aflevering

2023-10-17

Part I

1.

```
control <- toxData %>% filter(conc == 0)
mod <- lmer(fluorescence ~ day-1 + (1|plate) , data = control)
confint(mod)
```

```
## Computing profile confidence intervals ...
```

```
##            2.5 %    97.5 %
## .sig01  143.0122  441.2169
## .sigma  110.7260  166.1850
## day1    515.5940 1270.2631
## day2   2084.4615 2699.6218
## day3   2183.7303 2937.1447
```

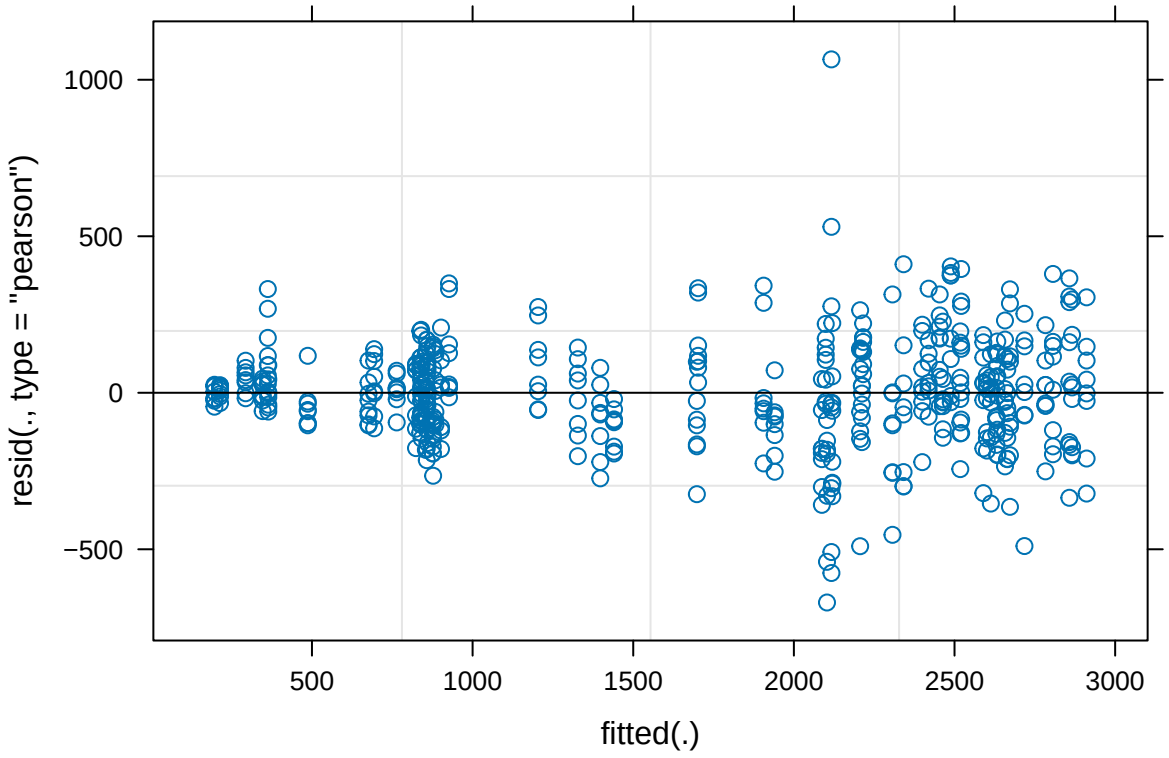
2.

Somewhat difference

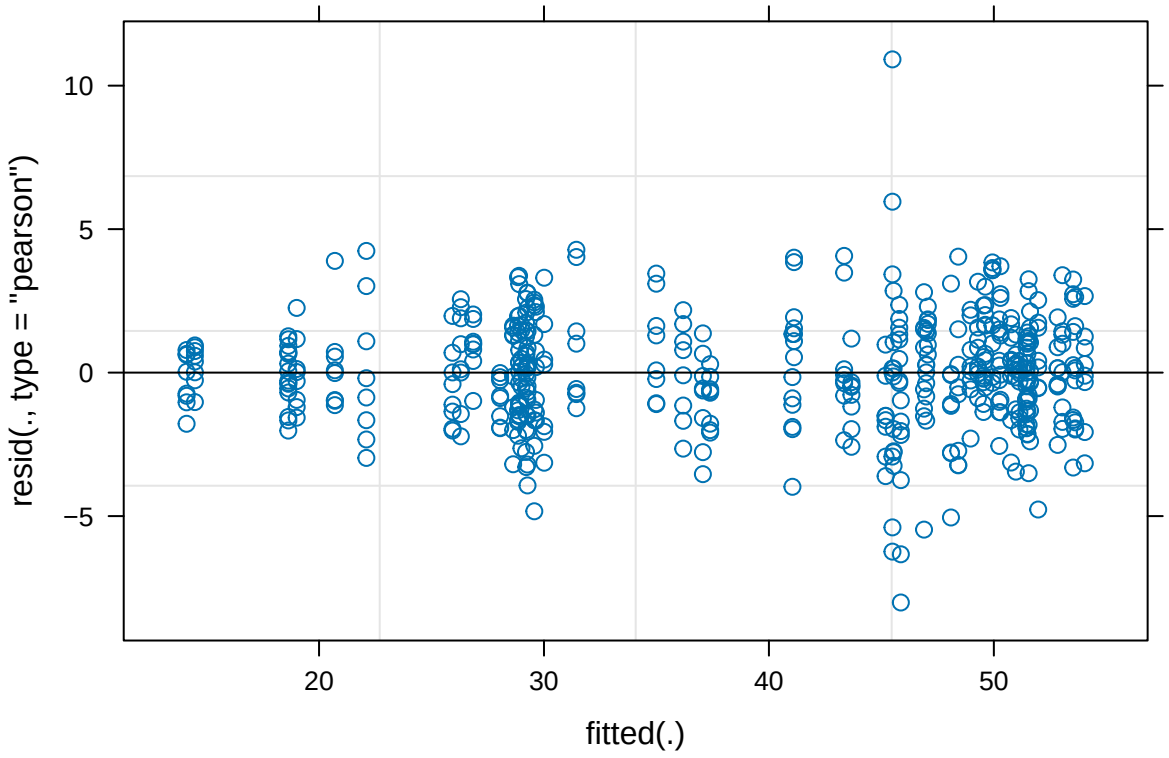
Part II

```
mod <- lmer(fluorescence ~ day*concFac-1 + (1|plate) , data = toxData)
mod_sqrt <- lmer(sqrt(fluorescence) ~ day*concFac + (1|plate) , data = toxData)
mod_log <- lmer(log(fluorescence) ~ day*concFac-1 + (1|plate) , data = toxData)
```

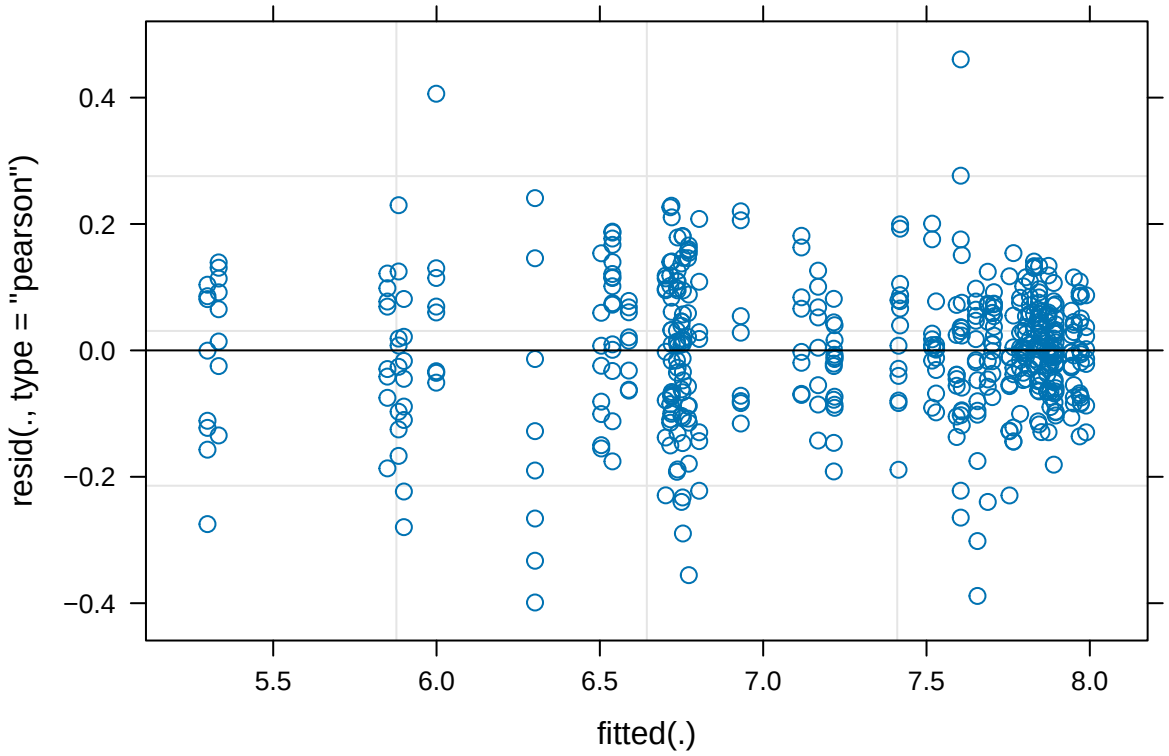
```
plot_mod <- function(mod, name){
  resid <- mod %>% residuals(type = "pearson")
  fitted <- mod %>% fitted()
  for_plot <- tibble(residuals = resid, fitted = fitted)
  for_plot %>% ggplot(aes(x=fitted, y = residuals)) + geom_point() + geom_hline(yintercept = 0) + theme_
}

mod %>% plot()
```




```
mod_sqrt %>% plot()
```



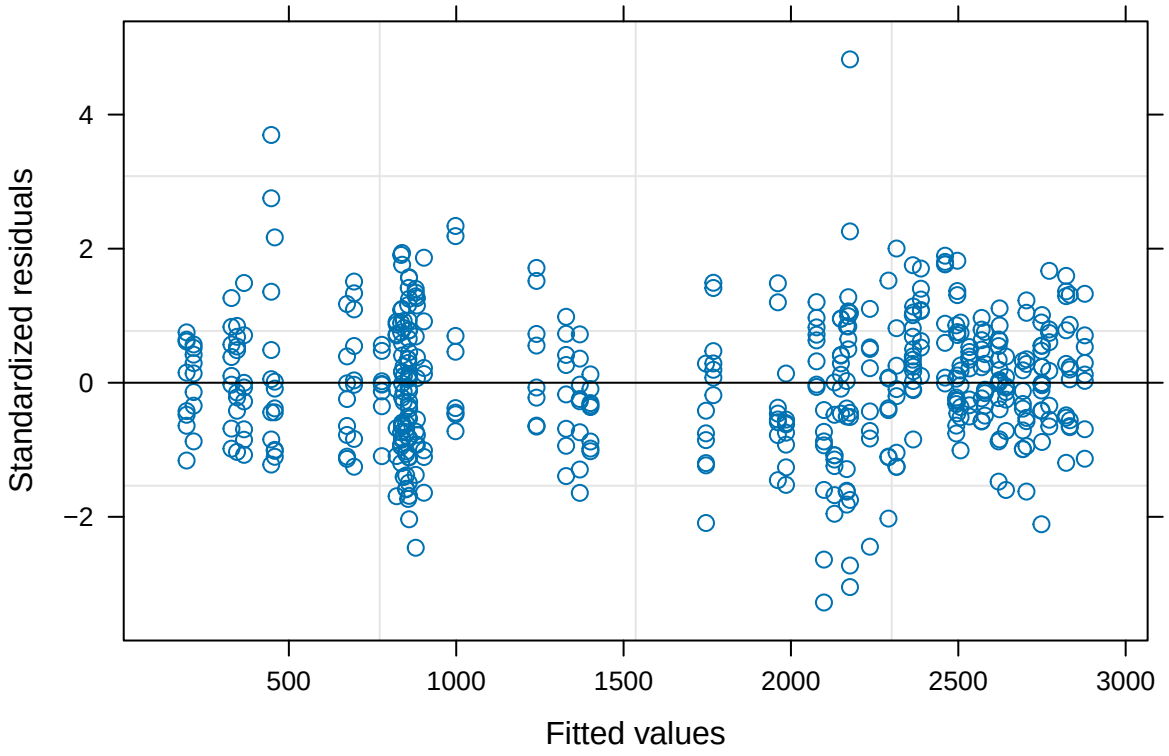

```
mod_log %>% plot()
```



We go log

4.

```
new_mod <- lme(fluorescence ~ day*concFac, random=~1|plate, data=toxData,
weights = varPower(form=~fitted(.)))
new_mod %>% plot()
```




```
summary(new_mod)
```

```
## Linear mixed-effects model fit by REML
##   Data: toxData
##        AIC      BIC    logLik
##   6218.882 6343.527 -3079.441
##
## Random effects:
##  Formula: ~1 | plate
##         (Intercept)  Residual
## StdDev:    159.7021 0.8225523
##
## Variance function:
##  Structure: Power of variance covariate
##  Formula: ~fitted(.)
##  Parameter estimates:
##     power
## 0.7202027
## Fixed effects:  fluorescence ~ day * concFac
##                         Value Std.Error  DF    t-value p-value
## (Intercept)          893.0931 116.67283 467   7.654679  0.0000
## day2                1481.5202 155.39486   4   9.533907  0.0007
## day3                1665.6699 172.59820   4   9.650564  0.0006
## concFac0.005         -24.4782  39.79025 467  -0.615181  0.5387
## concFac0.0158        -44.5094  39.48871 467  -1.127143  0.2603
## concFac0.05          -44.1773  39.49370 467  -1.118591  0.2639
```

```
## concFac0.158         -47.0214  39.45096 467  -1.191896  0.2339
## concFac0.5           -60.5521  39.24781 467  -1.542814  0.1236
## concFac1.58         -208.8120  37.05301 467  -5.635495  0.0000
## concFac5            -537.4895  32.55303 467 -16.511199  0.0000
## concFac15.8         -688.1037  30.82601 467 -22.322181  0.0000
## day2:concFac0.005   -337.3375  73.74311 467  -4.574496  0.0000
## day3:concFac0.005    223.3352  93.93503 467   2.377549  0.0178
## day2:concFac0.0158  -124.6180  73.58821 467  -1.693451  0.0910
## day3:concFac0.0158   192.9133  93.27167 467   2.068295  0.0392
## day2:concFac0.05    -100.6919  73.79072 467  -1.364561  0.1730
## day3:concFac0.05     298.5788  94.40136 467   3.162865  0.0017
## day2:concFac0.158     83.6430  75.27540 467   1.111160  0.2671
## day3:concFac0.158    256.6344  93.90627 467   2.732878  0.0065
## day2:concFac0.5      106.8776  75.25042 467   1.420293  0.1562
## day3:concFac0.5      187.0477  92.93732 467   2.012622  0.0447
## day2:concFac1.58    -175.0767  71.10738 467  -2.462145  0.0142
## day3:concFac1.58     -49.3415  87.95306 467  -0.560998  0.5751
## day2:concFac5       -594.6452  62.20532 467  -9.559394  0.0000
## day3:concFac5       -716.6774  76.01794 467  -9.427741  0.0000
## day2:concFac15.8    -994.5789  57.40552 467 -17.325493  0.0000
## day3:concFac15.8   -1477.4286  67.83022 467 -21.781275  0.0000
##  Correlation:
##                    (Intr) day2   day3   cF0.00 cF0.01 cF0.05 cF0.15 cnF0.5
## day2               -0.751
## day3               -0.676  0.508
## concFac0.005       -0.185  0.139  0.125
## concFac0.0158      -0.187  0.140  0.126  0.547
## concFac0.05        -0.187  0.140  0.126  0.547  0.552
## concFac0.158       -0.187  0.140  0.126  0.548  0.552  0.552
## concFac0.5         -0.188  0.141  0.127  0.551  0.555  0.555  0.556
## concFac1.58        -0.199  0.149  0.134  0.583  0.588  0.588  0.588  0.591
## concFac5           -0.226  0.170  0.153  0.664  0.669  0.669  0.670  0.673
## concFac15.8        -0.239  0.180  0.162  0.701  0.707  0.707  0.707  0.711
## day2:concFac0.005   0.100 -0.252 -0.068 -0.540 -0.295 -0.295 -0.296 -0.297
## day3:concFac0.005   0.078 -0.059 -0.264 -0.424 -0.232 -0.232 -0.232 -0.233
## day2:concFac0.0158  0.100 -0.253 -0.068 -0.294 -0.537 -0.296 -0.296 -0.298
## day3:concFac0.0158  0.079 -0.059 -0.266 -0.232 -0.423 -0.234 -0.234 -0.235
## day2:concFac0.05    0.100 -0.252 -0.068 -0.293 -0.295 -0.535 -0.295 -0.297
## day3:concFac0.05    0.078 -0.059 -0.263 -0.229 -0.231 -0.418 -0.231 -0.232
## day2:concFac0.158   0.098 -0.247 -0.066 -0.287 -0.289 -0.289 -0.524 -0.291
## day3:concFac0.158   0.079 -0.059 -0.264 -0.230 -0.232 -0.232 -0.420 -0.233
## day2:concFac0.5     0.098 -0.247 -0.066 -0.287 -0.289 -0.289 -0.290 -0.522
## day3:concFac0.5     0.079 -0.060 -0.267 -0.233 -0.234 -0.234 -0.235 -0.422
## day2:concFac1.58    0.104 -0.262 -0.070 -0.304 -0.306 -0.306 -0.307 -0.308
## day3:concFac1.58    0.084 -0.063 -0.282 -0.246 -0.248 -0.248 -0.248 -0.249
## day2:concFac5       0.119 -0.299 -0.080 -0.348 -0.350 -0.350 -0.351 -0.352
## day3:concFac5       0.097 -0.073 -0.327 -0.284 -0.287 -0.287 -0.287 -0.288
## day2:concFac15.8    0.128 -0.324 -0.087 -0.377 -0.379 -0.379 -0.380 -0.382
## day3:concFac15.8    0.109 -0.082 -0.366 -0.319 -0.321 -0.321 -0.321 -0.323
##                    cF1.58 cncFc5 cF15.8 d2:F0.00 d3:F0.00 d2:F0.01 d3:F0.01
## day2
## day3
## concFac0.005
## concFac0.0158
```

```
## concFac0.05
## concFac0.158
## concFac0.5
## concFac1.58
## concFac5            0.713
## concFac15.8         0.753  0.857
## day2:concFac0.005  -0.315 -0.358 -0.378
## day3:concFac0.005  -0.247 -0.281 -0.297  0.229
## day2:concFac0.0158 -0.315 -0.359 -0.379  0.533    0.124
## day3:concFac0.0158 -0.249 -0.283 -0.299  0.125    0.489    0.227
## day2:concFac0.05   -0.315 -0.358 -0.378  0.532    0.124    0.533    0.125
## day3:concFac0.05   -0.246 -0.280 -0.296  0.124    0.483    0.124    0.487
## day2:concFac0.158  -0.308 -0.351 -0.371  0.521    0.122    0.522    0.123
## day3:concFac0.158  -0.247 -0.281 -0.297  0.124    0.486    0.124    0.489
## day2:concFac0.5    -0.308 -0.351 -0.371  0.521    0.122    0.522    0.123
## day3:concFac0.5    -0.250 -0.284 -0.300  0.126    0.491    0.126    0.494
## day2:concFac1.58   -0.521 -0.372 -0.392  0.552    0.129    0.553    0.130
## day3:concFac1.58   -0.421 -0.300 -0.317  0.133    0.519    0.133    0.522
## day2:concFac5      -0.373 -0.523 -0.449  0.631    0.147    0.632    0.148
## day3:concFac5      -0.305 -0.428 -0.367  0.153    0.600    0.154    0.604
## day2:concFac15.8   -0.404 -0.460 -0.537  0.683    0.160    0.685    0.161
## day3:concFac15.8   -0.342 -0.390 -0.454  0.172    0.673    0.172    0.677
##                    d2:F0.05 d3:F0.05 d2:F0.1 d3:F0.1 d2:F0.5 d3:F0.5 d2:F1.
## day2
## day3
## concFac0.005
## concFac0.0158
## concFac0.05
## concFac0.158
## concFac0.5
## concFac1.58
## concFac5
## concFac15.8
## day2:concFac0.005
## day3:concFac0.005
## day2:concFac0.0158
## day3:concFac0.0158
## day2:concFac0.05
## day3:concFac0.05    0.224
## day2:concFac0.158   0.521    0.121
## day3:concFac0.158   0.124    0.483    0.220
## day2:concFac0.5     0.521    0.121    0.511   0.122
## day3:concFac0.5     0.125    0.488    0.123   0.491   0.220
## day2:concFac1.58    0.551    0.128    0.540   0.129   0.541   0.130
## day3:concFac1.58    0.133    0.516    0.130   0.519   0.130   0.524   0.220
## day2:concFac5       0.630    0.146    0.618   0.147   0.618   0.149   0.654
## day3:concFac5       0.153    0.597    0.150   0.600   0.150   0.607   0.159
## day2:concFac15.8    0.683    0.159    0.669   0.160   0.670   0.161   0.708
## day3:concFac15.8    0.172    0.669    0.168   0.673   0.169   0.680   0.178
##                    d3:F1. dy2:F5 dy3:F5 d2:F15
## day2
## day3
## concFac0.005
## concFac0.0158
```

```
## concFac0.05
## concFac0.158
## concFac0.5
## concFac1.58
## concFac5
## concFac15.8
## day2:concFac0.005
## day3:concFac0.005
## day2:concFac0.0158
## day3:concFac0.0158
## day2:concFac0.05
## day3:concFac0.05
## day2:concFac0.158
## day3:concFac0.158
## day2:concFac0.5
## day3:concFac0.5
## day2:concFac1.58
## day3:concFac1.58
## day2:concFac5       0.157
## day3:concFac5       0.641  0.224
## day2:concFac15.8    0.170  0.811  0.197
## day3:concFac15.8    0.718  0.204  0.831  0.244
##
## Standardized Within-Group Residuals:
##          Min           Q1          Med           Q3          Max
## -3.278168327 -0.648805182 -0.009855112  0.634164702  4.823772219
##
## Number of Observations: 498
## Number of Groups: 7
```

We go log still

5.

Estimates

```
reparm_log <- lmer(log(fluorescence) ~ day*concFac-1 + (1|plate) , data = toxData)
(reparm_log %>% fixef())[c(1,2,3)] %>% exp()
```

```
##      day1      day2      day3
##  886.2118 2361.3400 2554.9882
```

confints. This is the median.

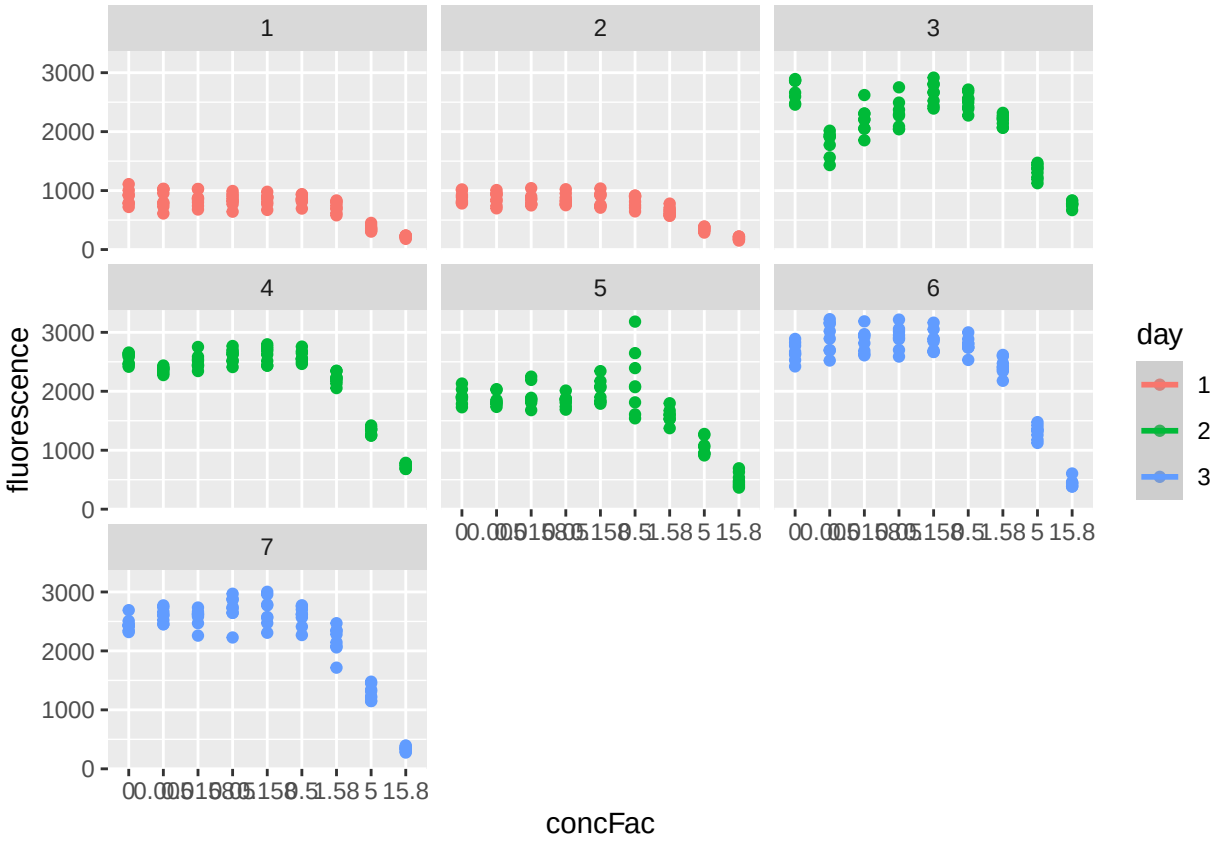
```
((reparm_log %>% confint()))[c(3,4,5),] %>% exp()
```

```
## Computing profile confidence intervals ...
```

```
##          2.5 %   97.5 %
## day1  764.2077 1027.694
## day2 2094.2014 2662.555
## day3 2205.6196 2959.697
```

```
toxData %>% ggplot(aes(x = concFac, y = fluorescence, color = day)) + geom_point() + geom_smooth(method=
```

```
## `geom_smooth()` using formula = 'y ~ x'
```



6

Want the concentration that gives half fluoresence corresponding to the baseline conc.

$$E(\log(f_b/2)) = E(log(f_b)) - \log(2)$$

Part III

8.

math. B_i are estimates of EC50 per day and D_i are estimates for baseline per day.

9.

10.

IV

11

```
library(rstan)
```

```
## Warning: package 'rstan' was built under R version 4.3.2
## Loading required package: StanHeaders
## Warning: package 'StanHeaders' was built under R version 4.3.2
##
## rstan version 2.32.3 (Stan version 2.26.1)
```

```
## For execution on a local, multicore CPU with excess RAM we recommend calling
## options(mc.cores = parallel::detectCores()).
## To avoid recompilation of unchanged Stan programs, we recommend calling
## rstan_options(auto_write = TRUE)
## For within-chain threading using `reduce_sum()` or `map_rect()` Stan functions,
## change `threads_per_chain` option:
## rstan_options(threads_per_chain = 1)
```

```
## Do not specify '-march=native' in 'LOCAL_CPPFLAGS' or a Makevars file
```

```
to_stan <- "data {
int N;
vector[N] day1dummy;
vector[N] day2dummy;
vector[N] day3dummy;
vector[N] Z;
vector[N] SE;
}
parameters {
real theta_1;
real theta_2;
real theta_3;
real<lower = 0> tau;
}
transformed parameters {
real ratio_3_1 = theta_3/theta_1;
}
model {
Z ~ normal(theta_1*day1dummy + theta_2*day2dummy + theta_3*day3dummy, sqrt(tau^2 + SE^2));
}
"
write(to_stan, file = "model.stan")
```

```
data <- list(N = length(bData$Estimate), Z=bData$Estimate, day1dummy = bData$day1dummy,
             day2dummy = bData$day2dummy, day3dummy = bData$day3dummy, SE = bData$SE)
fitted <- rstan::stan("model.stan", data = data, iter = 32000, chains = 4)
```

```
##
## SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 1).
## Chain 1:
## Chain 1: Gradient evaluation took 4.9e-05 seconds
## Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 0.49 seconds.
## Chain 1: Adjust your expectations accordingly!
## Chain 1:
## Chain 1:
## Chain 1: Iteration:     1 / 32000 [  0%]  (Warmup)
## Chain 1: Iteration:  3200 / 32000 [ 10%]  (Warmup)
## Chain 1: Iteration:  6400 / 32000 [ 20%]  (Warmup)
## Chain 1: Iteration:  9600 / 32000 [ 30%]  (Warmup)
## Chain 1: Iteration: 12800 / 32000 [ 40%]  (Warmup)
## Chain 1: Iteration: 16000 / 32000 [ 50%]  (Warmup)
## Chain 1: Iteration: 16001 / 32000 [ 50%]  (Sampling)
## Chain 1: Iteration: 19200 / 32000 [ 60%]  (Sampling)
## Chain 1: Iteration: 22400 / 32000 [ 70%]  (Sampling)
## Chain 1: Iteration: 25600 / 32000 [ 80%]  (Sampling)
```

```
## Chain 1: Iteration: 28800 / 32000 [ 90%]  (Sampling)
## Chain 1: Iteration: 32000 / 32000 [100%]  (Sampling)
## Chain 1:
## Chain 1:  Elapsed Time: 2.36 seconds (Warm-up)
## Chain 1:                2.653 seconds (Sampling)
## Chain 1:                5.013 seconds (Total)
## Chain 1:
##
## SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 2).
## Chain 2:
## Chain 2: Gradient evaluation took 2.8e-05 seconds
## Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 0.28 seconds.
## Chain 2: Adjust your expectations accordingly!
## Chain 2:
## Chain 2:
## Chain 2: Iteration:     1 / 32000 [  0%]  (Warmup)
## Chain 2: Iteration:  3200 / 32000 [ 10%]  (Warmup)
## Chain 2: Iteration:  6400 / 32000 [ 20%]  (Warmup)
## Chain 2: Iteration:  9600 / 32000 [ 30%]  (Warmup)
## Chain 2: Iteration: 12800 / 32000 [ 40%]  (Warmup)
## Chain 2: Iteration: 16000 / 32000 [ 50%]  (Warmup)
## Chain 2: Iteration: 16001 / 32000 [ 50%]  (Sampling)
## Chain 2: Iteration: 19200 / 32000 [ 60%]  (Sampling)
## Chain 2: Iteration: 22400 / 32000 [ 70%]  (Sampling)
## Chain 2: Iteration: 25600 / 32000 [ 80%]  (Sampling)
## Chain 2: Iteration: 28800 / 32000 [ 90%]  (Sampling)
## Chain 2: Iteration: 32000 / 32000 [100%]  (Sampling)
## Chain 2:
## Chain 2:  Elapsed Time: 2.476 seconds (Warm-up)
## Chain 2:                3.057 seconds (Sampling)
## Chain 2:                5.533 seconds (Total)
## Chain 2:
##
## SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 3).
## Chain 3:
## Chain 3: Gradient evaluation took 2.4e-05 seconds
## Chain 3: 1000 transitions using 10 leapfrog steps per transition would take 0.24 seconds.
## Chain 3: Adjust your expectations accordingly!
## Chain 3:
## Chain 3:
## Chain 3: Iteration:     1 / 32000 [  0%]  (Warmup)
## Chain 3: Iteration:  3200 / 32000 [ 10%]  (Warmup)
## Chain 3: Iteration:  6400 / 32000 [ 20%]  (Warmup)
## Chain 3: Iteration:  9600 / 32000 [ 30%]  (Warmup)
## Chain 3: Iteration: 12800 / 32000 [ 40%]  (Warmup)
## Chain 3: Iteration: 16000 / 32000 [ 50%]  (Warmup)
## Chain 3: Iteration: 16001 / 32000 [ 50%]  (Sampling)
## Chain 3: Iteration: 19200 / 32000 [ 60%]  (Sampling)
## Chain 3: Iteration: 22400 / 32000 [ 70%]  (Sampling)
## Chain 3: Iteration: 25600 / 32000 [ 80%]  (Sampling)
## Chain 3: Iteration: 28800 / 32000 [ 90%]  (Sampling)
## Chain 3: Iteration: 32000 / 32000 [100%]  (Sampling)
## Chain 3:
## Chain 3:  Elapsed Time: 2.377 seconds (Warm-up)
```

```
## Chain 3:                2.521 seconds (Sampling)
## Chain 3:                4.898 seconds (Total)
## Chain 3:
##
## SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 4).
## Chain 4:
## Chain 4: Gradient evaluation took 2.3e-05 seconds
## Chain 4: 1000 transitions using 10 leapfrog steps per transition would take 0.23 seconds.
## Chain 4: Adjust your expectations accordingly!
## Chain 4:
## Chain 4:
## Chain 4: Iteration:     1 / 32000 [  0%]  (Warmup)
## Chain 4: Iteration:  3200 / 32000 [ 10%]  (Warmup)
## Chain 4: Iteration:  6400 / 32000 [ 20%]  (Warmup)
## Chain 4: Iteration:  9600 / 32000 [ 30%]  (Warmup)
## Chain 4: Iteration: 12800 / 32000 [ 40%]  (Warmup)
## Chain 4: Iteration: 16000 / 32000 [ 50%]  (Warmup)
## Chain 4: Iteration: 16001 / 32000 [ 50%]  (Sampling)
## Chain 4: Iteration: 19200 / 32000 [ 60%]  (Sampling)
## Chain 4: Iteration: 22400 / 32000 [ 70%]  (Sampling)
## Chain 4: Iteration: 25600 / 32000 [ 80%]  (Sampling)
## Chain 4: Iteration: 28800 / 32000 [ 90%]  (Sampling)
## Chain 4: Iteration: 32000 / 32000 [100%]  (Sampling)
## Chain 4:
## Chain 4:  Elapsed Time: 2.327 seconds (Warm-up)
## Chain 4:                2.714 seconds (Sampling)
## Chain 4:                5.041 seconds (Total)
## Chain 4:
```

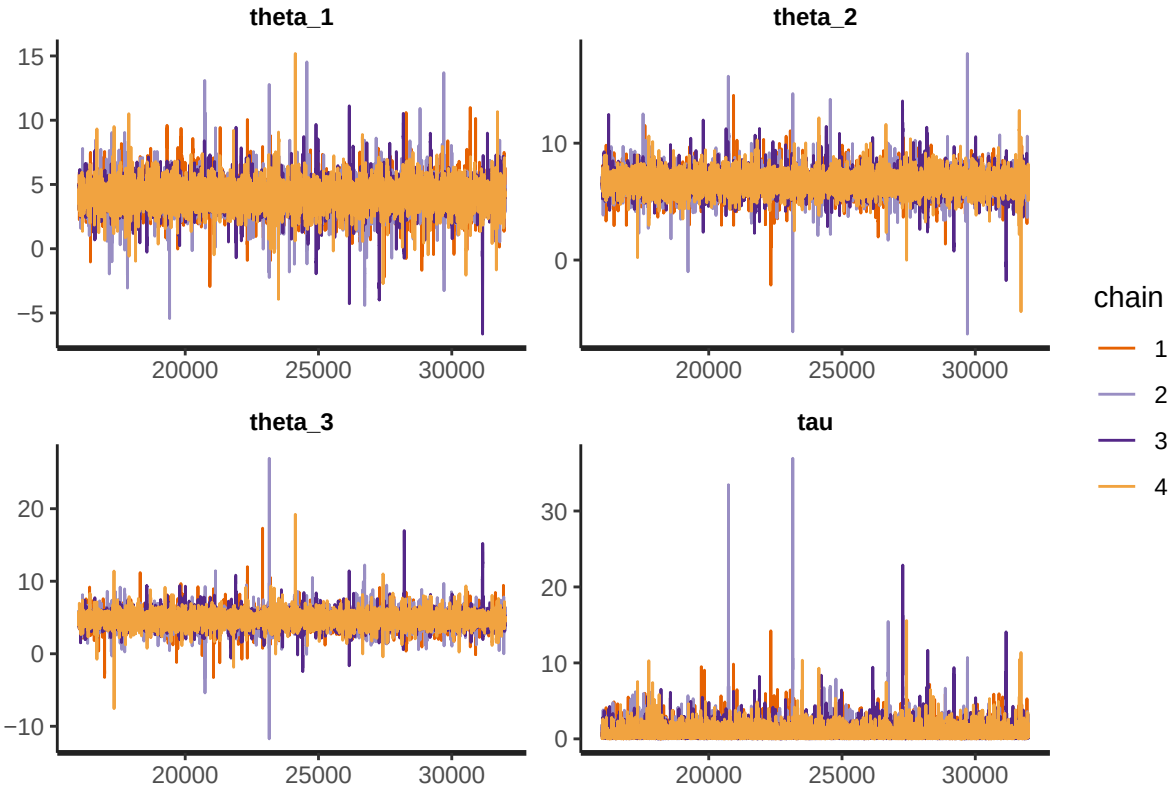
```
## Warning: There were 6 divergent transitions after warmup. See
## https://mc-stan.org/misc/warnings.html#divergent-transitions-after-warmup
## to find out why this is a problem and how to eliminate them.
```

```
## Warning: Examine the pairs() plot to diagnose sampling problems
```

```
fitted
```

```
## Inference for Stan model: anon_model.
## 4 chains, each with iter=32000; warmup=16000; thin=1;
## post-warmup draws per chain=16000, total post-warmup draws=64000.
##
##            mean se_mean   sd  2.5%   25%   50%   75% 97.5% n_eff Rhat
## theta_1    4.14    0.00 0.75  2.73  3.83  4.14  4.45  5.58 22860    1
## theta_2    6.62    0.00 0.65  5.46  6.31  6.60  6.91  7.87 29628    1
## theta_3    4.74    0.00 0.74  3.36  4.46  4.73  5.01  6.11 22372    1
## tau        0.70    0.01 0.75  0.03  0.28  0.53  0.89  2.39  8500    1
## ratio_3_1  1.17    0.01 3.55  0.71  1.04  1.14  1.26  1.82 65282    1
## lp__      -2.00    0.02 2.20 -7.69 -2.98 -1.44 -0.43  0.57  8710    1
##
## Samples were drawn using NUTS(diag_e) at Fri Jan 12 10:43:38 2024.
## For each parameter, n_eff is a crude measure of effective sample size,
## and Rhat is the potential scale reduction factor on split chains (at
## convergence, Rhat=1).
```

```
traceplot(fitted, pars = c("theta_1","theta_2","theta_3","tau"))
```


theta_1
theta_2
theta_3
tau
15
10
5
0
−5
10
0
20
10
0
−10
30
20
10
0
20000
25000
30000
chain
1
2
3
4