Exercise 1

- The standard deviation of measurements at low level for a method for detecting benzene in blood is 52 ng/L.
    - What is the Critical Level if we use a 1% probability criterion?
    - What is the Minimum Detectable Value?
    - If we can use 52 ng/L as the standard deviation, what is a 95% confidence interval for the true concentration if the measured concentration is 175 ng/L?
    - If the CV at high levels is 12%, about what is the standard deviation at high levels for the natural log measured concentration? Find a 95% confidence interval for the concentration if the measured concentration is 1850 ng/L?

$$\sigma = 52 \text{ ng/L}$$

$$\alpha = 0.01$$

$$\beta = 0.01$$

$$\text{CL} = 0 + \sigma z(\alpha) = (52)(2.326) = 121 \text{ ng/L}$$

$$\text{MDV} = 0 + \sigma z(\alpha) + \sigma z(\beta) = (52)(2.326 + 2.326) = 242 \text{ ng/L}$$

$$\begin{aligned} 95\%\ \text{CI} &= 175 \pm (52)(1.960) \\ &= 175 \pm 102 \\ &= [73, 277] \text{ ng/L} \end{aligned}$$

If the high level CV is about 12%, then the natural log of the measurement has

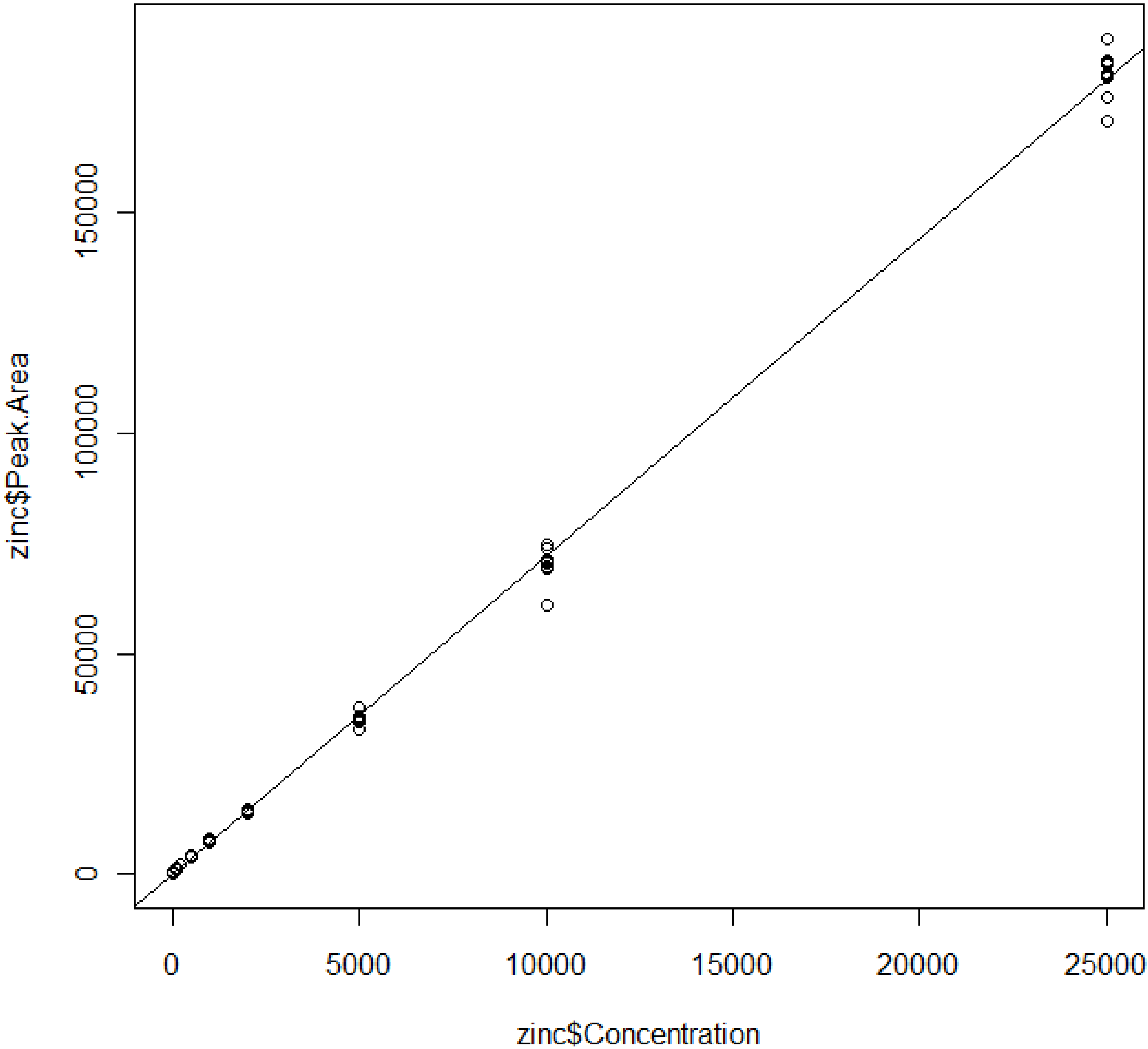
$$\sigma = 0.12$$

$$\begin{aligned} 95\%\ \text{CI} &= \ln(1850) \pm (0.12)(1.960) \\ &= 7.523 \pm 0.235 \\ &= [7.288, 7.758] \text{ in ln units} \\ &= [1462, 2341] \text{ ng/L} \end{aligned}$$

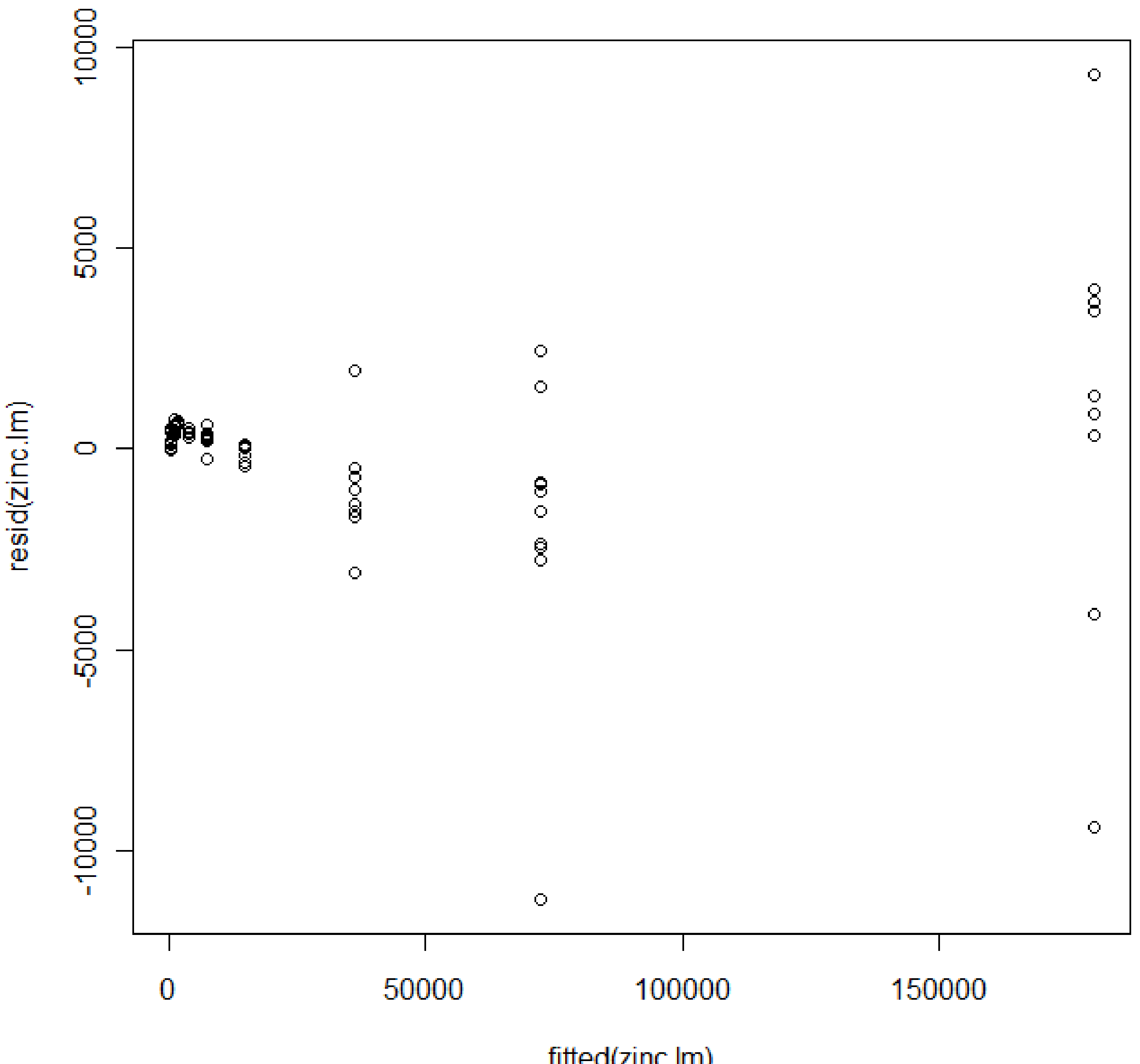
Exercise 2

- Download data on measurement of zinc in water by ICP/MS (“Zinc.csv”). Use read.csv() to load.
- Conduct a regression analysis in which you predict peak area from concentration
- Which of the usual regression assumptions appears to be satisfied and which do not?
- What would the estimated concentration be if the peak area of a new sample was 1850?
- From the blanks part of the data, how big should a result be to indicate the presence of zinc with some degree of certainty?

```
zinc <- read.csv("zinc.csv")
> names(zinc)
[1] "Concentration" "Peak.Area"
> zinc.lm <- lm(Peak.Area ~ Concentration,data=zinc)
> summary(zinc.lm)

Call:
lm(formula = Peak.Area ~ Concentration, data = zinc)

Residuals:
      Min         1Q    Median        3Q       Max
-11242.22    -82.01    333.28    485.89   9353.28

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)   104.5429   267.1370   0.391    0.696
Concentration   7.2080     0.0307 234.769   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2201 on 89 degrees of freedom
Multiple R-squared: 0.9984,     Adjusted R-squared: 0.9984
F-statistic: 5.512e+04 on 1 and 89 DF,  p-value: < 2.2e-16

> plot(zinc$Concentration,zinc$Peak.Area)
> abline(coef(zinc.lm))
> plot(fitted(zinc.lm),resid(zinc.lm))
> (1850-104.5429)/7.2080
[1] 242.1555
```



zinc$Peak.Area
0
50000
100000
150000
0
5000
10000
15000
20000
25000
zinc$Concentration


10000
5000
0
-5000
-10000
resid(zinc.lm)
0
50000
100000
150000
fitted(zinc.lm)

```
> zinc[zinc$Concentration==0,]
  Concentration Peak.Area
1             0       115
2             0       631
3             0       508
4             0       317
5             0       220
6             0        93
7             0        99
8             0       135

> mean(zinc[zinc$Concentration==0,2])
[1] 264.75

> sd(zinc[zinc$Concentration==0,2])
[1] 205.0343

264.75+2.326*205.3
[1] 742.2778
```

The CL in peak area terms is 742, with zero concentration indicated at 265.
The CL in ppt is
$(742 - 104.5429)/7.2080 = 88$ ppt.
The MDV is 176 ppt.

No samples for true concentrations of 0, 10, or 20 had peak areas above the CL.
For the samples at 100ppt or above, all had peak areas above the CL of 742.

References

- Lloyd Currie (1995) “Nomenclature in Evaluation of Analytical Methods Including Detection and Quantification Capabilities,” *Pure & Applied Chemistry*, **67**, 1699–1723.
- David M. Rocke and Stefan Lorenzato (1995) “A Two-Component Model For Measurement Error In Analytical Chemistry,” *Technometrics*, **37**, 176–184.
- Machelle Wilson, David M. Rocke, Blythe Durbin, and Henry Kahn (2004) “Detection Limits And Goodness-of-Fit Measures For The Two-component Model Of Chemical Analytical Error,” *Analytica Chimica Acta*, **509**, 197–208.