AA Data Analysis

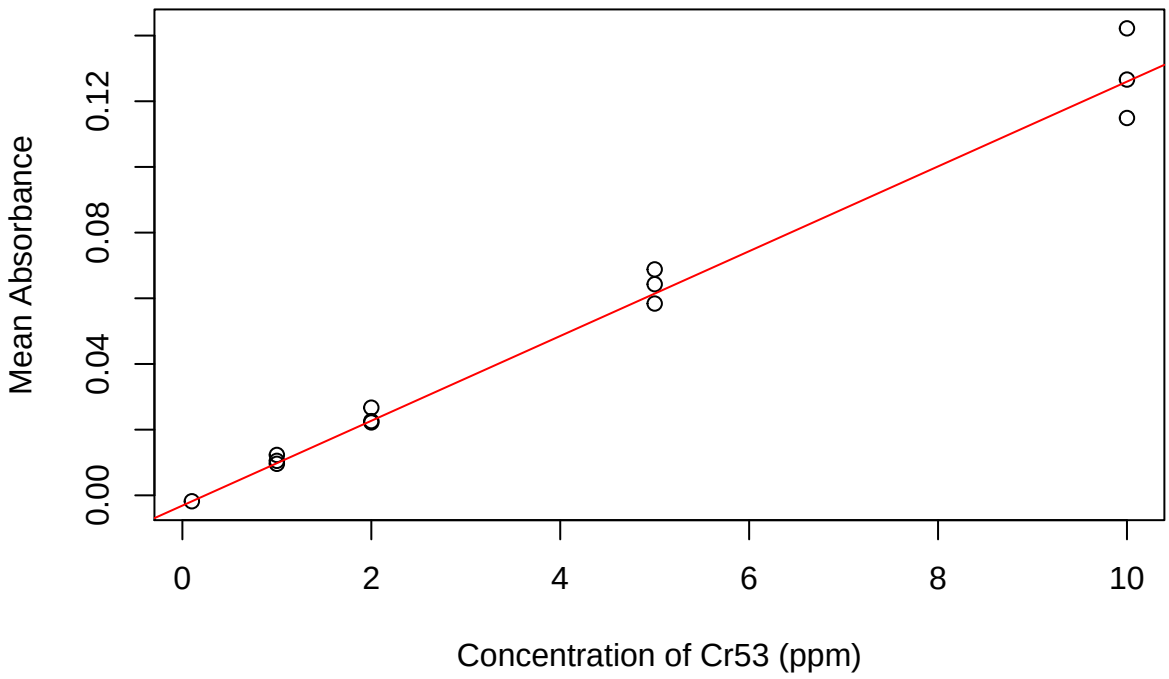
```
library(tidyverse)
library(readr)
```

```
AA <- read.csv("~/chem313/313_icpms/data/tidy_AA.csv") %>%
  mutate(rsd = as.numeric(percent_rsd)*100)
```

```
cal <- AA %>%
  filter(type != "Sample", percent_rsd != "HIGH") %>%
  select(mean_abs, rsd, concentration)
#weighted linear regression
w <- 1/(cal$mean_abs*cal$rsd)^2
model <- lm(cal$mean_abs ~ cal$concentration, weights = w)

slope <- model$coefficients[2]
intercept <- model$coefficients[1]
slope_std <- summary(model)$coefficients[2,2]
intercept_std <- summary(model)$coefficients[1,2]

plot(cal$mean_abs ~ cal$concentration,
       xlab = paste("Concentration of Cr53 (ppm)"),
       ylab = "Mean Absorbance") +
    abline(model, col = "red") +
    title(paste("Calibration for Cr53"))
```




```
## integer(0)
```

```
equation <- tibble(metal = "Cr53", slope, slope_std, intercept, intercept_std)
cal <- rbind(equation)
cal
```

```
## # A tibble: 1 x 5
##   metal  slope slope_std intercept intercept_std
##   <chr>  <dbl>     <dbl>     <dbl>         <dbl>
## 1 Cr53  0.0129  0.000112  -0.00312      0.000133
```

```
sample_sites <- unique(filter(AA, site != "MB", site != "")$site)
#inputs: unique_site (as a character)
#outputs: concentration vector
sample_analysis <- function(unique_site){
#unique_site <- "A"
  concentration_data <- NULL
  sample <- filter(AA, site == unique_site)
  data <- NULL
  for (ID in sample$sample_key){
    sample_data_aa <- filter(sample, sample_key == ID)

    m <- cal$slope
    b <- cal$intercept
    y <- sample_data_aa$mean_abs

    b_e <- cal$intercept_std
    m_e <- cal$slope_std
    x <- (y-b)/m #The units are dependent on the calibration standards (Kg/mL)

    RSD <- ((sample_data_aa$rsd/100)*sample_data_aa$mean_abs)
```

```
    abs <- sample_data_aa$mean_abs
    #error propagation
    e_yb <- sqrt((RSD)^2 + (b_e)^2) #error in y-b from calibration
    yb <- abs - b
    e_x <- x*sqrt((e_yb/yb)^2 +(m_e/m)^2) #error in x from calibration
    data <- rbind(data, data_frame(sample_key = ID, x, e_x))
    if(unique_site != "MB"){
      concentration_data <- data_frame(sample_key = sample_data_aa$sample_key,
                                       analyst = sample_data_aa$analyst,
                                       metal = "Cr53",
                                       site = unique_site,
                                       conc_dil = x,
                                       conc_dil_error = e_x) %>%
        rbind(concentration_data)
    }
    if (unique_site == "MB"){
      x <- mean(data$x)
      e_x <- sd(data$x)
      concentration_data <- data_frame(metal = "Cr53",
                                       site = unique_site,
                                       conc_dil = x,
                                       conc_dil_error = e_x) %>%
        rbind(concentration_data)
  }
  }

  return(concentration_data)
}
```

```
#inputs: a function
#outputs: a data frame with the function outputs from each site

run_sites <- function(Function){
  value <- NULL
  for (site in sample_sites){
    site_value <- Function(site)
    value <- rbind(site_value, value)
  }
  return(value)
}
```

```
MB <- sample_analysis("MB") #(ug/kg)
```

```
## Warning: `data_frame()` is deprecated as of tibble 1.1.0.
## Please use `tibble()` instead.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_warnings()` to see where this warning was generated.
```

```
uncor_sample <- run_sites(sample_analysis) #values do not account for dilutions (ug/kg)

MB
```

```
## # A tibble: 10 x 4
##    metal site  conc_dil conc_dil_error
##    <chr> <chr>    <dbl>          <dbl>
```

```
##  1 Cr53  MB      0.130          0.0464
##  2 Cr53  MB      0.134          0.0473
##  3 Cr53  MB      0.136          0.0502
##  4 Cr53  MB      0.132          0.0528
##  5 Cr53  MB      0.132          0.0578
##  6 Cr53  MB      0.129          0.0640
##  7 Cr53  MB      0.114          0.0634
##  8 Cr53  MB      0.0845         0.0272
##  9 Cr53  MB      0.0987         0.0164
## 10 Cr53  MB      0.110         NA
```

```
uncor_sample
```

```
## # A tibble: 34 x 6
##    sample_key analyst metal site  conc_dil conc_dil_error
##         <int> <fct>   <chr> <chr>    <dbl>          <dbl>
##  1         56 AVM     Cr53  A        0.769          23.2
##  2         54 LAK     Cr53  A        0.730          13.2
##  3         48 AH      Cr53  A        1.26           42.9
##  4         46 LML     Cr53  A        1.03           27.7
##  5         58 SS      Cr53  B        0.854          14.1
##  6         52 MF      Cr53  B        0.707          17.2
##  7         45 KAD     Cr53  B        0.738           8.92
##  8         41 LF      Cr53  B        0.691           1.80
##  9         40 AB      Cr53  B        0.622          15.2
## 10          6 MRMJ    Cr53  C        0.908          32.0
## # ... with 24 more rows
```

```
sample_data_mb <- NULL
#error propagation: subtraction of MB
conc_dil_blanked <- uncor_sample$conc_dil-MB$conc_dil
```

```
## Warning in uncor_sample$conc_dil - MB$conc_dil: longer object length is not a
## multiple of shorter object length
```

```
conc_dil_blanked_error <- sqrt(uncor_sample$conc_dil_error)^2 + (MB$conc_dil_error)^2
```

```
## Warning in sqrt(uncor_sample$conc_dil_error)^2 + (MB$conc_dil_error)^2: longer
## object length is not a multiple of shorter object length
```

```
sample_data_mb <- uncor_sample %>%
  mutate(conc_dil_blanked, conc_dil_blanked_error) %>%
  rbind(sample_data_mb)
sample_data_mb
```

```
## # A tibble: 34 x 8
##    sample_key analyst metal site  conc_dil conc_dil_error conc_dil_blanked
##         <int> <fct>   <chr> <chr>    <dbl>          <dbl>            <dbl>
##  1         56 AVM     Cr53  A        0.769          23.2             0.638
##  2         54 LAK     Cr53  A        0.730          13.2             0.596
##  3         48 AH      Cr53  A        1.26           42.9             1.13
##  4         46 LML     Cr53  A        1.03           27.7             0.900
##  5         58 SS      Cr53  B        0.854          14.1             0.722
##  6         52 MF      Cr53  B        0.707          17.2             0.578
##  7         45 KAD     Cr53  B        0.738           8.92            0.624
##  8         41 LF      Cr53  B        0.691           1.80            0.607
##  9         40 AB      Cr53  B        0.622          15.2             0.523
```

```
## 10          6 MRMJ    Cr53  C        0.908          32.0             0.798
## # ... with 24 more rows, and 1 more variable: conc_dil_blanked_error <dbl>
```

```
#error propagation
vol_e <- 1
mass_e <- 0.001
dil_1010_e <- sqrt(1^2 + 10^2)
dil_e <- sqrt((dil_1010_e/1010)^2 + (1/10)^2) #error in 101 dilution factor

#correct for dilution and propagate error
sample_data_aa <- merge(AA, sample_data_mb) %>%
  unique() %>%
  mutate(conc_blanked = conc_dil_blanked*(total_volume/1000)/(mass_of_soil/1000),
         conc_blanked_error = conc_blanked *
           sqrt((conc_dil_blanked_error/conc_dil_blanked)^2 +
           (dil_e/101)^2 +
           (mass_e/mass_of_soil)^2 +
           (vol_e/total_volume)^2),
         conc_unblanked = conc_dil*(total_volume/1000)/(mass_of_soil/1000),
         conc_unblanked_error = conc_unblanked*
           sqrt((conc_dil_error/conc_dil)^2 +
                  (dil_e/101)^2 +
                  (mass_e/mass_of_soil)^2 +
                  (vol_e/total_volume)^2)) %>%
  select(-concentration,
         -type,
         -mass_of_soil,
         -total_volume,
         -rsd,
         -conc_dil_blanked,
         -conc_dil_blanked_error,
         -conc_dil,
         -conc_dil_error,
         -mean_abs,
         -percent_rsd)
```

```
sample_conc_aa <- sample_data_aa %>%
  filter(site != "QC") %>%
  group_by(metal, site) %>%
  summarize(conc_mean = mean(conc_blanked),
            conc_sd = sd(conc_blanked),
            count = n()) %>%
  mutate(error = qnorm(0.975)*conc_sd/sqrt(count),
         lower_ci = conc_mean - error,
         upper_ci = conc_mean + error) %>%
  select(-count,
         -error)
```

```
## `summarise()` regrouping output by 'metal' (override with `.groups` argument)
```

```
write.csv(sample_conc_aa, "~/chem313/313_icpms/data/sample_aa.csv")
```

```
qc_conc_aa <- sample_data_aa %>%
  filter(site == "QC") %>%
  group_by(metal) %>%
  summarize(conc_mean = mean(conc_unblanked),
```

```
            conc_sd = sd(conc_unblanked),
            count = n()) %>%
  mutate(error = qnorm(0.975)*conc_sd/sqrt(count),
         lower_ci = conc_mean - error,
         upper_ci = conc_mean + error,
         mass_frac = conc_mean/1000) %>%
  select(-count,
         -error)
```

```
## `summarise()` ungrouping output (override with `.groups` argument)
```