regressions

Load libraries

```
library(readxl)
library(here)
```

```
here() starts at /Users/updates1/Downloads/tandy_foram_cal2
```

```
library(bayclumpr)
```

Test 1

Calibration

```
Table1 <- read_excel(here("data", "Test 1.xlsx"))
Table1$Material <- rep(1, nrow(Table1))
colnames(Table1)[c(5, 6, 2, 3, 8)] <- c("D47", "D47error", "Temperature", "TempError", "Ion")

# Check basic regression model
lm(Table1$D47 ~ Table1$Temperature)
```

```
Call:
lm(formula = Table1$D47 ~ Table1$Temperature)

Coefficients:
       (Intercept)  Table1$Temperature
            0.2981              0.0277
```

```r
# Fit Bayesian regression
ionmodel <- cal.ion.bayesian(calibrationData = Table1,
                             IonError = Table1$`Ion error`[1])
```

```
Trying to compile a simple C file

Running /Library/Frameworks/R.framework/Resources/bin/R CMD SHLIB foo.c
using C compiler: 'Apple clang version 14.0.3 (clang-1403.0.22.14.1)'
using SDK: 'MacOSX13.3.sdk'
clang -arch x86_64 -I"/Library/Frameworks/R.framework/Resources/include" -DNDEBUG   -I"/Libra
In file included from <built-in>:1:
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/S
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
/Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/RcppEigen/include/Eigen
#include <cmath>
         ^~~~~~~
1 error generated.
make: *** [foo.o] Error 1

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 1).

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 2).
Chain 1:
Chain 1: Gradient evaluation took 8.2e-05 seconds
Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 0.82 seconds.
Chain 1: Adjust your expectations accordingly!
Chain 1:
Chain 1:
Chain 2:
Chain 2: Gradient evaluation took 7.8e-05 seconds
Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 0.78 seconds.
Chain 2: Adjust your expectations accordingly!
Chain 2:
Chain 2:
Chain 1: Iteration:    1 / 2500 [  0%]  (Warmup)
Chain 2: Iteration:    1 / 2500 [  0%]  (Warmup)
Chain 1: Iteration:  250 / 2500 [ 10%]  (Warmup)
Chain 2: Iteration:  250 / 2500 [ 10%]  (Warmup)
Chain 1: Iteration:  500 / 2500 [ 20%]  (Warmup)
Chain 2: Iteration:  500 / 2500 [ 20%]  (Warmup)
Chain 1: Iteration:  750 / 2500 [ 30%]  (Warmup)
```

```
Chain 2: Iteration:  750 / 2500 [ 30%]  (Warmup)
Chain 1: Iteration: 1000 / 2500 [ 40%]  (Warmup)
Chain 1: Iteration: 1001 / 2500 [ 40%]  (Sampling)
Chain 2: Iteration: 1000 / 2500 [ 40%]  (Warmup)
Chain 2: Iteration: 1001 / 2500 [ 40%]  (Sampling)
Chain 1: Iteration: 1250 / 2500 [ 50%]  (Sampling)
Chain 2: Iteration: 1250 / 2500 [ 50%]  (Sampling)
Chain 1: Iteration: 1500 / 2500 [ 60%]  (Sampling)
Chain 2: Iteration: 1500 / 2500 [ 60%]  (Sampling)
Chain 1: Iteration: 1750 / 2500 [ 70%]  (Sampling)
Chain 2: Iteration: 1750 / 2500 [ 70%]  (Sampling)
Chain 1: Iteration: 2000 / 2500 [ 80%]  (Sampling)
Chain 2: Iteration: 2000 / 2500 [ 80%]  (Sampling)
Chain 1: Iteration: 2250 / 2500 [ 90%]  (Sampling)
Chain 2: Iteration: 2250 / 2500 [ 90%]  (Sampling)
Chain 1: Iteration: 2500 / 2500 [100%]  (Sampling)
Chain 1:
Chain 1:  Elapsed Time: 7.127 seconds (Warm-up)
Chain 1:                7.347 seconds (Sampling)
Chain 1:                14.474 seconds (Total)
Chain 1:
Chain 2: Iteration: 2500 / 2500 [100%]  (Sampling)
Chain 2:
Chain 2:  Elapsed Time: 7.419 seconds (Warm-up)
Chain 2:                7.509 seconds (Sampling)
Chain 2:                14.928 seconds (Total)
Chain 2:
```

```r
parameters <- data.frame(rstan::summary(ionmodel[[1]])$summary)
parameters
```

```
              mean      se_mean           sd        X2.5.         X25.
alpha 1.874393e-01 1.002284e-03 4.209427e-02 1.042909e-01 1.589569e-01
beta  3.568244e-02 7.545035e-05 3.173264e-03 2.938559e-02 3.360510e-02
gamma 1.915828e-04 1.130581e-06 5.163513e-05 9.018044e-05 1.564742e-04
sigma 1.129180e-02 2.523088e-05 1.161702e-03 9.214442e-03 1.048775e-02
lp__  1.343750e+02 2.025869e-01 8.201380e+00 1.179770e+02 1.289621e+02
              X50.         X75.       X97.5.    n_eff      Rhat
alpha 1.875568e-01 2.150656e-01 2.703110e-01 1763.860 1.0011798
beta  3.568003e-02 3.781564e-02 4.198793e-02 1768.846 1.0012394
gamma 1.927091e-04 2.263956e-04 2.892532e-04 2085.869 1.0002111
sigma 1.122899e-02 1.203672e-02 1.375343e-02 2119.946 0.9999176
```

```
lp__  1.347038e+02 1.402500e+02 1.496207e+02 1638.895 0.9997077
```

Reconstructions

```
ionRec <- read.csv(here("data", "reconstructions_ion.csv"))
PredsBay <- rec.bayesian(calModel = ionmodel[[1]],
                              recData = ionRec,
                              iter = 1000,
                              postcalsamples = 100, MC = FALSE)
```

```
Trying to compile a simple C file


Running /Library/Frameworks/R.framework/Resources/bin/R CMD SHLIB foo.c
using C compiler: ‘Apple clang version 14.0.3 (clang-1403.0.22.14.1)’
using SDK: ‘MacOSX13.3.sdk’
clang -arch x86_64 -I"/Library/Frameworks/R.framework/Resources/include" -DNDEBUG   -I"/Libra
In file included from <built-in>:1:
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/S
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
/Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/RcppEigen/include/Eigen
#include <cmath>
         ^~~~~~~
1 error generated.
make: *** [foo.o] Error 1

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 1).
Chain 1:
Chain 1: Gradient evaluation took 0.000932 seconds
Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 9.32 seconds.
Chain 1: Adjust your expectations accordingly!
Chain 1:
Chain 1:
Chain 1: Iteration:   1 / 1000 [  0%]  (Warmup)
Chain 1: Iteration: 100 / 1000 [ 10%]  (Warmup)
Chain 1: Iteration: 200 / 1000 [ 20%]  (Warmup)
Chain 1: Iteration: 300 / 1000 [ 30%]  (Warmup)
Chain 1: Iteration: 400 / 1000 [ 40%]  (Warmup)
Chain 1: Iteration: 500 / 1000 [ 50%]  (Warmup)
Chain 1: Iteration: 501 / 1000 [ 50%]  (Sampling)
```

```
Chain 1: Iteration: 600 / 1000 [ 60%]  (Sampling)
Chain 1: Iteration: 700 / 1000 [ 70%]  (Sampling)
Chain 1: Iteration: 800 / 1000 [ 80%]  (Sampling)
Chain 1: Iteration: 900 / 1000 [ 90%]  (Sampling)
Chain 1: Iteration: 1000 / 1000 [100%]  (Sampling)
Chain 1:
Chain 1:  Elapsed Time: 7.031 seconds (Warm-up)
Chain 1:                7.644 seconds (Sampling)
Chain 1:                14.675 seconds (Total)
Chain 1:

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 2).
Chain 2:
Chain 2: Gradient evaluation took 0.000423 seconds
Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 4.23 seconds.
Chain 2: Adjust your expectations accordingly!
Chain 2:
Chain 2:
Chain 2: Iteration:   1 / 1000 [  0%]  (Warmup)
Chain 2: Iteration: 100 / 1000 [ 10%]  (Warmup)
Chain 2: Iteration: 200 / 1000 [ 20%]  (Warmup)
Chain 2: Iteration: 300 / 1000 [ 30%]  (Warmup)
Chain 2: Iteration: 400 / 1000 [ 40%]  (Warmup)
Chain 2: Iteration: 500 / 1000 [ 50%]  (Warmup)
Chain 2: Iteration: 501 / 1000 [ 50%]  (Sampling)
Chain 2: Iteration: 600 / 1000 [ 60%]  (Sampling)
Chain 2: Iteration: 700 / 1000 [ 70%]  (Sampling)
Chain 2: Iteration: 800 / 1000 [ 80%]  (Sampling)
Chain 2: Iteration: 900 / 1000 [ 90%]  (Sampling)
Chain 2: Iteration: 1000 / 1000 [100%]  (Sampling)
Chain 2:
Chain 2:  Elapsed Time: 7.287 seconds (Warm-up)
Chain 2:                7.901 seconds (Sampling)
Chain 2:                15.188 seconds (Total)
Chain 2:
```

```
PredsBay
```

```
   Sample       D47    D47error  meanTemp     error
1       1 0.6810000 0.008000000 -4.361824 0.3971245
2       2 0.6840000 0.008000000 -5.178247 0.3799968
3       3 0.6760000 0.004000000 -2.955371 0.3447445
```

4	4	0.6820000	0.008000000	-4.627058	0.4167773
5	5	0.6710000	0.006000000	-1.554342	0.3633100
6	6	0.6770000	0.006000000	-3.252226	0.3734195
7	7	0.6730000	0.006000000	-2.128177	0.3856844
8	8	0.6610000	0.009000000	1.329341	0.3852396
9	9	0.6460000	0.009000000	5.826560	0.4694032
10	10	0.6576115	0.010148864	2.317773	0.4563891
11	11	0.6550000	0.006000000	3.098069	0.4056669
12	12	0.6490941	0.006795659	4.881994	0.4035266
13	13	0.6548070	0.006238050	3.159858	0.3840421
14	14	0.6490000	0.007000000	4.900517	0.4237026
15	15	0.6497333	0.005281993	4.675436	0.4011676
16	16	0.6510000	0.006000000	4.289560	0.3641039
17	17	0.6500000	0.006000000	4.599571	0.3649938
18	18	0.6440000	0.004000000	6.429001	0.3571945
19	19	0.6460000	0.004000000	5.832171	0.3847125
20	20	0.6520000	0.004000000	3.990999	0.3790308
21	21	0.6480000	0.005000000	5.213782	0.3879961
22	22	0.6570000	0.008000000	2.497336	0.4366788
23	23	0.6490000	0.005000000	4.900748	0.4001049
24	24	0.6590000	0.004000000	1.912706	0.3568275
25	25	0.6600000	0.004000000	1.625039	0.3586478
26	26	0.6611273	0.006271371	1.292575	0.4040331
27	27	0.6540000	0.004000000	3.406456	0.3574539
28	28	0.6400000	0.005000000	7.673451	0.3932754
29	29	0.6420000	0.003000000	7.057679	0.3600672
30	30	0.6390000	0.005000000	8.006650	0.3672983
31	31	0.6460000	0.004000000	5.822036	0.3666498
32	32	0.6500000	0.004000000	4.590553	0.3766551
33	33	0.6420000	0.004000000	7.060393	0.3734748
34	34	0.6450000	0.006000000	6.129239	0.4197043
35	35	0.6550000	0.004000000	3.115784	0.3553703
36	36	0.6460000	0.004000000	5.821549	0.3861166
37	37	0.6410000	0.006000000	7.376355	0.3936603
38	38	0.6380000	0.005000000	8.312190	0.4196052
39	39	0.6470000	0.004000000	5.510897	0.3728805
40	40	0.6460000	0.004000000	5.829941	0.3969684
41	41	0.6400000	0.004000000	7.697255	0.3630209
42	42	0.6630000	0.007000000	0.740646	0.3846718
43	43	0.6360000	0.005000000	8.950897	0.4069421
44	44	0.6390516	0.004761713	7.983201	0.4011882
45	45	0.6350000	0.006000000	9.263032	0.4193045
46	46	0.6350000	0.008000000	9.277108	0.4072827

```
47     47 0.6330000 0.007000000  9.904392 0.4415947
48     48 0.6389423 0.004672495  8.035150 0.3899529
49     49 0.6120000 0.007000000 16.908109 0.4425900
50     50 0.6280000 0.008000000 11.534758 0.4530863
51     51 0.6170000 0.007000000 15.205366 0.4896464
52     52 0.6140000 0.006000000 16.237678 0.4538210
53     53 0.6410000 0.007000000  7.372366 0.3920648
54     54 0.6454762 0.006751232  5.986298 0.3977512
55     55 0.6330000 0.009000000  9.908157 0.4872907
56     56 0.6361071 0.004430934  8.919700 0.3709104
57     57 0.6281071 0.004497306 11.503496 0.4142326
58     58 0.6140000 0.007000000 16.211753 0.4582119
59     59 0.6190000 0.008000000 14.517105 0.4786082
60     60 0.6310000 0.010000000 10.549184 0.5029699
61     61 0.6260000 0.008000000 12.187410 0.5096085
62     62 0.6440000 0.005000000  6.445126 0.4151501
63     63 0.6420000 0.011000000  7.059300 0.4993247
```

Test 2

Calibration

```
Table1 <- read_excel(here("data", "Test 2.xlsx"))
Table1$Material <- rep(1, nrow(Table1))
colnames(Table1)[c(5, 6, 2, 3, 8)] <- c("D47", "D47error", "Temperature", "TempError", "Ion"

# Check basic regression model
lm(Table1$D47 ~ Table1$Temperature)
```

```
Call:
lm(formula = Table1$D47 ~ Table1$Temperature)

Coefficients:
       (Intercept)  Table1$Temperature
            0.2137              0.0343
```

```
# Fit Bayesian regression
ionmodel <- cal.ion.bayesian(calibrationData = Table1,
                             IonError = Table1$`Ion error`[1])
```

```
Trying to compile a simple C file


Running /Library/Frameworks/R.framework/Resources/bin/R CMD SHLIB foo.c
using C compiler: ‘Apple clang version 14.0.3 (clang-1403.0.22.14.1)’
using SDK: ‘MacOSX13.3.sdk’
clang -arch x86_64 -I"/Library/Frameworks/R.framework/Resources/include" -DNDEBUG   -I"/Libra
In file included from <built-in>:1:
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/S
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
/Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/RcppEigen/include/Eigen
#include <cmath>
         ^~~~~~
1 error generated.
make: *** [foo.o] Error 1

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 1).

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 2).
Chain 1:
Chain 1: Gradient evaluation took 0.000148 seconds
Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 1.48 seconds.
Chain 1: Adjust your expectations accordingly!
Chain 1:
Chain 1:
Chain 1: Iteration:    1 / 2500 [  0%]  (Warmup)
Chain 2:
Chain 2: Gradient evaluation took 0.000136 seconds
Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 1.36 seconds.
Chain 2: Adjust your expectations accordingly!
Chain 2:
Chain 2:
Chain 2: Iteration:    1 / 2500 [  0%]  (Warmup)
Chain 2: Iteration:  250 / 2500 [ 10%]  (Warmup)
Chain 1: Iteration:  250 / 2500 [ 10%]  (Warmup)
Chain 1: Iteration:  500 / 2500 [ 20%]  (Warmup)
Chain 2: Iteration:  500 / 2500 [ 20%]  (Warmup)
Chain 2: Iteration:  750 / 2500 [ 30%]  (Warmup)
Chain 1: Iteration:  750 / 2500 [ 30%]  (Warmup)
Chain 2: Iteration: 1000 / 2500 [ 40%]  (Warmup)
Chain 2: Iteration: 1001 / 2500 [ 40%]  (Sampling)
Chain 1: Iteration: 1000 / 2500 [ 40%]  (Warmup)
```

```
Chain 1: Iteration: 1001 / 2500 [ 40%]  (Sampling)
Chain 2: Iteration: 1250 / 2500 [ 50%]  (Sampling)
Chain 1: Iteration: 1250 / 2500 [ 50%]  (Sampling)
Chain 2: Iteration: 1500 / 2500 [ 60%]  (Sampling)
Chain 1: Iteration: 1500 / 2500 [ 60%]  (Sampling)
Chain 2: Iteration: 1750 / 2500 [ 70%]  (Sampling)
Chain 1: Iteration: 1750 / 2500 [ 70%]  (Sampling)
Chain 2: Iteration: 2000 / 2500 [ 80%]  (Sampling)
Chain 1: Iteration: 2000 / 2500 [ 80%]  (Sampling)
Chain 2: Iteration: 2250 / 2500 [ 90%]  (Sampling)
Chain 1: Iteration: 2250 / 2500 [ 90%]  (Sampling)
Chain 2: Iteration: 2500 / 2500 [100%]  (Sampling)
Chain 2:
Chain 2:  Elapsed Time: 5.276 seconds (Warm-up)
Chain 2:                6.345 seconds (Sampling)
Chain 2:                11.621 seconds (Total)
Chain 2:
Chain 1: Iteration: 2500 / 2500 [100%]  (Sampling)
Chain 1:
Chain 1:  Elapsed Time: 5.322 seconds (Warm-up)
Chain 1:                6.353 seconds (Sampling)
Chain 1:                11.675 seconds (Total)
Chain 1:
```

```r
parameters <- data.frame(rstan::summary(ionmodel[[1]])$summary)
parameters
```

```
              mean      se_mean           sd        X2.5.         X25.
alpha 1.484213e-01 7.800694e-04 4.945469e-02 4.785806e-02 1.156304e-01
beta  3.880663e-02 5.897658e-05 3.748919e-03 3.139795e-02 3.637523e-02
gamma 1.802189e-04 1.311042e-06 7.417042e-05 3.525595e-05 1.324717e-04
sigma 1.176404e-02 2.107493e-05 1.470091e-03 9.327901e-03 1.067766e-02
lp__  8.213318e+01 1.969157e-01 6.532562e+00 6.789672e+01 7.798191e+01
              X50.         X75.       X97.5.    n_eff      Rhat
alpha 1.479362e-01 1.806324e-01 2.446452e-01 4019.282 0.9996638
beta  3.884326e-02 4.123557e-02 4.640208e-02 4040.665 0.9996222
gamma 1.789954e-04 2.286449e-04 3.285403e-04 3200.577 0.9997364
sigma 1.162419e-02 1.267206e-02 1.501313e-02 4865.822 0.9998789
lp__  8.251298e+01 8.685646e+01 9.359486e+01 1100.541 1.0008149
```

Reconstructions

```
ionRec <- read.csv(here("data", "reconstructions_ion.csv"))
PredsBay <- rec.bayesian(calModel = ionmodel[[1]],
                             recData = ionRec,
                             iter = 1000,
                             postcalsamples = 100, MC = FALSE)
```

```
Trying to compile a simple C file

Running /Library/Frameworks/R.framework/Resources/bin/R CMD SHLIB foo.c
using C compiler: 'Apple clang version 14.0.3 (clang-1403.0.22.14.1)'
using SDK: 'MacOSX13.3.sdk'
clang -arch x86_64 -I"/Library/Frameworks/R.framework/Resources/include" -DNDEBUG   -I"/Libra
In file included from <built-in>:1:
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/S
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
/Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/RcppEigen/include/Eigen
#include <cmath>
         ^~~~~~~
1 error generated.
make: *** [foo.o] Error 1

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 1).
Chain 1:
Chain 1: Gradient evaluation took 0.000895 seconds
Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 8.95 seconds.
Chain 1: Adjust your expectations accordingly!
Chain 1:
Chain 1:
Chain 1: Iteration:   1 / 1000 [  0%]  (Warmup)
Chain 1: Iteration: 100 / 1000 [ 10%]  (Warmup)
Chain 1: Iteration: 200 / 1000 [ 20%]  (Warmup)
Chain 1: Iteration: 300 / 1000 [ 30%]  (Warmup)
Chain 1: Iteration: 400 / 1000 [ 40%]  (Warmup)
Chain 1: Iteration: 500 / 1000 [ 50%]  (Warmup)
Chain 1: Iteration: 501 / 1000 [ 50%]  (Sampling)
Chain 1: Iteration: 600 / 1000 [ 60%]  (Sampling)
Chain 1: Iteration: 700 / 1000 [ 70%]  (Sampling)
Chain 1: Iteration: 800 / 1000 [ 80%]  (Sampling)
```

```
Chain 1: Iteration: 900 / 1000 [ 90%]  (Sampling)
Chain 1: Iteration: 1000 / 1000 [100%]  (Sampling)
Chain 1:
Chain 1:  Elapsed Time: 8.143 seconds (Warm-up)
Chain 1:                8.363 seconds (Sampling)
Chain 1:                16.506 seconds (Total)
Chain 1:

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 2).
Chain 2:
Chain 2: Gradient evaluation took 0.000382 seconds
Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 3.82 seconds.
Chain 2: Adjust your expectations accordingly!
Chain 2:
Chain 2:
Chain 2: Iteration:   1 / 1000 [  0%]  (Warmup)
Chain 2: Iteration: 100 / 1000 [ 10%]  (Warmup)
Chain 2: Iteration: 200 / 1000 [ 20%]  (Warmup)
Chain 2: Iteration: 300 / 1000 [ 30%]  (Warmup)
Chain 2: Iteration: 400 / 1000 [ 40%]  (Warmup)
Chain 2: Iteration: 500 / 1000 [ 50%]  (Warmup)
Chain 2: Iteration: 501 / 1000 [ 50%]  (Sampling)
Chain 2: Iteration: 600 / 1000 [ 60%]  (Sampling)
Chain 2: Iteration: 700 / 1000 [ 70%]  (Sampling)
Chain 2: Iteration: 800 / 1000 [ 80%]  (Sampling)
Chain 2: Iteration: 900 / 1000 [ 90%]  (Sampling)
Chain 2: Iteration: 1000 / 1000 [100%]  (Sampling)
Chain 2:
Chain 2:  Elapsed Time: 8.162 seconds (Warm-up)
Chain 2:                8.078 seconds (Sampling)
Chain 2:                16.24 seconds (Total)
Chain 2:
```

```
PredsBay
```

```
   Sample       D47    D47error   meanTemp     error
1       1 0.6810000 0.008000000 -3.2368651 0.3711406
2       2 0.6840000 0.008000000 -3.9953806 0.3732399
3       3 0.6760000 0.004000000 -1.9389658 0.3002777
4       4 0.6820000 0.008000000 -3.4892724 0.3713567
5       5 0.6710000 0.006000000 -0.6142037 0.3473179
6       6 0.6770000 0.006000000 -2.1898763 0.3498301
```

7	7	0.6730000	0.006000000	-1.1520221	0.3360321
8	8	0.6610000	0.009000000	2.0375881	0.4144897
9	9	0.6460000	0.009000000	6.2372207	0.4030548
10	10	0.6576115	0.010148864	2.9741723	0.4391511
11	11	0.6550000	0.006000000	3.7071696	0.3517128
12	12	0.6490941	0.006795659	5.3616545	0.4039918
13	13	0.6548070	0.006238050	3.7562424	0.3673356
14	14	0.6490000	0.007000000	5.3741024	0.3952439
15	15	0.6497333	0.005281993	5.1762805	0.3558534
16	16	0.6510000	0.006000000	4.8219797	0.3684348
17	17	0.6500000	0.006000000	5.0975043	0.3792794
18	18	0.6440000	0.004000000	6.7970404	0.3896916
19	19	0.6460000	0.004000000	6.2234347	0.3679054
20	20	0.6520000	0.004000000	4.5448150	0.3785168
21	21	0.6480000	0.005000000	5.6685289	0.3659069
22	22	0.6570000	0.008000000	3.1314159	0.4054097
23	23	0.6490000	0.005000000	5.3785433	0.3727296
24	24	0.6590000	0.004000000	2.6102325	0.3294835
25	25	0.6600000	0.004000000	2.3272759	0.3580205
26	26	0.6611273	0.006271371	2.0284047	0.3618594
27	27	0.6540000	0.004000000	3.9741113	0.3621980
28	28	0.6400000	0.005000000	7.9611678	0.3653019
29	29	0.6420000	0.003000000	7.3749732	0.3403467
30	30	0.6390000	0.005000000	8.2402805	0.3729271
31	31	0.6460000	0.004000000	6.2205526	0.3527257
32	32	0.6500000	0.004000000	5.1034912	0.3348643
33	33	0.6420000	0.004000000	7.3673951	0.3538384
34	34	0.6450000	0.006000000	6.5116647	0.3751588
35	35	0.6550000	0.004000000	3.6950139	0.3256008
36	36	0.6460000	0.004000000	6.2241429	0.3518449
37	37	0.6410000	0.006000000	7.6440946	0.3767960
38	38	0.6380000	0.005000000	8.5255087	0.3421291
39	39	0.6470000	0.004000000	5.9378636	0.3490139
40	40	0.6460000	0.004000000	6.2153902	0.3363310
41	41	0.6400000	0.004000000	7.9489678	0.3539651
42	42	0.6630000	0.007000000	1.4998668	0.3651459
43	43	0.6360000	0.005000000	9.1228096	0.3892187
44	44	0.6390516	0.004761713	8.2276812	0.3750703
45	45	0.6350000	0.006000000	9.4031687	0.4185461
46	46	0.6350000	0.008000000	9.4135954	0.3961193
47	47	0.6330000	0.007000000	10.0068092	0.4332533
48	48	0.6389423	0.004672495	8.2635072	0.3769571
49	49	0.6120000	0.007000000	16.4309558	0.4231706

```
50     50 0.6280000 0.008000000 11.4962553 0.4395305
51     51 0.6170000 0.007000000 14.8746598 0.4177176
52     52 0.6140000 0.006000000 15.8056956 0.4220225
53     53 0.6410000 0.007000000  7.6602218 0.3874780
54     54 0.6454762 0.006751232  6.3745825 0.3859253
55     55 0.6330000 0.009000000  9.9981712 0.4401960
56     56 0.6361071 0.004430934  9.0747781 0.4016184
57     57 0.6281071 0.004497306 11.4581109 0.3961706
58     58 0.6140000 0.007000000 15.7999161 0.4251337
59     59 0.6190000 0.008000000 14.2554297 0.4810442
60     60 0.6310000 0.010000000 10.6014603 0.4676986
61     61 0.6260000 0.008000000 12.0956303 0.4280241
62     62 0.6440000 0.005000000  6.8004437 0.3777523
63     63 0.6420000 0.011000000  7.3838578 0.4531584
```

Test 3

Calibration

```
Table1 <- read_excel(here("data", "Test 3.xlsx"))
Table1$Material <- rep(1, nrow(Table1))
colnames(Table1)[c(5, 6, 2, 3, 8)] <- c("D47", "D47error", "Temperature", "TempError", "Ion"

# Check basic regression model
lm(Table1$D47 ~ Table1$Temperature)
```

```
Call:
lm(formula = Table1$D47 ~ Table1$Temperature)

Coefficients:
       (Intercept)  Table1$Temperature
           0.18944             0.03624
```

```
# Fit Bayesian regression
ionmodel <- cal.ion.bayesian(calibrationData = Table1,
                             IonError = Table1$`Ion error`[1])
```

```
Trying to compile a simple C file
```

```
Running /Library/Frameworks/R.framework/Resources/bin/R CMD SHLIB foo.c
using C compiler: ‘Apple clang version 14.0.3 (clang-1403.0.22.14.1)’
using SDK: ‘MacOSX13.3.sdk’
clang -arch x86_64 -I"/Library/Frameworks/R.framework/Resources/include" -DNDEBUG   -I"/Libra
In file included from <built-in>:1:
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/S
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
/Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/RcppEigen/include/Eigen
#include <cmath>
         ^~~~~~~
1 error generated.
make: *** [foo.o] Error 1

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 2).

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 1).
Chain 2:
Chain 2: Gradient evaluation took 7e-05 seconds
Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 0.7 seconds.
Chain 2: Adjust your expectations accordingly!
Chain 2:
Chain 2:
Chain 1:
Chain 1: Gradient evaluation took 7.2e-05 seconds
Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 0.72 seconds.
Chain 1: Adjust your expectations accordingly!
Chain 1:
Chain 1:
Chain 2: Iteration:    1 / 2500 [  0%]  (Warmup)
Chain 1: Iteration:    1 / 2500 [  0%]  (Warmup)
Chain 1: Iteration:  250 / 2500 [ 10%]  (Warmup)
Chain 2: Iteration:  250 / 2500 [ 10%]  (Warmup)
Chain 2: Iteration:  500 / 2500 [ 20%]  (Warmup)
Chain 1: Iteration:  500 / 2500 [ 20%]  (Warmup)
Chain 2: Iteration:  750 / 2500 [ 30%]  (Warmup)
Chain 1: Iteration:  750 / 2500 [ 30%]  (Warmup)
Chain 2: Iteration: 1000 / 2500 [ 40%]  (Warmup)
Chain 2: Iteration: 1001 / 2500 [ 40%]  (Sampling)
Chain 1: Iteration: 1000 / 2500 [ 40%]  (Warmup)
Chain 1: Iteration: 1001 / 2500 [ 40%]  (Sampling)
Chain 2: Iteration: 1250 / 2500 [ 50%]  (Sampling)
Chain 1: Iteration: 1250 / 2500 [ 50%]  (Sampling)
```

```
Chain 2: Iteration: 1500 / 2500 [ 60%]  (Sampling)
Chain 1: Iteration: 1500 / 2500 [ 60%]  (Sampling)
Chain 2: Iteration: 1750 / 2500 [ 70%]  (Sampling)
Chain 1: Iteration: 1750 / 2500 [ 70%]  (Sampling)
Chain 2: Iteration: 2000 / 2500 [ 80%]  (Sampling)
Chain 1: Iteration: 2000 / 2500 [ 80%]  (Sampling)
Chain 2: Iteration: 2250 / 2500 [ 90%]  (Sampling)
Chain 1: Iteration: 2250 / 2500 [ 90%]  (Sampling)
Chain 2: Iteration: 2500 / 2500 [100%]  (Sampling)
Chain 2:
Chain 2:  Elapsed Time: 3.276 seconds (Warm-up)
Chain 2:                2.378 seconds (Sampling)
Chain 2:                5.654 seconds (Total)
Chain 2:
Chain 1: Iteration: 2500 / 2500 [100%]  (Sampling)
Chain 1:
Chain 1:  Elapsed Time: 3.45 seconds (Warm-up)
Chain 1:                2.428 seconds (Sampling)
Chain 1:                5.878 seconds (Total)
Chain 1:
```

```
parameters <- data.frame(rstan::summary(ionmodel[[1]])$summary)
parameters
```

```
              mean      se_mean           sd         X2.5.         X25.
alpha 1.431644e-01 1.850668e-03 7.282417e-02 -5.381023e-03 9.647244e-02
beta  3.934038e-02 1.422659e-04 5.626281e-03  2.824252e-02 3.570913e-02
gamma 1.497969e-04 1.979652e-06 9.775299e-05 -4.861004e-05 8.665487e-05
sigma 1.298425e-02 5.309659e-05 2.246144e-03  9.400855e-03 1.147096e-02
lp__  4.129965e+01 1.351336e-01 5.114954e+00  3.025819e+01 3.804337e+01
              X50.          X75.       X97.5.    n_eff      Rhat
alpha 1.407560e-01  0.190197053 2.857066e-01 1548.440 0.9999058
beta  3.954372e-02  0.042989675 5.059389e-02 1564.016 0.9999427
gamma 1.487664e-04  0.000213968 3.360281e-04 2438.272 0.9998613
sigma 1.268429e-02  0.014229532 1.793771e-02 1789.542 0.9994646
lp__  4.166145e+01 44.910646258 5.048924e+01 1432.705 1.0037514
```

Reconstructions

```r
ionRec <- read.csv(here("data", "reconstructions_ion.csv"))
PredsBay <- rec.bayesian(calModel = ionmodel[[1]],
                         recData = ionRec,
                         iter = 1000,
                         postcalsamples = 100, MC = FALSE)
```

```
Trying to compile a simple C file


Running /Library/Frameworks/R.framework/Resources/bin/R CMD SHLIB foo.c
using C compiler: ‘Apple clang version 14.0.3 (clang-1403.0.22.14.1)’
using SDK: ‘MacOSX13.3.sdk’
clang -arch x86_64 -I"/Library/Frameworks/R.framework/Resources/include" -DNDEBUG   -I"/Libra
In file included from <built-in>:1:
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/S
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
/Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/RcppEigen/include/Eigen
#include <cmath>
         ^~~~~~~
1 error generated.
make: *** [foo.o] Error 1

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 1).
Chain 1:
Chain 1: Gradient evaluation took 0.000772 seconds
Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 7.72 seconds.
Chain 1: Adjust your expectations accordingly!
Chain 1:
Chain 1:
Chain 1: Iteration:   1 / 1000 [  0%]  (Warmup)
Chain 1: Iteration: 100 / 1000 [ 10%]  (Warmup)
Chain 1: Iteration: 200 / 1000 [ 20%]  (Warmup)
Chain 1: Iteration: 300 / 1000 [ 30%]  (Warmup)
Chain 1: Iteration: 400 / 1000 [ 40%]  (Warmup)
Chain 1: Iteration: 500 / 1000 [ 50%]  (Warmup)
Chain 1: Iteration: 501 / 1000 [ 50%]  (Sampling)
Chain 1: Iteration: 600 / 1000 [ 60%]  (Sampling)
Chain 1: Iteration: 700 / 1000 [ 70%]  (Sampling)
Chain 1: Iteration: 800 / 1000 [ 80%]  (Sampling)
Chain 1: Iteration: 900 / 1000 [ 90%]  (Sampling)
Chain 1: Iteration: 1000 / 1000 [100%]  (Sampling)
```

```
Chain 1:
Chain 1:  Elapsed Time: 7.646 seconds (Warm-up)
Chain 1:                7.9 seconds (Sampling)
Chain 1:                15.546 seconds (Total)
Chain 1:

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 2).
Chain 2:
Chain 2: Gradient evaluation took 0.00038 seconds
Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 3.8 seconds.
Chain 2: Adjust your expectations accordingly!
Chain 2:
Chain 2:
Chain 2: Iteration:   1 / 1000 [  0%]  (Warmup)
Chain 2: Iteration: 100 / 1000 [ 10%]  (Warmup)
Chain 2: Iteration: 200 / 1000 [ 20%]  (Warmup)
Chain 2: Iteration: 300 / 1000 [ 30%]  (Warmup)
Chain 2: Iteration: 400 / 1000 [ 40%]  (Warmup)
Chain 2: Iteration: 500 / 1000 [ 50%]  (Warmup)
Chain 2: Iteration: 501 / 1000 [ 50%]  (Sampling)
Chain 2: Iteration: 600 / 1000 [ 60%]  (Sampling)
Chain 2: Iteration: 700 / 1000 [ 70%]  (Sampling)
Chain 2: Iteration: 800 / 1000 [ 80%]  (Sampling)
Chain 2: Iteration: 900 / 1000 [ 90%]  (Sampling)
Chain 2: Iteration: 1000 / 1000 [100%]  (Sampling)
Chain 2:
Chain 2:  Elapsed Time: 7.354 seconds (Warm-up)
Chain 2:                7.863 seconds (Sampling)
Chain 2:                15.217 seconds (Total)
Chain 2:
```

```
PredsBay
```

```
   Sample       D47    D47error    meanTemp     error
1       1 0.6810000 0.008000000 -2.48317501 0.3826064
2       2 0.6840000 0.008000000 -3.22383352 0.3764459
3       3 0.6760000 0.004000000 -1.23949907 0.3693994
4       4 0.6820000 0.008000000 -2.73701159 0.3762498
5       5 0.6710000 0.006000000  0.02246633 0.4005778
6       6 0.6770000 0.006000000 -1.48736299 0.3761610
7       7 0.6730000 0.006000000 -0.47990728 0.3894862
8       8 0.6610000 0.009000000  2.60428333 0.4221158
```

9	9	0.6460000	0.009000000	6.62329262	0.4538915
10	10	0.6576115	0.010148864	3.50896419	0.4237958
11	11	0.6550000	0.006000000	4.19663425	0.3890616
12	12	0.6490941	0.006795659	5.76660340	0.4204701
13	13	0.6548070	0.006238050	4.24638915	0.4026896
14	14	0.6490000	0.007000000	5.80861285	0.4207746
15	15	0.6497333	0.005281993	5.60685353	0.4200198
16	16	0.6510000	0.006000000	5.26564486	0.4025539
17	17	0.6500000	0.006000000	5.53162963	0.4038171
18	18	0.6440000	0.004000000	7.16340158	0.3815362
19	19	0.6460000	0.004000000	6.61842959	0.3860267
20	20	0.6520000	0.004000000	4.98705739	0.3864800
21	21	0.6480000	0.005000000	6.07683789	0.4008975
22	22	0.6570000	0.008000000	3.66288966	0.4345241
23	23	0.6490000	0.005000000	5.80941587	0.3828174
24	24	0.6590000	0.004000000	3.13899819	0.3937081
25	25	0.6600000	0.004000000	2.86217092	0.3877546
26	26	0.6611273	0.006271371	2.55996743	0.3843673
27	27	0.6540000	0.004000000	4.46845114	0.3827902
28	28	0.6400000	0.005000000	8.28071260	0.4189174
29	29	0.6420000	0.003000000	7.72981590	0.3500892
30	30	0.6390000	0.005000000	8.55155004	0.3999516
31	31	0.6460000	0.004000000	6.61631784	0.3774293
32	32	0.6500000	0.004000000	5.53315893	0.3874776
33	33	0.6420000	0.004000000	7.72639368	0.3886603
34	34	0.6450000	0.006000000	6.90109498	0.4167015
35	35	0.6550000	0.004000000	4.20199964	0.3738494
36	36	0.6460000	0.004000000	6.62276774	0.3884107
37	37	0.6410000	0.006000000	8.00174167	0.4148907
38	38	0.6380000	0.005000000	8.83744586	0.4108564
39	39	0.6470000	0.004000000	6.36389814	0.3823901
40	40	0.6460000	0.004000000	6.62304998	0.3912833
41	41	0.6400000	0.004000000	8.27312767	0.4027980
42	42	0.6630000	0.007000000	2.09404057	0.3756448
43	43	0.6360000	0.005000000	9.39992617	0.4182927
44	44	0.6390516	0.004761713	8.54269176	0.3894145
45	45	0.6350000	0.006000000	9.68190453	0.4252597
46	46	0.6350000	0.008000000	9.68484699	0.4414243
47	47	0.6330000	0.007000000	10.23986955	0.4363252
48	48	0.6389423	0.004672495	8.56990816	0.4116610
49	49	0.6120000	0.007000000	16.41155406	0.4616299
50	50	0.6280000	0.008000000	11.67313296	0.4370357
51	51	0.6170000	0.007000000	14.90742073	0.4596349

```
52     52 0.6140000 0.006000000 15.80126476 0.4207439
53     53 0.6410000 0.007000000  8.00065674 0.4229742
54     54 0.6454762 0.006751232  6.76745188 0.4267237
55     55 0.6330000 0.009000000 10.25685848 0.4676162
56     56 0.6361071 0.004430934  9.37452485 0.4040930
57     57 0.6281071 0.004497306 11.64933773 0.4020064
58     58 0.6140000 0.007000000 15.80792353 0.4465374
59     59 0.6190000 0.008000000 14.31068943 0.4517615
60     60 0.6310000 0.010000000 10.81610162 0.4755016
61     61 0.6260000 0.008000000 12.25455491 0.4314101
62     62 0.6440000 0.005000000  7.16729825 0.3936367
63     63 0.6420000 0.011000000  7.72684727 0.4678229
```

Test 4

Calibration

```
Table1 <- read_excel(here("data", "Test 4.xlsx"))
Table1$Material <- rep(1, nrow(Table1))
colnames(Table1)[c(5, 6, 2, 3, 8)] <- c("D47", "D47error", "Temperature", "TempError", "Ion"
)

# Check basic regression model
lm(Table1$D47 ~ Table1$Temperature)
```

```
Call:
lm(formula = Table1$D47 ~ Table1$Temperature)

Coefficients:
       (Intercept)  Table1$Temperature
           0.24681             0.03173
```

```
# Fit Bayesian regression
ionmodel <- cal.ion.bayesian(calibrationData = Table1,
                             IonError = Table1$`Ion error`[1])
```

```
Trying to compile a simple C file
```

```
Running /Library/Frameworks/R.framework/Resources/bin/R CMD SHLIB foo.c
using C compiler: ‘Apple clang version 14.0.3 (clang-1403.0.22.14.1)’
using SDK: ‘MacOSX13.3.sdk’
clang -arch x86_64 -I"/Library/Frameworks/R.framework/Resources/include" -DNDEBUG   -I"/Libra
In file included from <built-in>:1:
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/S
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/R
/Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/RcppEigen/include/Eigen
#include <cmath>
         ^~~~~~~
1 error generated.
make: *** [foo.o] Error 1

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 1).

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 2).
Chain 1:
Chain 1: Gradient evaluation took 6.4e-05 seconds
Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 0.64 seconds.
Chain 1: Adjust your expectations accordingly!
Chain 1:
Chain 1:
Chain 2:
Chain 2: Chain 1: Iteration:    1 / 2500 [  0%]  (Warmup)
Gradient evaluation took 7.4e-05 seconds
Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 0.74 seconds.
Chain 2: Adjust your expectations accordingly!
Chain 2:
Chain 2:
Chain 2: Iteration:    1 / 2500 [  0%]  (Warmup)
Chain 1: Iteration:  250 / 2500 [ 10%]  (Warmup)
Chain 2: Iteration:  250 / 2500 [ 10%]  (Warmup)
Chain 2: Iteration:  500 / 2500 [ 20%]  (Warmup)
Chain 1: Iteration:  500 / 2500 [ 20%]  (Warmup)
Chain 2: Iteration:  750 / 2500 [ 30%]  (Warmup)
Chain 1: Iteration:  750 / 2500 [ 30%]  (Warmup)
Chain 2: Iteration: 1000 / 2500 [ 40%]  (Warmup)
Chain 2: Iteration: 1001 / 2500 [ 40%]  (Sampling)
Chain 1: Iteration: 1000 / 2500 [ 40%]  (Warmup)
Chain 1: Iteration: 1001 / 2500 [ 40%]  (Sampling)
Chain 2: Iteration: 1250 / 2500 [ 50%]  (Sampling)
Chain 1: Iteration: 1250 / 2500 [ 50%]  (Sampling)
```

```
Chain 2: Iteration: 1500 / 2500 [ 60%]  (Sampling)
Chain 1: Iteration: 1500 / 2500 [ 60%]  (Sampling)
Chain 2: Iteration: 1750 / 2500 [ 70%]  (Sampling)
Chain 1: Iteration: 1750 / 2500 [ 70%]  (Sampling)
Chain 2: Iteration: 2000 / 2500 [ 80%]  (Sampling)
Chain 1: Iteration: 2000 / 2500 [ 80%]  (Sampling)
Chain 2: Iteration: 2250 / 2500 [ 90%]  (Sampling)
Chain 1: Iteration: 2250 / 2500 [ 90%]  (Sampling)
Chain 2: Iteration: 2500 / 2500 [100%]  (Sampling)
Chain 2:
Chain 2:  Elapsed Time: 2.947 seconds (Warm-up)
Chain 2:                2.288 seconds (Sampling)
Chain 2:                5.235 seconds (Total)
Chain 2:
Chain 1: Iteration: 2500 / 2500 [100%]  (Sampling)
Chain 1:
Chain 1:  Elapsed Time: 3.282 seconds (Warm-up)
Chain 1:                2.292 seconds (Sampling)
Chain 1:                5.574 seconds (Total)
Chain 1:

Warning: There were 2 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
```

```r
parameters <- data.frame(rstan::summary(ionmodel[[1]])$summary)
parameters
```

```
              mean      se_mean           sd         X2.5.         X25.
alpha 1.475750e-01 3.153279e-03 0.1090330483 -7.256418e-02 8.037341e-02
beta  3.873250e-02 2.344614e-04 0.0081334514  2.367579e-02 3.345255e-02
gamma 2.283575e-04 3.739255e-06 0.0001524572 -7.722088e-05 1.316113e-04
sigma 1.235099e-02 7.015664e-05 0.0027629675  8.050826e-03 1.044974e-02
lp__  3.518645e+01 1.301816e-01 4.6496910787  2.491998e+01 3.239775e+01
              X50.         X75.       X97.5.    n_eff      Rhat
alpha 1.502507e-01 2.176775e-01 3.508374e-01 1195.616 1.0001738
beta  3.847614e-02 4.377693e-02 5.518219e-02 1203.392 1.0001963
gamma 2.268861e-04 3.240952e-04 5.261085e-04 1662.363 1.0005415
sigma 1.197324e-02 1.384168e-02 1.882249e-02 1551.008 0.9994483
lp__  3.554419e+01 3.842438e+01 4.333442e+01 1275.701 1.0006395
```

Reconstructions

```
ionRec <- read.csv(here("data", "reconstructions_ion.csv"))
PredsBay <- rec.bayesian(calModel = ionmodel[[1]],
                             recData = ionRec,
                             iter = 1000,
                             postcalsamples = 100, MC = FALSE)
```

```
Trying to compile a simple C file

Running /Library/Frameworks/R.framework/Resources/bin/R CMD SHLIB foo.c
using C compiler: ‘Apple clang version 14.0.3 (clang-1403.0.22.14.1)’
using SDK: ‘MacOSX13.3.sdk’
clang -arch x86_64 -I"/Library/Frameworks/R.framework/Resources/include" -DNDEBUG   -I"/Libra
In file included from <built-in>:1:
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/S
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/I
In file included from /Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/I
/Library/Frameworks/R.framework/Versions/4.5-x86_64/Resources/library/RcppEigen/include/Eigen
#include <cmath>
         ^~~~~~~
1 error generated.
make: *** [foo.o] Error 1

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 1).
Chain 1:
Chain 1: Gradient evaluation took 0.00071 seconds
Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 7.1 seconds.
Chain 1: Adjust your expectations accordingly!
Chain 1:
Chain 1:
Chain 1: Iteration:   1 / 1000 [  0%]  (Warmup)
Chain 1: Iteration: 100 / 1000 [ 10%]  (Warmup)
Chain 1: Iteration: 200 / 1000 [ 20%]  (Warmup)
Chain 1: Iteration: 300 / 1000 [ 30%]  (Warmup)
Chain 1: Iteration: 400 / 1000 [ 40%]  (Warmup)
Chain 1: Iteration: 500 / 1000 [ 50%]  (Warmup)
Chain 1: Iteration: 501 / 1000 [ 50%]  (Sampling)
Chain 1: Iteration: 600 / 1000 [ 60%]  (Sampling)
Chain 1: Iteration: 700 / 1000 [ 70%]  (Sampling)
Chain 1: Iteration: 800 / 1000 [ 80%]  (Sampling)
```

```
Chain 1: Iteration: 900 / 1000 [ 90%]  (Sampling)
Chain 1: Iteration: 1000 / 1000 [100%]  (Sampling)
Chain 1:
Chain 1:  Elapsed Time: 8.943 seconds (Warm-up)
Chain 1:                9.967 seconds (Sampling)
Chain 1:                18.91 seconds (Total)
Chain 1:

SAMPLING FOR MODEL 'anon_model' NOW (CHAIN 2).
Chain 2:
Chain 2: Gradient evaluation took 0.000392 seconds
Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 3.92 seconds.
Chain 2: Adjust your expectations accordingly!
Chain 2:
Chain 2:
Chain 2: Iteration:   1 / 1000 [  0%]  (Warmup)
Chain 2: Iteration: 100 / 1000 [ 10%]  (Warmup)
Chain 2: Iteration: 200 / 1000 [ 20%]  (Warmup)
Chain 2: Iteration: 300 / 1000 [ 30%]  (Warmup)
Chain 2: Iteration: 400 / 1000 [ 40%]  (Warmup)
Chain 2: Iteration: 500 / 1000 [ 50%]  (Warmup)
Chain 2: Iteration: 501 / 1000 [ 50%]  (Sampling)
Chain 2: Iteration: 600 / 1000 [ 60%]  (Sampling)
Chain 2: Iteration: 700 / 1000 [ 70%]  (Sampling)
Chain 2: Iteration: 800 / 1000 [ 80%]  (Sampling)
Chain 2: Iteration: 900 / 1000 [ 90%]  (Sampling)
Chain 2: Iteration: 1000 / 1000 [100%]  (Sampling)
Chain 2:
Chain 2:  Elapsed Time: 8.939 seconds (Warm-up)
Chain 2:                9.397 seconds (Sampling)
Chain 2:                18.336 seconds (Total)
Chain 2:
```

```
PredsBay
```

```
   Sample       D47    D47error   meanTemp     error
1       1 0.6810000 0.008000000 -3.6526368 0.3954588
2       2 0.6840000 0.008000000 -4.4296900 0.4114876
3       3 0.6760000 0.004000000 -2.3422673 0.3647710
4       4 0.6820000 0.008000000 -3.8993684 0.3971269
5       5 0.6710000 0.006000000 -0.9989978 0.3954455
6       6 0.6770000 0.006000000 -2.5825888 0.3620319
```

7	7	0.6730000	0.006000000	-1.5365882	0.3691315
8	8	0.6610000	0.009000000	1.7326162	0.4388650
9	9	0.6460000	0.009000000	5.9946194	0.4647390
10	10	0.6576115	0.010148864	2.7063253	0.4723358
11	11	0.6550000	0.006000000	3.4212007	0.4280090
12	12	0.6490941	0.006795659	5.1203734	0.4459297
13	13	0.6548070	0.006238050	3.4695149	0.4114285
14	14	0.6490000	0.007000000	5.1312029	0.4018929
15	15	0.6497333	0.005281993	4.9214506	0.3731613
16	16	0.6510000	0.006000000	4.5443766	0.4222364
17	17	0.6500000	0.006000000	4.8399403	0.4106816
18	18	0.6440000	0.004000000	6.5849246	0.4056249
19	19	0.6460000	0.004000000	6.0067914	0.4449167
20	20	0.6520000	0.004000000	4.2662133	0.4020670
21	21	0.6480000	0.005000000	5.4178795	0.4143410
22	22	0.6570000	0.008000000	2.8712013	0.4142531
23	23	0.6490000	0.005000000	5.1339094	0.4109961
24	24	0.6590000	0.004000000	2.2968200	0.3813868
25	25	0.6600000	0.004000000	2.0139845	0.3658855
26	26	0.6611273	0.006271371	1.6950032	0.4038747
27	27	0.6540000	0.004000000	3.6985836	0.3837712
28	28	0.6400000	0.005000000	7.7637196	0.4301241
29	29	0.6420000	0.003000000	7.1655928	0.3924954
30	30	0.6390000	0.005000000	8.0515251	0.4321632
31	31	0.6460000	0.004000000	6.0073098	0.3928467
32	32	0.6500000	0.004000000	4.8474880	0.3992404
33	33	0.6420000	0.004000000	7.1822361	0.4050143
34	34	0.6450000	0.006000000	6.2870413	0.4101947
35	35	0.6550000	0.004000000	3.3991615	0.4030992
36	36	0.6460000	0.004000000	6.0052882	0.4187261
37	37	0.6410000	0.006000000	7.4586403	0.4281555
38	38	0.6380000	0.005000000	8.3358555	0.3952466
39	39	0.6470000	0.004000000	5.7078408	0.3846034
40	40	0.6460000	0.004000000	5.9977704	0.3920959
41	41	0.6400000	0.004000000	7.7586761	0.4102210
42	42	0.6630000	0.007000000	1.1907685	0.3961747
43	43	0.6360000	0.005000000	8.9551640	0.3941332
44	44	0.6390516	0.004761713	8.0452687	0.4458638
45	45	0.6350000	0.006000000	9.2486715	0.4140660
46	46	0.6350000	0.008000000	9.2541564	0.4801803
47	47	0.6330000	0.007000000	9.8723528	0.4478617
48	48	0.6389423	0.004672495	8.0653378	0.4020133
49	49	0.6120000	0.007000000	16.4296944	0.4594295

50	50	0.6280000	0.008000000	11.3876600	0.4663336
51	51	0.6170000	0.007000000	14.8207454	0.4827343
52	52	0.6140000	0.006000000	15.8046666	0.4679357
53	53	0.6410000	0.007000000	7.4649034	0.4308621
54	54	0.6454762	0.006751232	6.1391924	0.4415681
55	55	0.6330000	0.009000000	9.8648300	0.5052773
56	56	0.6361071	0.004430934	8.9119613	0.4145514
57	57	0.6281071	0.004497306	11.3358953	0.4157555
58	58	0.6140000	0.007000000	15.7956130	0.4731783
59	59	0.6190000	0.008000000	14.1942090	0.4706135
60	60	0.6310000	0.010000000	10.4600551	0.4885191
61	61	0.6260000	0.008000000	12.0133061	0.4977756
62	62	0.6440000	0.005000000	6.5674336	0.4345780
63	63	0.6420000	0.011000000	7.1717107	0.5201491