Linear Calibration Example 1

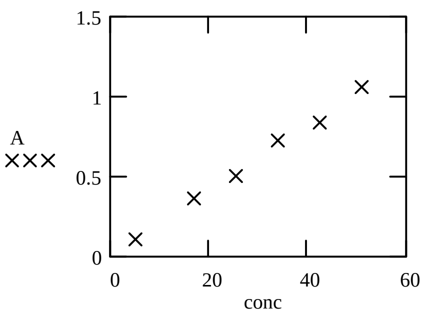
$conc := (5.1\ \ 17.0\ \ 25.5\ \ 34.0\ \ 42.5\ \ 51.0)^T$ calibration standards, ppm

$T := (78.1\ \ 43.2\ \ 31.4\ \ 18.8\ \ 14.5\ \ 8.7)^T$ transmittance, as percentages

Although the calibration measurements are recorded as transmittances, Beer's Law specifies that the concentration of analyte is linearly proportional to the absorbance. Thus, we must first calculate the absorbance of the cabliration standards.

$A := \overrightarrow{-\log\left(\frac{T}{100}\right)}$ $A^T = [\,0.1073\ \ 0.3645\ \ 0.5031\ \ 0.7258\ \ 0.8386\ \ 1.0605\,]$ calculate absorbances

Always check a plot of the calibration data to make sure it looks okay.



A linear fit seems reasonable for this data. Let's obtain the least-squares estimates of slope and intercept.

$b_0 := \text{intercept}(conc, A)$ $b_0 = 4.9876 \cdot 10^{-3}$ $b_1 := \text{slope}(conc, A)$ $b_1 = 0.0204$

Now we can calculate a point estimate of the analyte concentration for the "unknown"

$T_u := 35.6$ $y_u := -\log\left(\frac{T_u}{100}\right)$ $y_u = 0.4486$ absorbance of the unknown

$x_u := \frac{y_u - b_0}{b_1}$ $x_u = 21.7559$ point estimate of analyte concentration, in ppm

A confidence interval for the analyte concentration can be obtained by assuming homogeneous noise on the calibration measurements.

First calculate the standard deviation of the residuals

$fit := b_1 \cdot conc + b_0$ $res := A - fit$ $res^T = [\,-1.6182 \cdot 10^{-3}\ \ 0.0129\ \ -0.0218\ \ 0.0277\ \ -0.0329\ \ 0.0157\,]$

$s_{res} := \sqrt{\frac{1}{4} \cdot \sum \overrightarrow{res^2}}$ $s_{res} = 0.0262$ an estimate of the homogeneous noise

$S_{xx} := 5 \cdot \text{Var}(conc)$ $xbar := \text{mean}(conc)$ A few other things we need.

Now we are ready to calculate the standard error of our point estimate.

$se_u := \frac{s_{res}}{b_1} \sqrt{1 + \frac{1}{6} + \frac{(x_u - xbar)^2}{S_{xx}}}$ $se_u = 1.4085$

If the calibration measurements are normally distributed, so is our point estimate. Thus, we can use t-tables to calculate a confidence interval.

$t := qt(.975, 4)$ $t = 2.7764$ 4 degrees of freedom, 95% confidence

$t \cdot se_u = 3.9107$ width of the confidence interval

Thus, the analyte concentration in the "unknown" is 21.8 ± 3.9 ppm (95% CL)