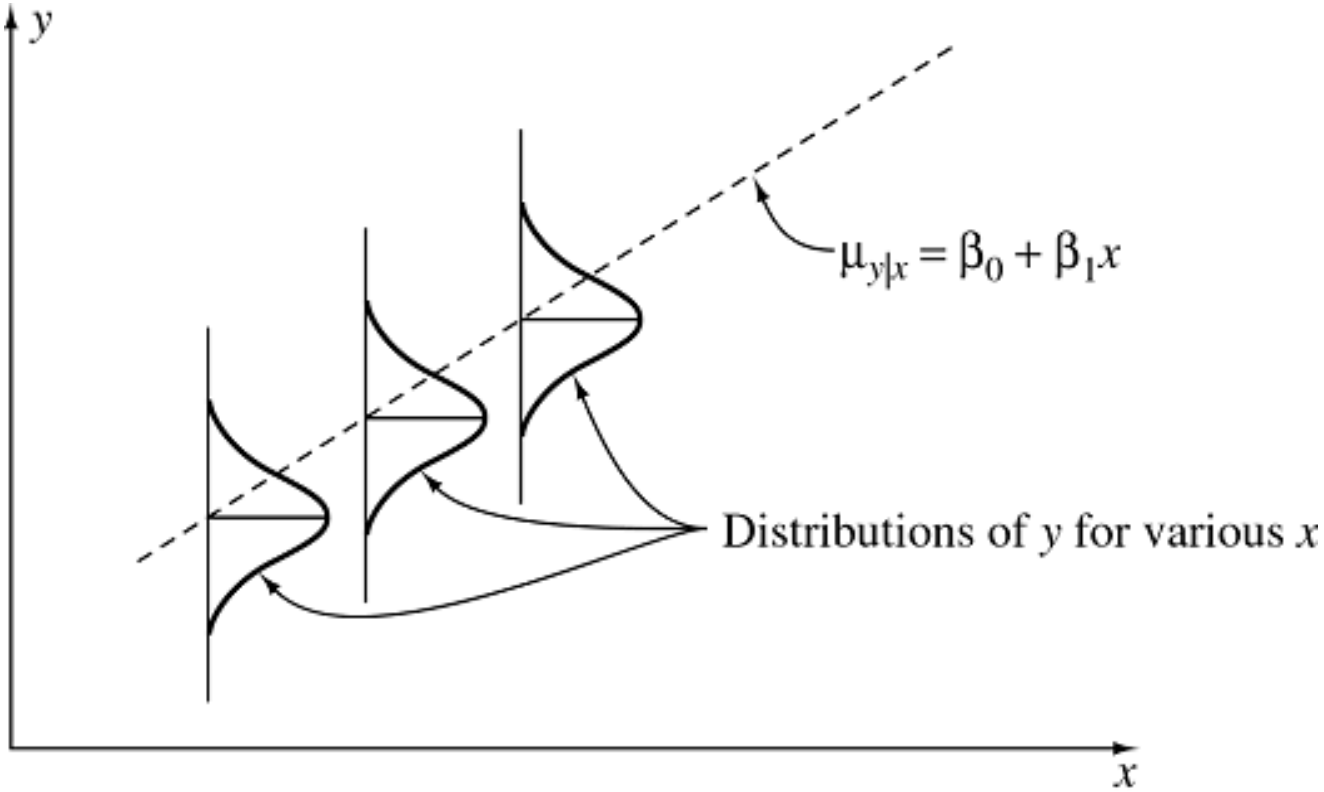


Figure: Normal Simple Linear Regression Model

Regression Analysis and Calibration

For n data pairs (x_i, y_i), simple linear regression methodology allows one to make confidence intervals and tests associated with the model, and what is more important for our present purposes, *prediction limits for a new y associated with a new x*. These are of the form

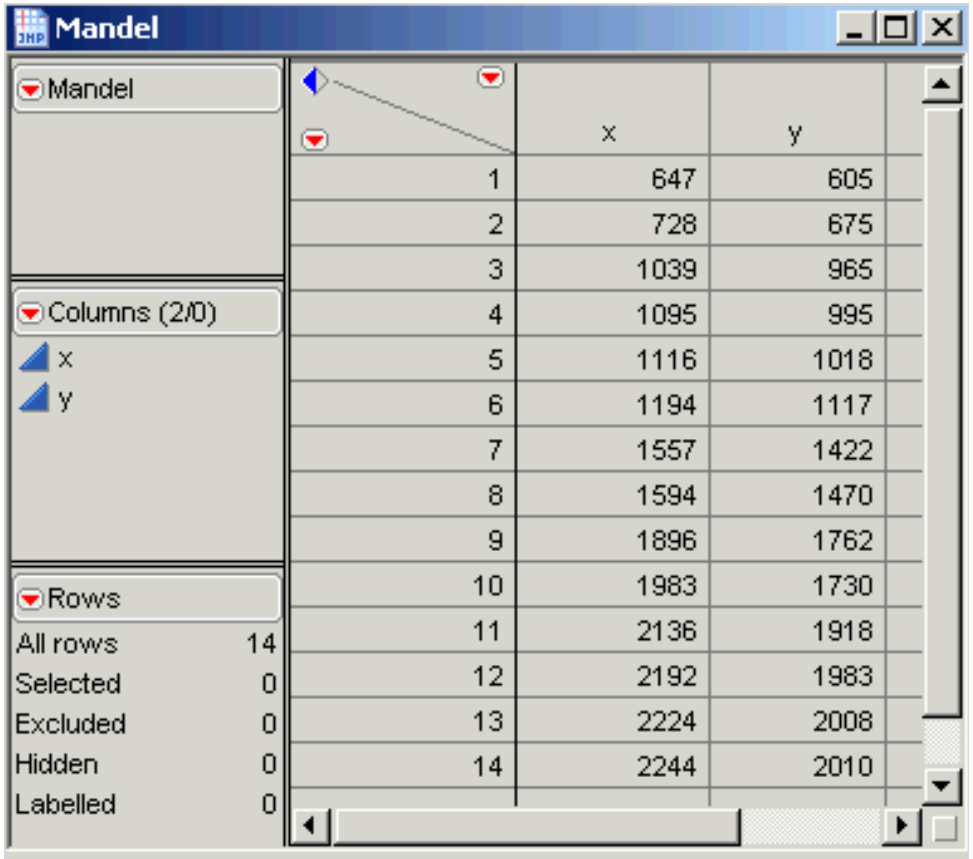
$$(b_0 + b_1 x) \pm t s_{\mathrm{LF}} \sqrt{1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{\sum (x - \bar{x})^2}}$$

where the least squares line is $\hat{y} = b_0 + b_1 x$ and s_{LF} is an estimate of σ derived from the fit of the line to the data. Any good statistical package will compute and plot these limits along with a least squares line through the data set.

Regression Analysis and Calibration

Example 7-1 (Mandel NBS/NIST)

"Gold-standard" and "local" measurements on $n = 14$ specimens (units not given) are as below.



	x	y
1	647	605
2	728	675
3	1039	965
4	1095	995
5	1116	1018
6	1194	1117
7	1557	1422
8	1594	1470
9	1896	1762
10	1983	1730
11	2136	1918
12	2192	1983
13	2224	2008
14	2244	2010

Figure: JMP Data Table for Mandel's Calibration Example

Regression Analysis and Calibration

Example 7-1 (Mandel NBS/NIST)

A JMP report for simple linear regression including prediction limits for an additional value of y (that, of course, change with x) plotted is below.

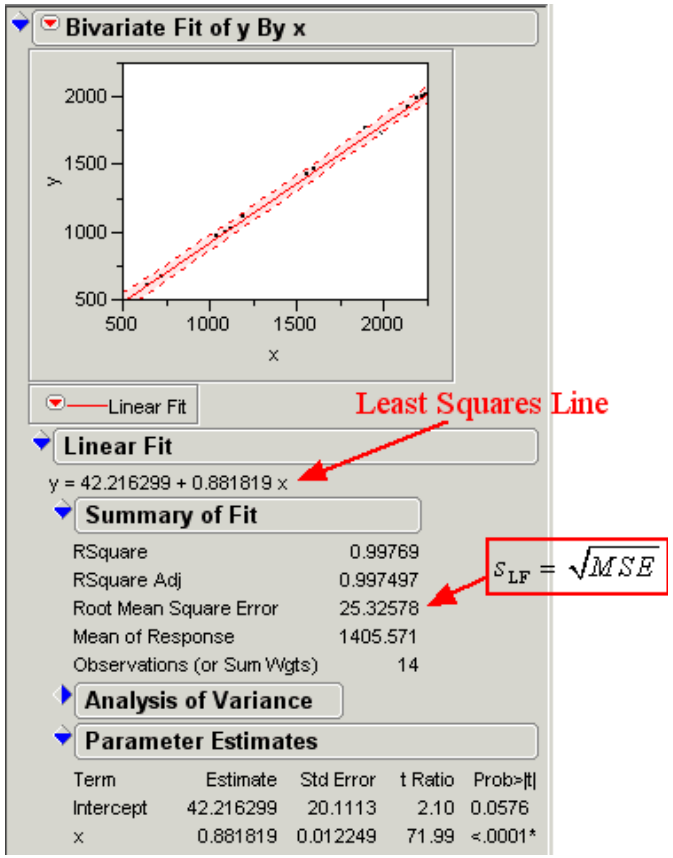


Figure: JMP Report for Simple Linear Regression With Mandel's Data

Regression Analysis and Calibration

What is of most interest here is (of course) what regression technology indicates about measurement and calibration. In particular:

- From a simple linear regression output,

$$s_{\mathrm{LF}} = \sqrt{MSE} = \text{"root mean square error"}$$

  is a kind of estimated repeatability standard deviation. One may make confidence intervals for $\sigma_{\text{repeatability}}$ based on this "sample standard deviation" using $\nu = n - 2$ degrees of freedom and limits

$$s_{\mathrm{LF}}\sqrt{\frac{n-2}{\chi^2_{\text{upper}}}} \quad \text{and} \quad s_{\mathrm{LF}}\sqrt{\frac{n-2}{\chi^2_{\text{lower}}}}$$

- The least squares equation $\hat{y} = b_0 + b_1 x$ can be solved for x, giving

$$\hat{x} = \frac{y - b_0}{b_1}$$

  as a way of estimating a "gold-standard" value of a measurand x from a measured local value y.

Regression Analysis and Calibration

- It turns out that one can take the prediction limits for y and "turn them around" to get confidence limits for the x corresponding to a measured local y. This provides a defensible way to set "error bounds" on what y indicates about x.

Since from the JMP report

$$y = 42.216299 + 0.881819x \quad \text{with } s_{\text{LF}} = 25.32578$$

we might expect a local (y) repeatability standard deviation of around 25 (in the y units). In fact, 95% confidence limits for σ can be made (using $n - 2 = 12$ degrees of freedom) limits

$$25.3\sqrt{\frac{12}{23.337}} \quad \text{and} \quad 25.3\sqrt{\frac{12}{4.4004}}$$

i.e.

$$18.1 \quad \text{and} \quad 41.8$$

Making use of the slope and intercept of the least squares line, a "conversion formula" for going from y to x is

$$\hat{x} = \frac{y - 42.216299}{0.881819}$$

Regression Analysis and Calibration

Example 7-1 (Mandel NBS/NIST)

The following figure shows how one can set 95% confidence limits on x if $y = 1500$ is observed, using a plot of 95% prediction limits for y given x.

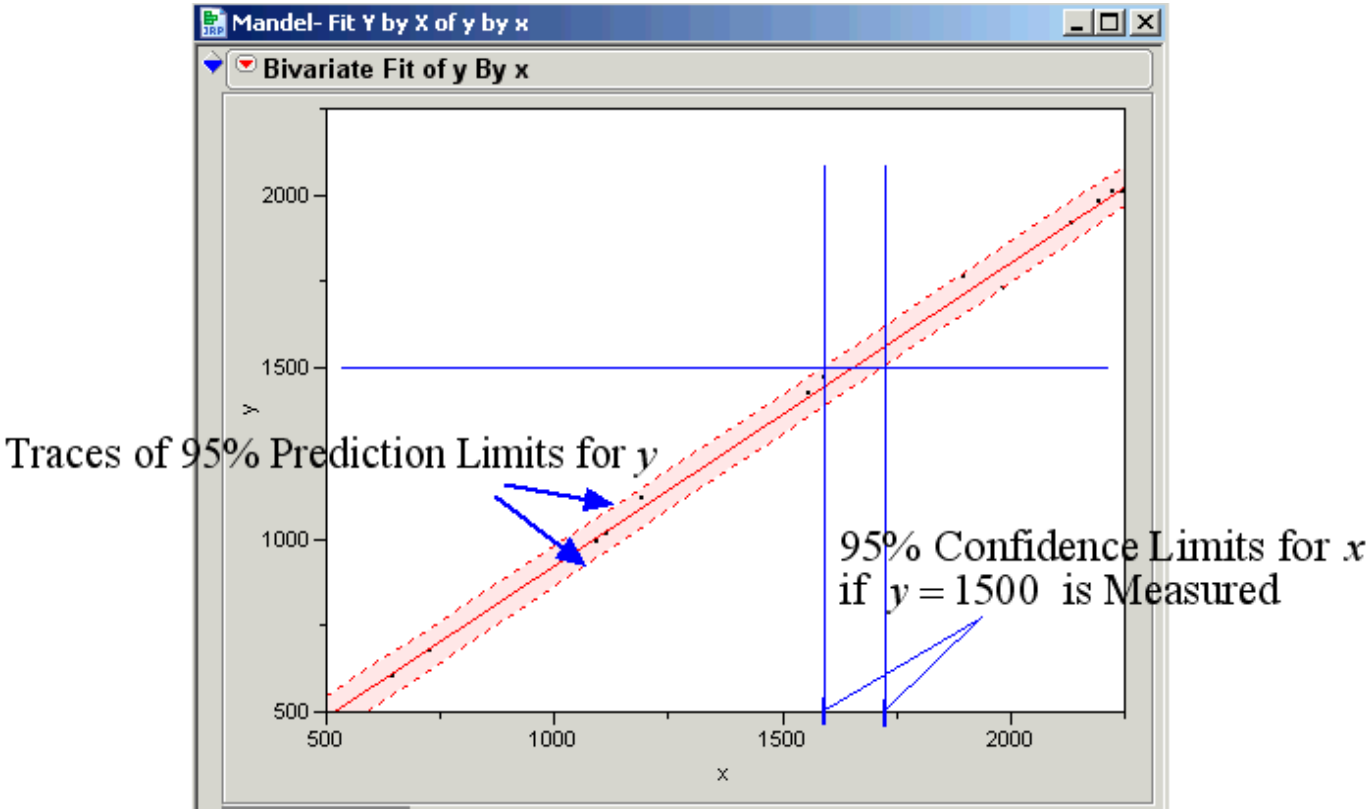


Figure: 95% Confidence Limits for x When $y = 1500$ is Measured, Derived From Traces of 95% Prediction Limits for y at Given x Values

Regression Analysis and Calibration

As one final consideration in this example, it is worthwhile to note what a standard simple linear regression analysis has to say about the "linearity" of the local measurement device assuming that the (unavailable) units of x and y are meant to be the same. While a scatterplot of the n data pairs (x_i, y_i) is reasonably straight-line, that is not really the issue to be discussed, but rather something stronger. As we mentioned in Module 2, the term "linearity" as typically employed in metrology contexts concerns the matter of *constant bias*. In regression terms, this requires a straight-line relationship between measurand and average measurement *with slope of 1*.

The methods of elementary regression analysis say that confidence limits for the slope β_1 of the simple linear regression model are

$$b_1 \pm t \frac{s_{\mathrm{LF}}}{\sqrt{\sum (x_i - \bar{x})^2}}$$

The report on panel 7 shows that

$$b_1 = .882 \quad \text{and} \quad \frac{s_{\text{LF}}}{\sqrt{\sum (x_i - \bar{x})^2}} = \text{SE}_{b_1} = .012$$

so that (using the upper 2.5% point of the t_{12} distribution, 2.179) 95% confidence limits for β_1 are

$$.882 \pm 2.179\,(.012)$$

or

$$.882 \pm .026$$

A 95% confidence interval for β_1 clearly does not include 1.0. So if the intent was that the local measurement device be "linear," at least before calibration it was not. Bias was not constant.