Qusage: Speeding up in Rcpp

Timothy J. Triche, Jr, Anthony R. Colombo

17 February, 2016

Contents

1 SpeedSage Intro

qusage is published software that is slow for large runs, SpeedSage corrects for speed and efficiency at large orders #Bottlenecking of Functions Qusage can improve the speed of its algorithm by minimizing the cost of computaiton.

1.1 changes Armadillo C++

trading NA flexibility slows down qusage runs, but having the user input no NAs enforcing good input, this speeds up calcIndividualExpressions, as well as using C++ libraries.

2 Individual Expression Function

This test the local version which enforces no NA in Baseline or PostTreatment object, this reduces the flexibility. this test data is from the vignette where postTreatment was modified to be Baseline+20.4, a simple training set from the QuSAGE vignette.

```
library(inline)
library(microbenchmark)
library(Rcpp)
```

```
##
## Attaching package: 'Rcpp'

## The following object is masked from 'package:inline':
##
##     registerPlugin
```

```
library(parallel)
library(speedSage)
```

```
## Loading required package: limma
```

```
library(qusage)
```

```
##
## Attaching package: 'qusage'
```

```
## The following objects are masked from 'package:speedSage':
##
##     aggregateGeneSet, calcBayesCI, calcVIF, getXcoords,
##     makeComparison, read.gmt
```

```
library(ggplot2)
eset<-system.file("extdata","eset.RData",package="speedSage")
load(eset)
labels<-c(rep("t0",134),rep("t1",134))
contrast<-"t1-t0"
colnames(eset)<-c(rep("t0",134),rep("t1",134))
fileISG<-system.file("extdata","c2.cgp.v5.1.symbols.gmt",package="speedSage")
ISG.geneSet<-read.gmt(fileISG)
ISG.geneSet<-ISG.geneSet[grepl("DER_IFN_GAMMA_RESPONSE_UP",names(ISG.geneSet))]
Baseline<-eset
PostTreatment<-eset+20.4
ncol(Baseline) #not splitting up eset
```

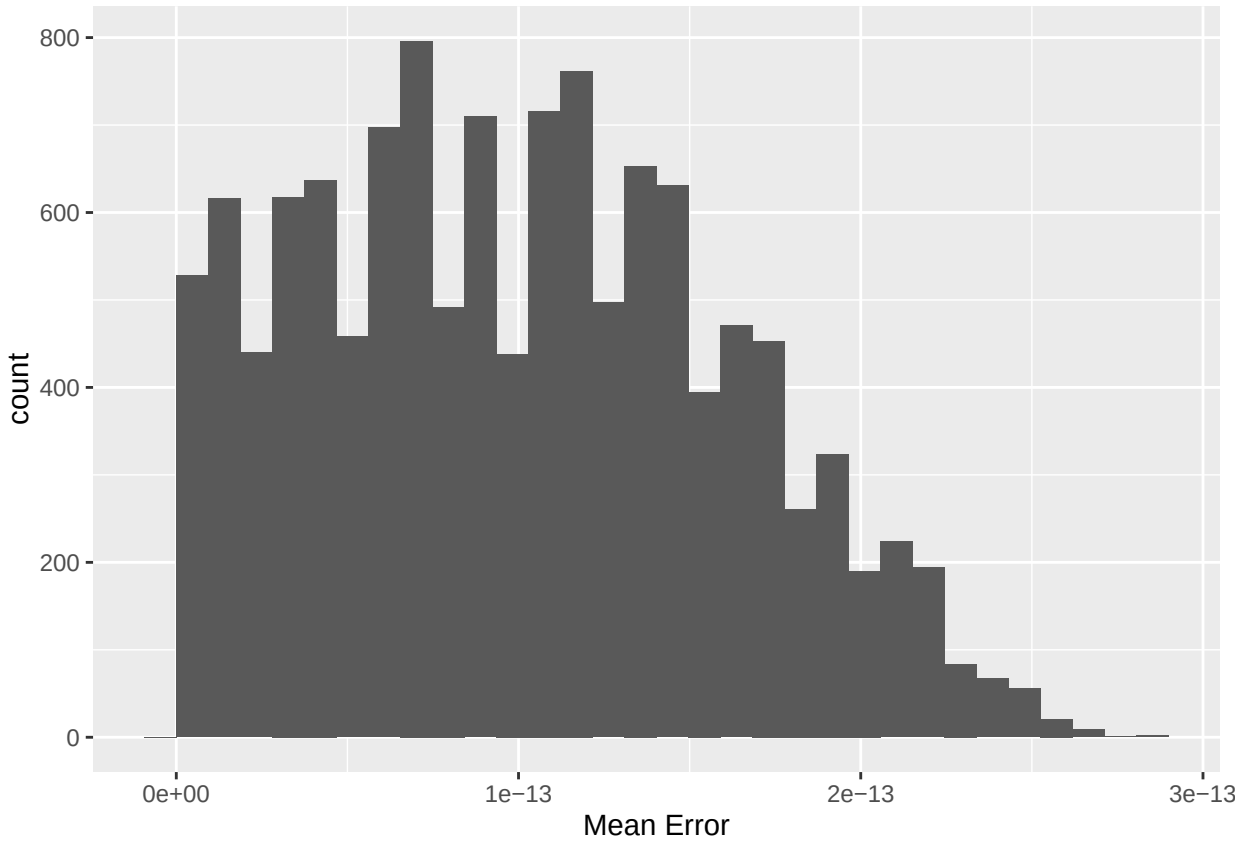
```
## [1] 268
```

```
#paired
sourceCpp(file="/home/anthonycolombo/Documents/qusage/qusage_repos/qusage_speed/R/sigmaArm.cpp")
sourceCpp(file="/home/anthonycolombo/Documents/qusage/qusage_repos/qusage_speed/R/sigmasCpp.cpp")
test1<-calcIndividualExpressionsArm(Baseline,PostTreatment,paired=TRUE,min.variance.factor=10^-6)
```

```
## Found more than one class "QSarray" in cache; using the first, from namespace 'speedSage'
```

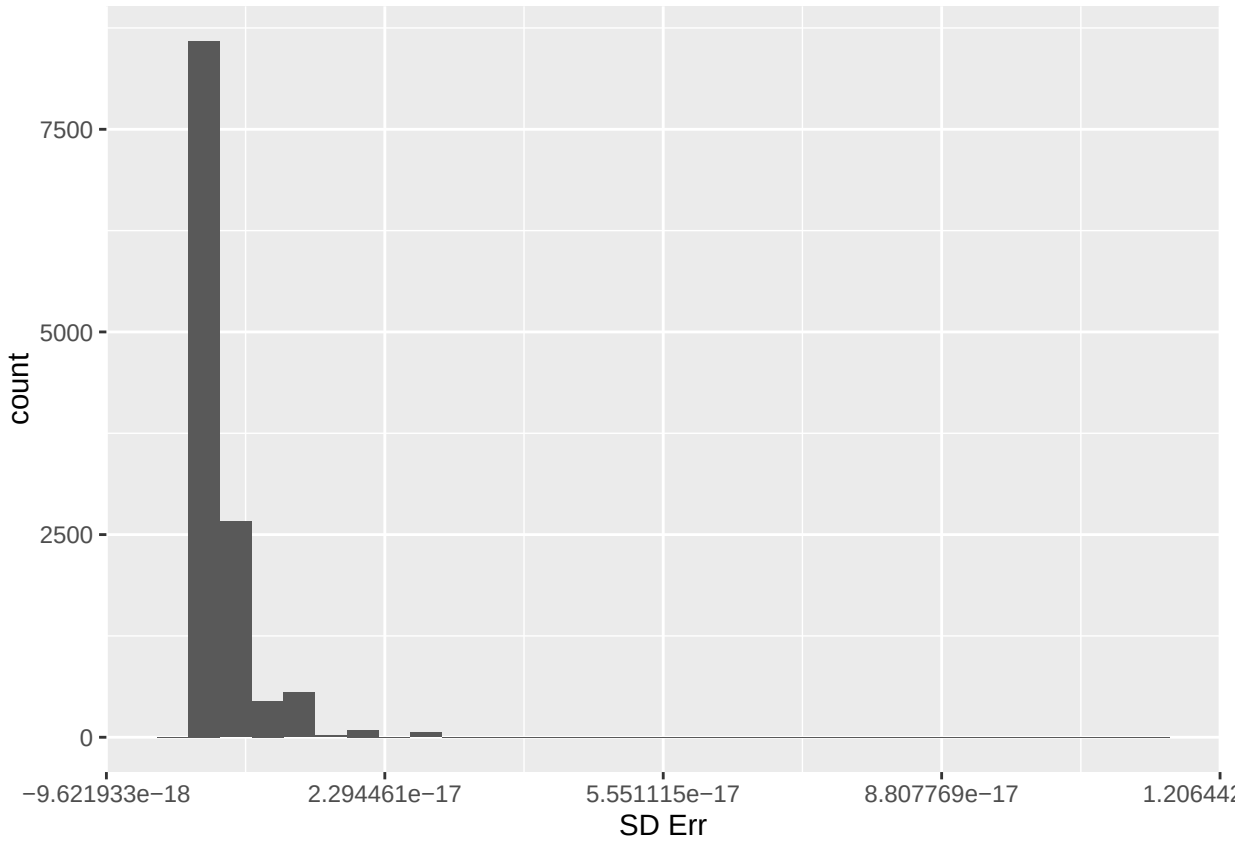
```
test2<-calcIndividualExpressionsC(Baseline,PostTreatment,paired=TRUE,min.variance.factor=10^-6)
test3<-calcIndividualExpressions(Baseline,PostTreatment,paired=TRUE,min.variance.factor=10^-6,na.rm=TRU
qplot(abs(test1[[1]]-test3[[1]]), xlab="Mean Error")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



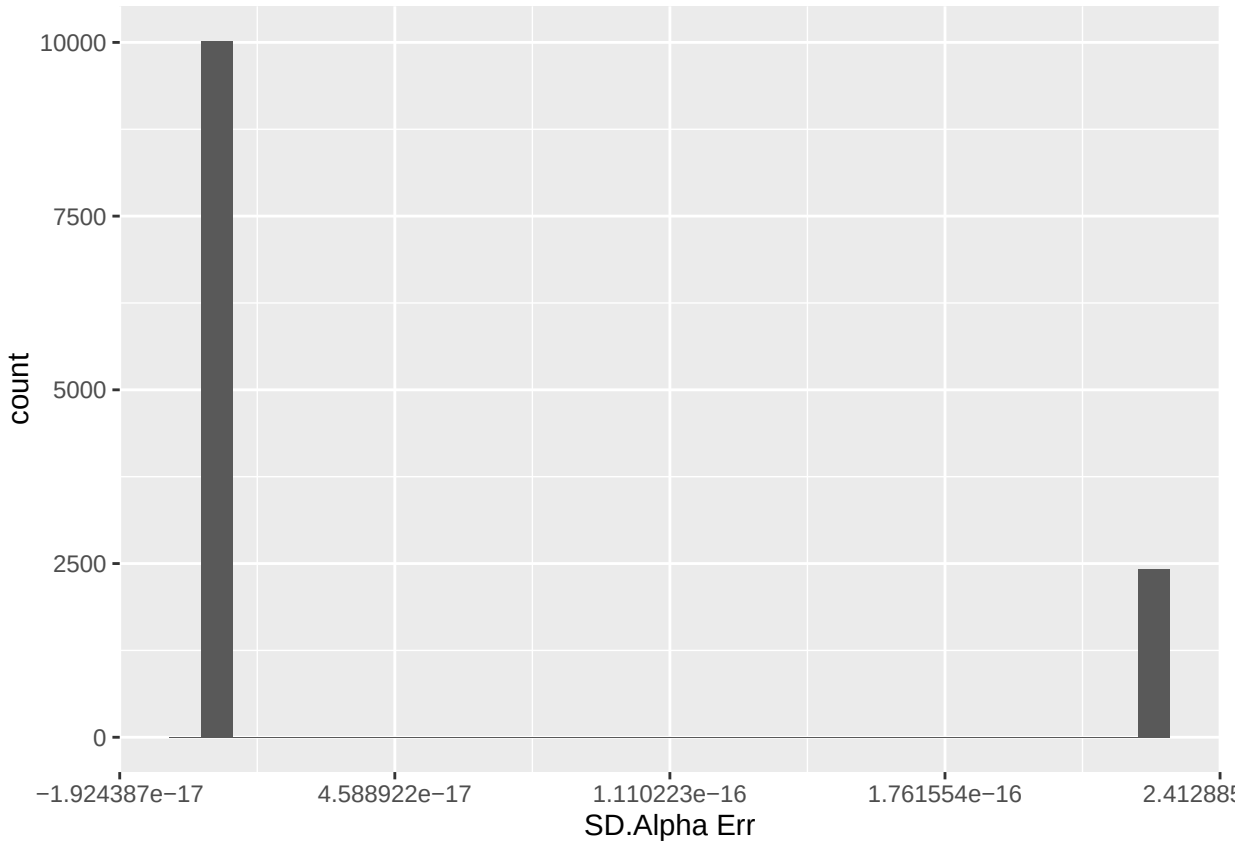

```
qplot(abs(test1[[2]]-test3[[2]]), xlab="SD Err")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



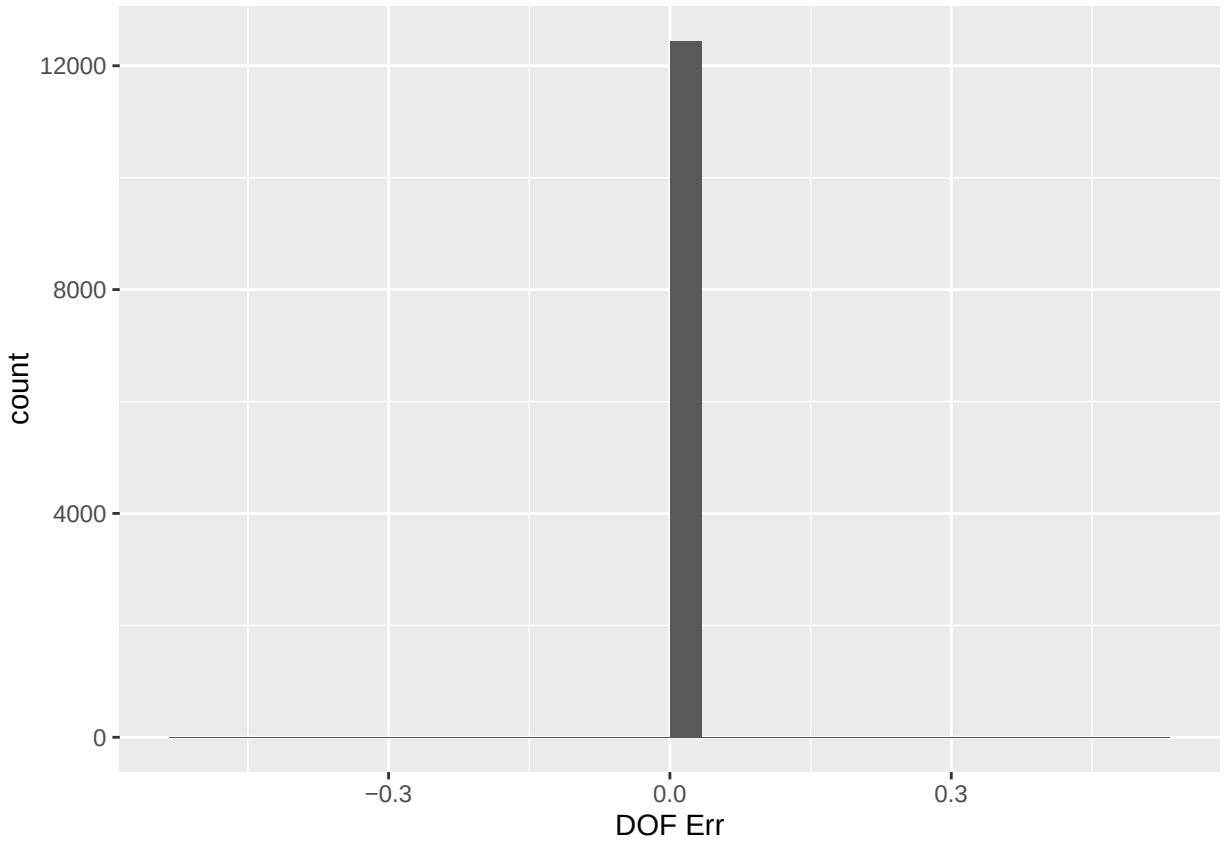

```
qplot(abs(test1[[3]]-test3[[3]]), xlab="SD.Alpha Err")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```




```
qplot(abs(test1[[4]]-test3[[4]]), xlab="DOF Err")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



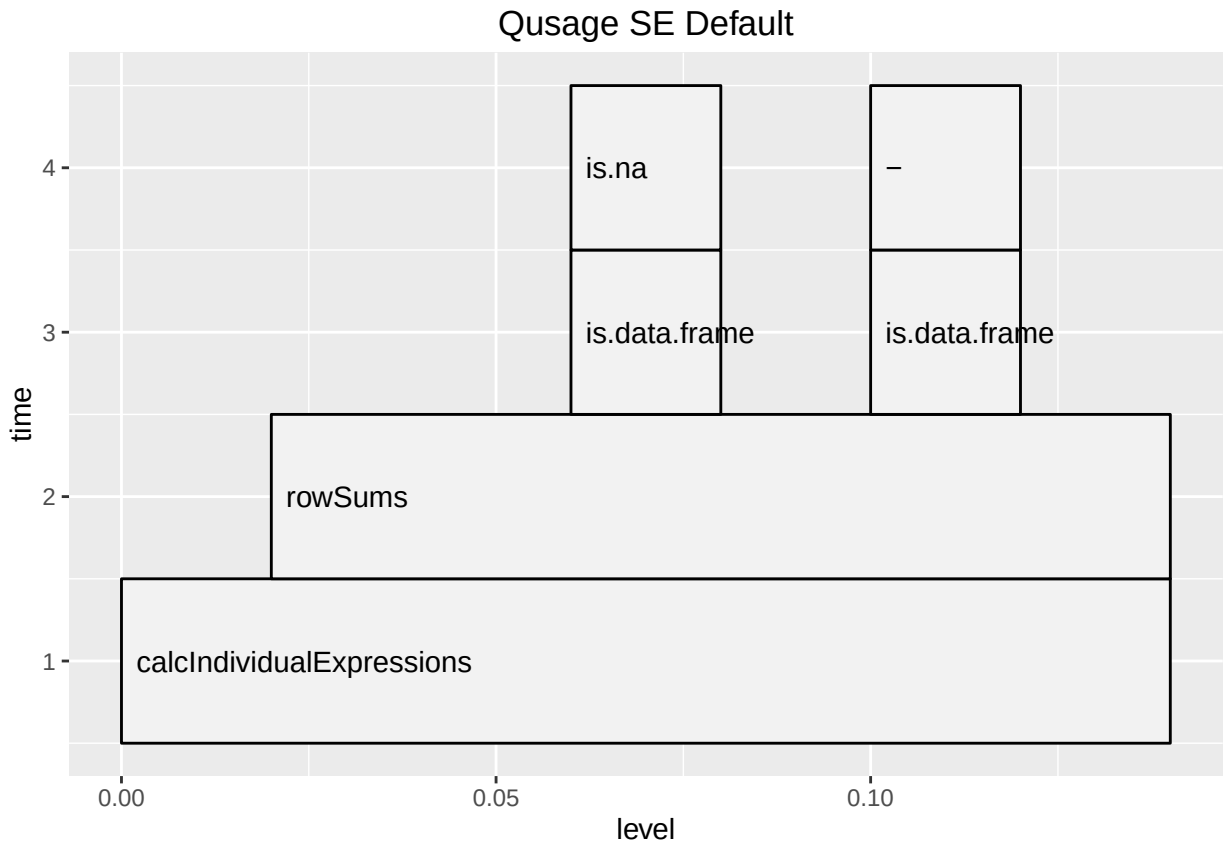

```
mb<-microbenchmark(
test1<-calcIndividualExpressionsArm(Baseline,PostTreatment,paired=TRUE,min.variance.factor=10^-6),
test2<-calcIndividualExpressionsC(Baseline,PostTreatment,paired=TRUE,min.variance.factor=10^-6),
test3<-calcIndividualExpressions(Baseline,PostTreatment,paired=TRUE,min.variance.factor=10^-6,na.rm=TRU
mb
```

```
## Unit: milliseconds
##
##             test1 <- calcIndividualExpressionsArm(Baseline, PostTreatment,      paired = TRUE, min.va
##               test2 <- calcIndividualExpressionsC(Baseline, PostTreatment,      paired = TRUE, min.va
##  test3 <- calcIndividualExpressions(Baseline, PostTreatment, paired = TRUE,      min.variance.factor
##        min       lq      mean    median       uq      max neval cld
##   87.08107  90.0902  98.15651  91.85961  95.9504 156.4834   100 a
##  124.44351 127.7931 140.03864 129.59273 133.5002 192.9120   100  b
##  142.06105 146.1056 170.80863 149.61460 204.3039 211.7414   100   c
```

```
require(profr)
```

```
## Loading required package: profr
```

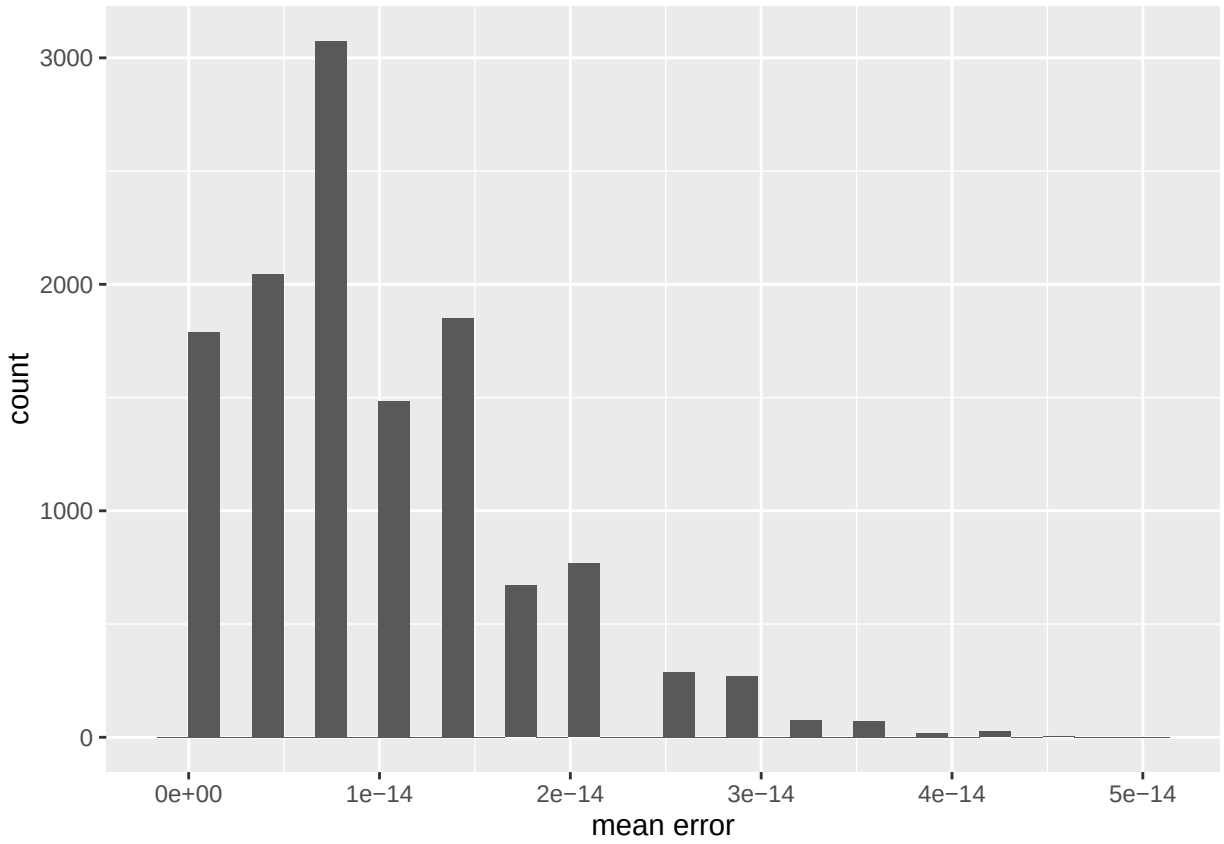
```
require(ggplot2)
x1<-profr(calcIndividualExpressions(Baseline,PostTreatment,paired=TRUE,min.variance.factor=10^-6,na.rm=
ggplot(x1)+labs(title="Qusage SE Default")
```




```
x2<-profr(calcIndividualExpressionsArm(Baseline,PostTreatment,paired=TRUE,min.variance.factor=10^-6))
ggplot(x2)+labs(title="Qusage SE Armadillo")
```

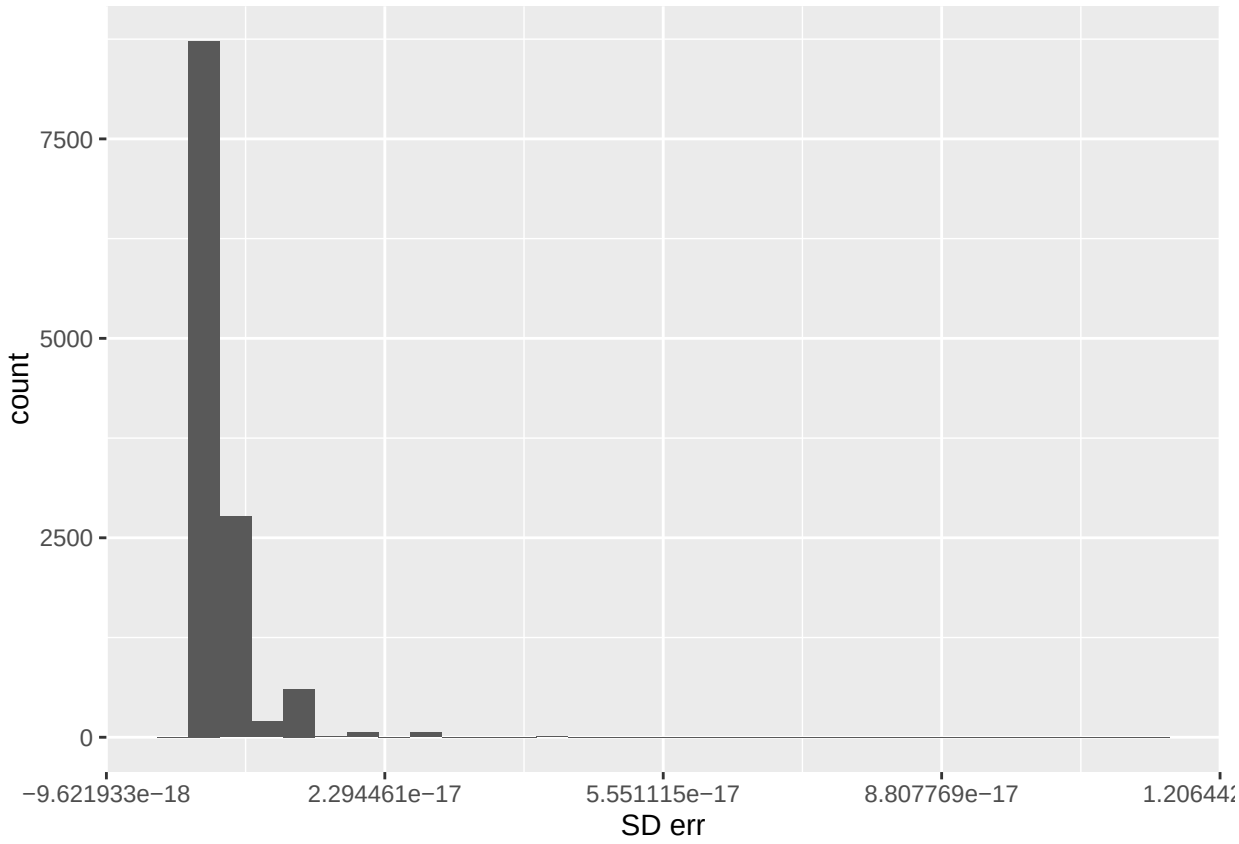

```
#single end testing
sourceCpp("/home/anthonycolombo/Documents/qusage/qusage_repos/qusage_speed/R/sigmaSingle.cpp")
testSE1<-calcIndividualExpressions(Baseline,PostTreatment,paired=FALSE,min.variance.factor=10^-6,na.rm='
testSE2<-calcIndividualExpressionsArm(Baseline,PostTreatment,paired=FALSE,min.variance.factor=10^-6)
testSE3<-calcIndividualExpressionsC(Baseline,PostTreatment,paired=FALSE,min.variance.factor=10^-6)


e1<-(abs(testSE1[[1]]-testSE2[[1]]))
e2<-(abs(testSE1[[2]]-testSE2[[2]]))
e3<-(abs(testSE1[[3]]-testSE2[[3]]))
e4<-(abs(testSE1[[4]]-testSE2[[4]]))
qplot(as.vector(e1), xlab="mean error")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



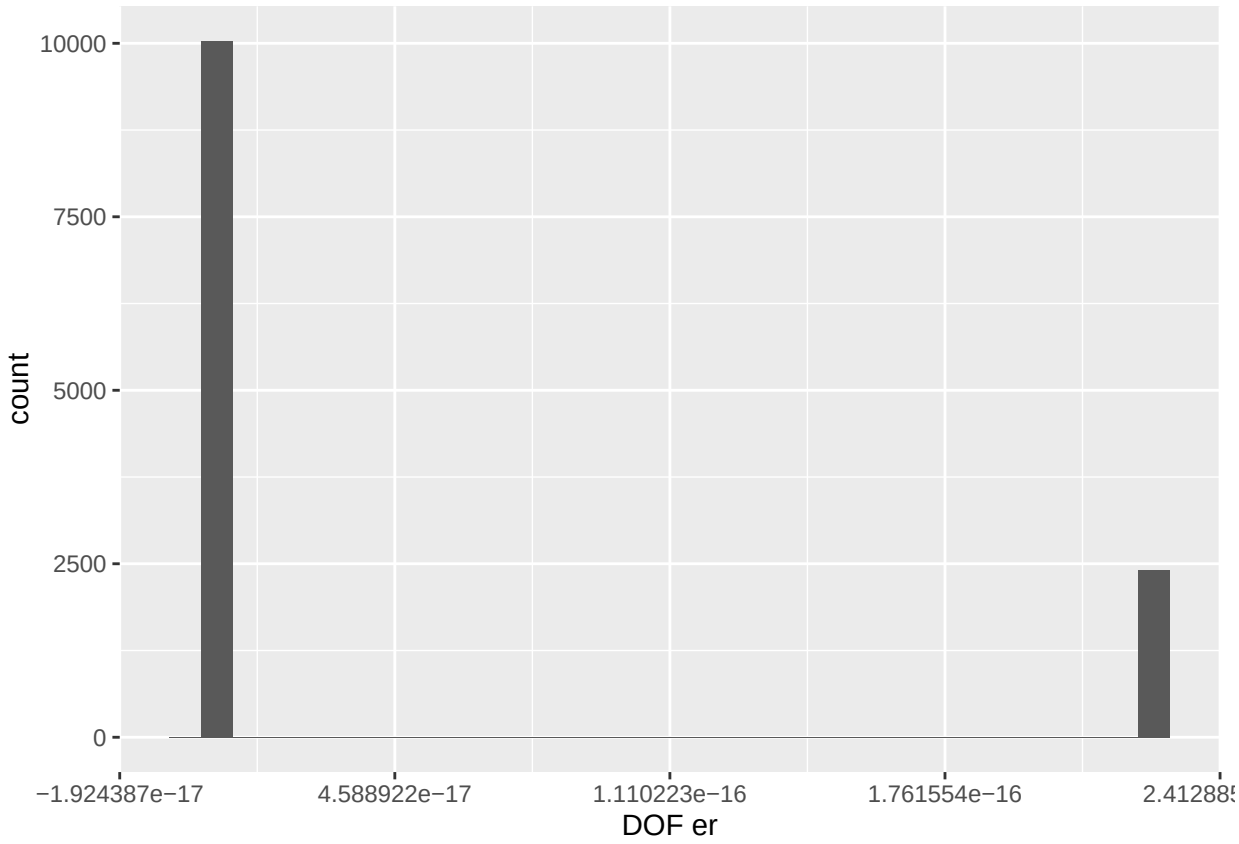

```
qplot(as.vector(e2), xlab="SD err")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



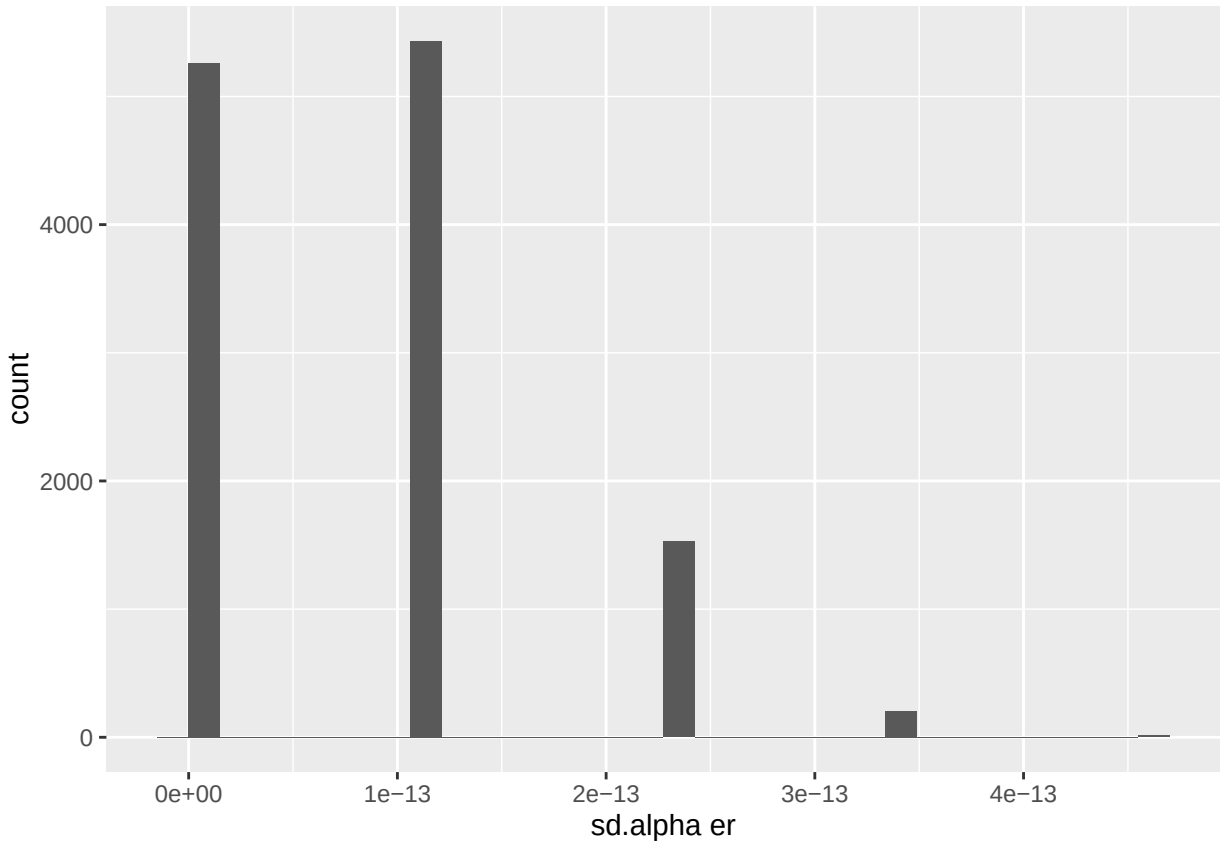

```
qplot(as.vector(e3), xlab= "DOF er")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

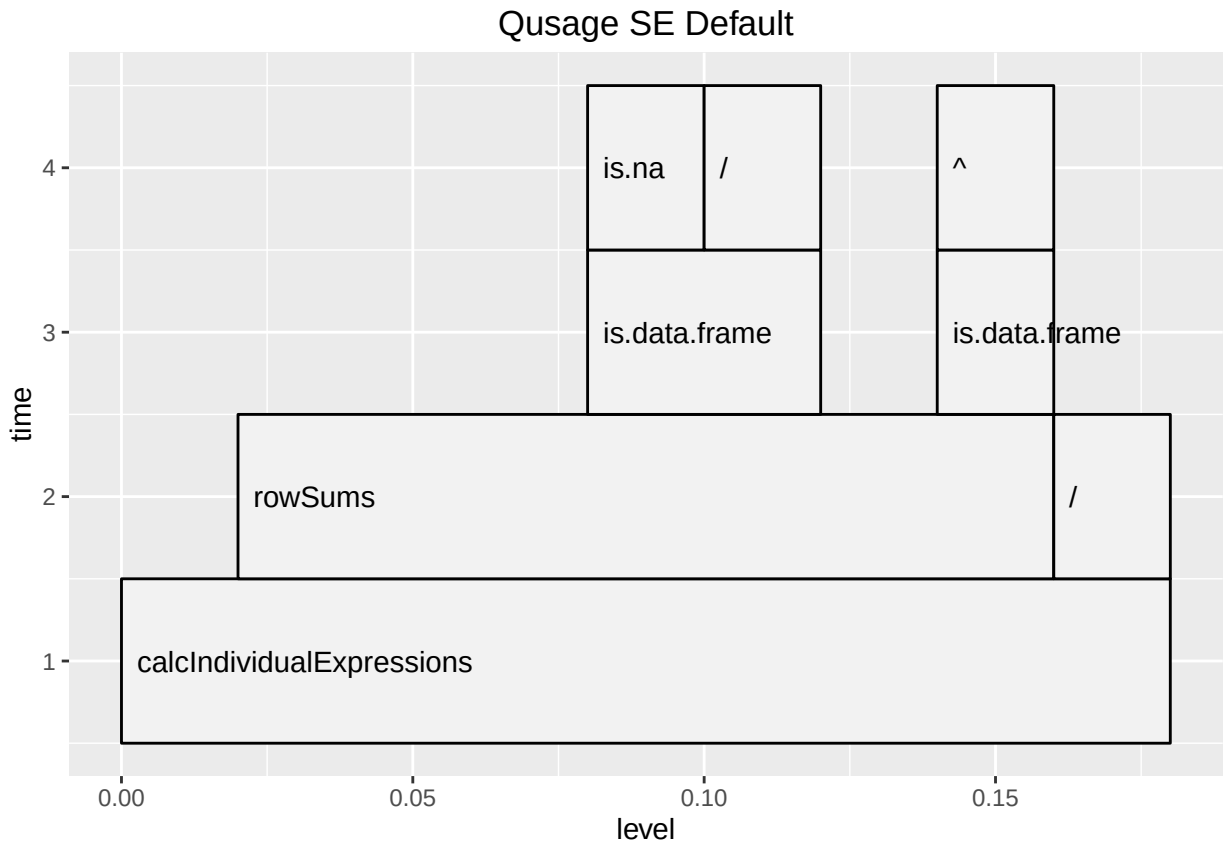



```
qplot(as.vector(e4), xlab="sd.alpha er")
```

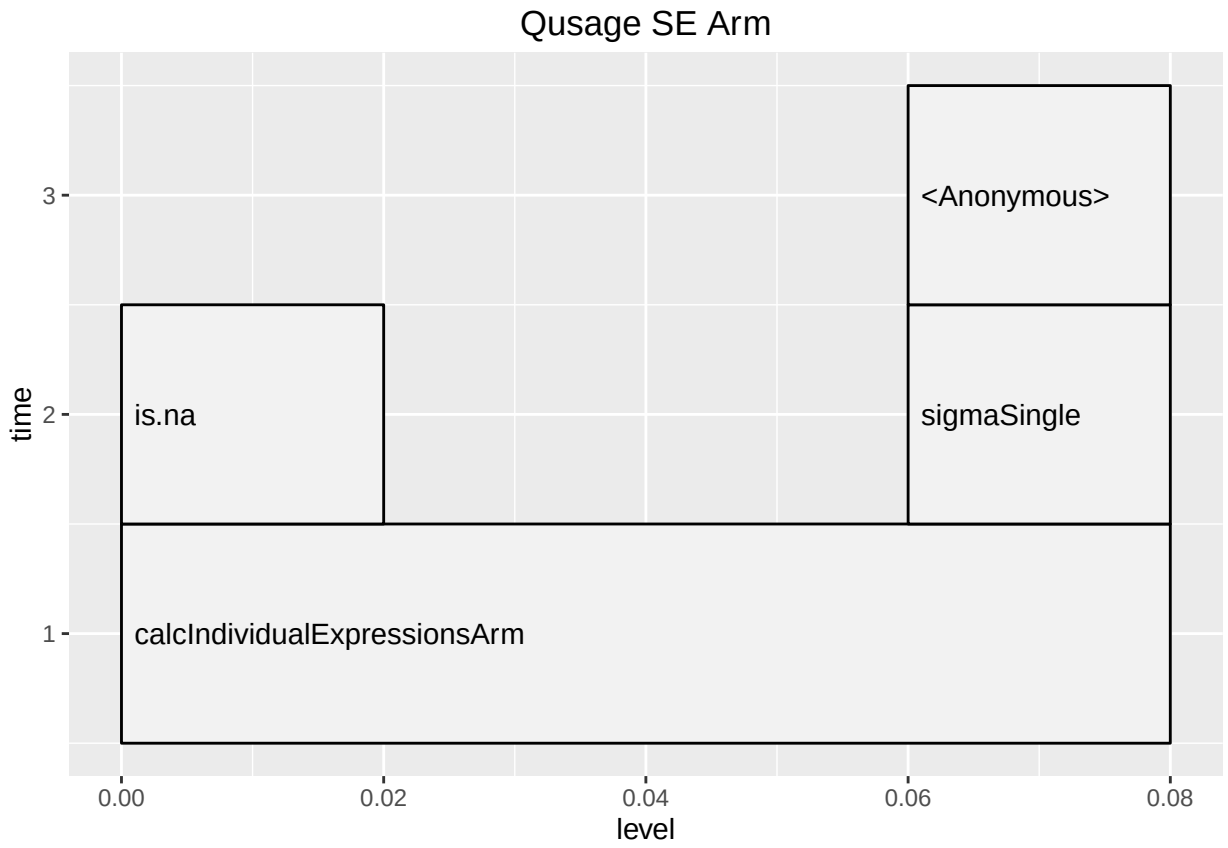
```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```




```
require(profr)
require(ggplot2)
y1<-profr(calcIndividualExpressions(Baseline,PostTreatment,paired=FALSE,min.variance.factor=10^-6,na.rm=
y2<-profr(calcIndividualExpressionsArm(Baseline,PostTreatment,paired=FALSE,min.variance.factor=10^-6))
ggplot(y1)+labs(title="Qusage SE Default")
```




```
ggplot(y2)+labs(title="Qusage SE Arm")
```




```
#this shows that the only difference is the vector of Non-NA columns per each row; which is the same as
seMB<-microbenchmark(
testSE1<-calcIndividualExpressions(Baseline,PostTreatment,paired=FALSE,min.variance.factor=10^-6,na.rm=
testSE2<-calcIndividualExpressionsArm(Baseline,PostTreatment,paired=FALSE,min.variance.factor=10^-6)
)
seMB
```

```
## Unit: milliseconds
##
##  testSE1 <- calcIndividualExpressions(Baseline, PostTreatment,      paired = FALSE, min.variance.fac
##             testSE2 <- calcIndividualExpressionsArm(Baseline, PostTreatment,      paired = FALSE, mi
##        min        lq     mean    median       uq      max neval cld
##  174.29680 181.14035 216.9777 201.35234 245.0851 341.6823   100   b
##   83.15912  89.48346 100.3642  91.98409 101.2754 178.0744   100  a
```

```
#add NAs and test
testPT<-PostTreatment[1:20,]
testPT<-cbind(rbind(testPT,NaN),NA)
rownames(testPT)[nrow(testPT)]<-"NA"
testB<-Baseline[1:20,]
testB<-cbind(rbind(testB,NaN),NA)
rownames(testB)[nrow(testB)]<-"NA"
#calcIndividualExpressionsC(testB,testPT)) will produce error and stop if NA
```

3 Alternate training sets

there is an issue when calling makeComparisons on eset.1 and eset.2 test object, the mclapply is dispatching twice which causes slowness, also I wish to compile R computations for certain functions to speed up before run-time. This eset was then created from makeCompairson funciton which compares two different labels after splitting the eset by column names label type.

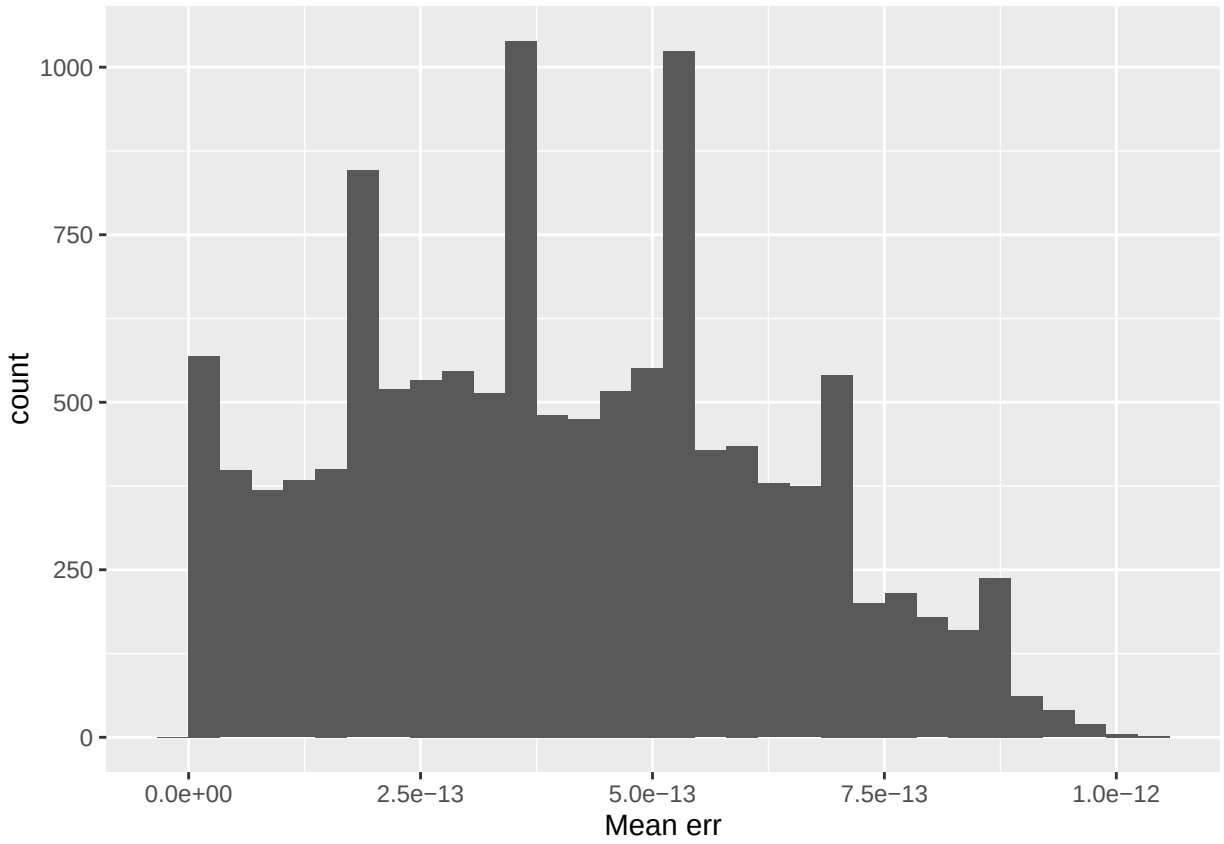
4 Paired end revised demo set , not split by label

```
library(Rcpp)
library(parallel)
library(speedSage)
library(qusage)
eset<-system.file("extdata","eset.RData",package="speedSage")
load(eset)
labels<-c(rep("t0",134),rep("t1",134))
contrast<-"t1-t0"
colnames(eset)<-c(rep("t0",134),rep("t1",134))
fileISG<-system.file("extdata","c2.cgp.v5.1.symbols.gmt",package="speedSage")
ISG.geneSet<-read.gmt(fileISG)
ISG.geneSet<-ISG.geneSet[grepl("DER_IFN_GAMMA_RESPONSE_UP",names(ISG.geneSet))]
sourceCpp(file="/home/anthonycolombo/Documents/qusage/qusage_repos/qusage_speed/R/sigmasCpp.cpp")
sourceCpp(file="/home/anthonycolombo/Documents/qusage/qusage_repos/qusage_speed/R/sigmaArm.cpp")
sourceCpp(file="/home/anthonycolombo/Documents/qusage/qusage_repos/qusage_speed/R/sigmaSingle.cpp")

eset.1<-eset-40.3
eset.2<-eset+100.5
ncol(eset.1) #splitting eset in half
```

```
## [1] 268
```

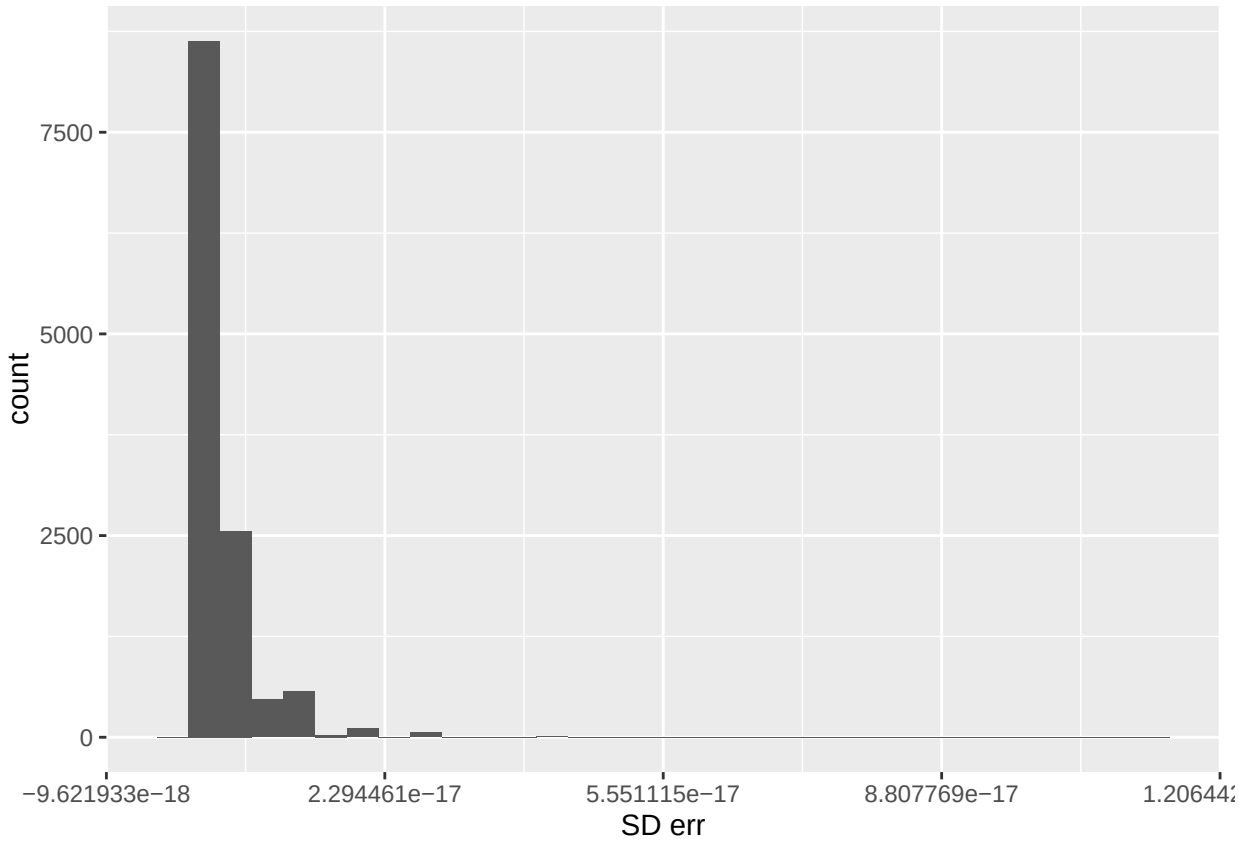
```
original<-calcIndividualExpressions(eset.1,eset.2,paired=TRUE)
cpp<-calcIndividualExpressionsC(eset.1,eset.2,paired=TRUE)
arm<-calcIndividualExpressionsArm(eset.1,eset.2,paired=TRUE)

e1<-(abs(original[[1]]-arm[[1]]))
e2<-(abs(original[[2]]-arm[[2]]))
e3<-(abs(original[[3]]-arm[[3]]))
e4<-(abs(original[[4]]-arm[[4]]))
qplot(as.vector(e1),xlab="Mean err")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



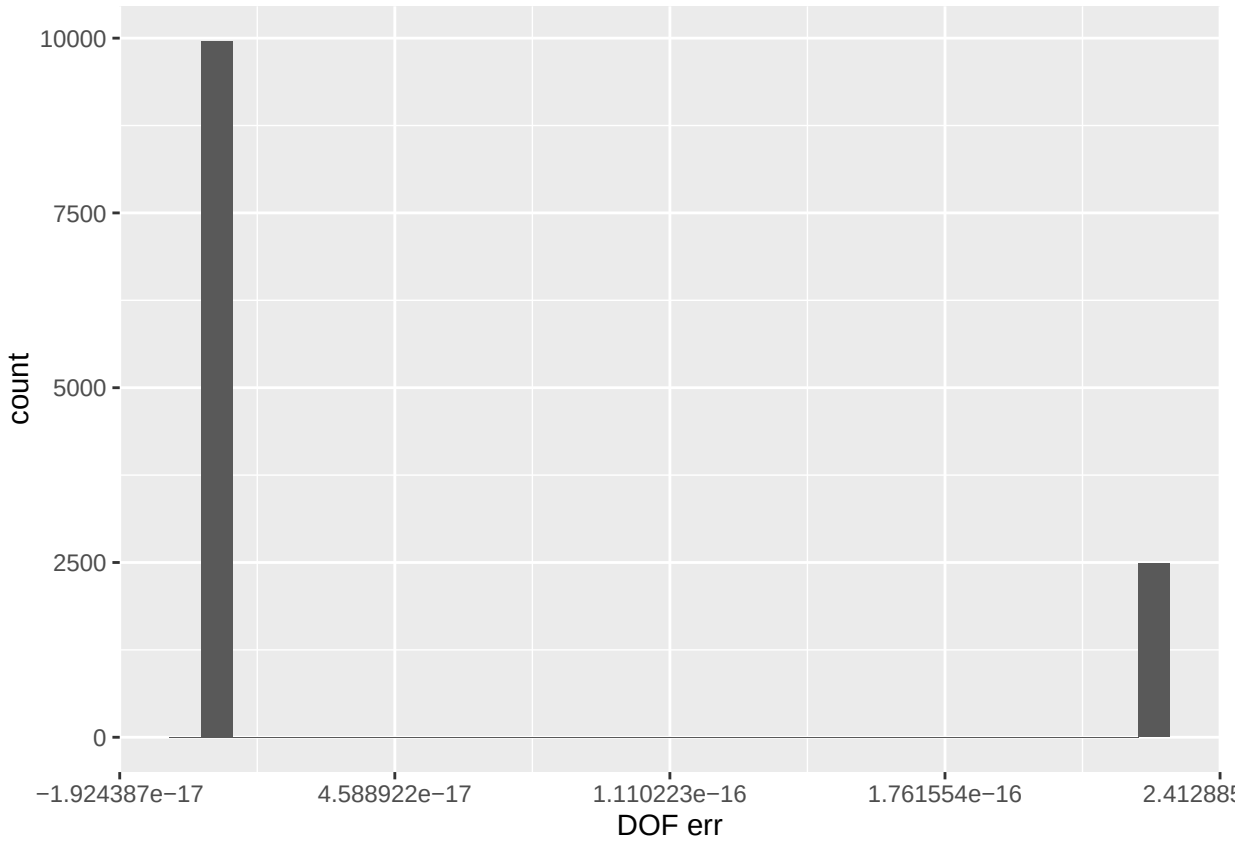

```
qplot(as.vector(e2), xlab="SD err")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



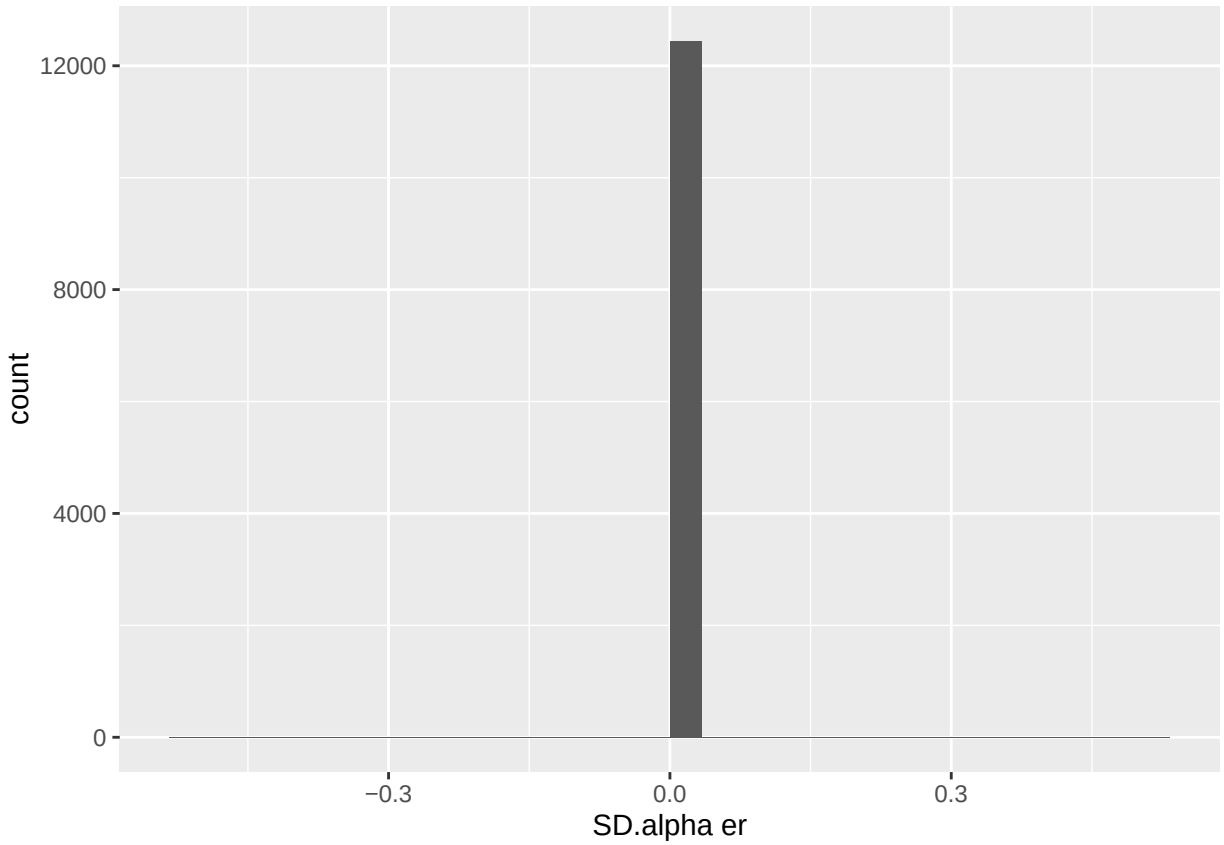

```
qplot(as.vector(e3), xlab="DOF err")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```




```
qplot(as.vector(e4), xlab="SD.alpha er")
```

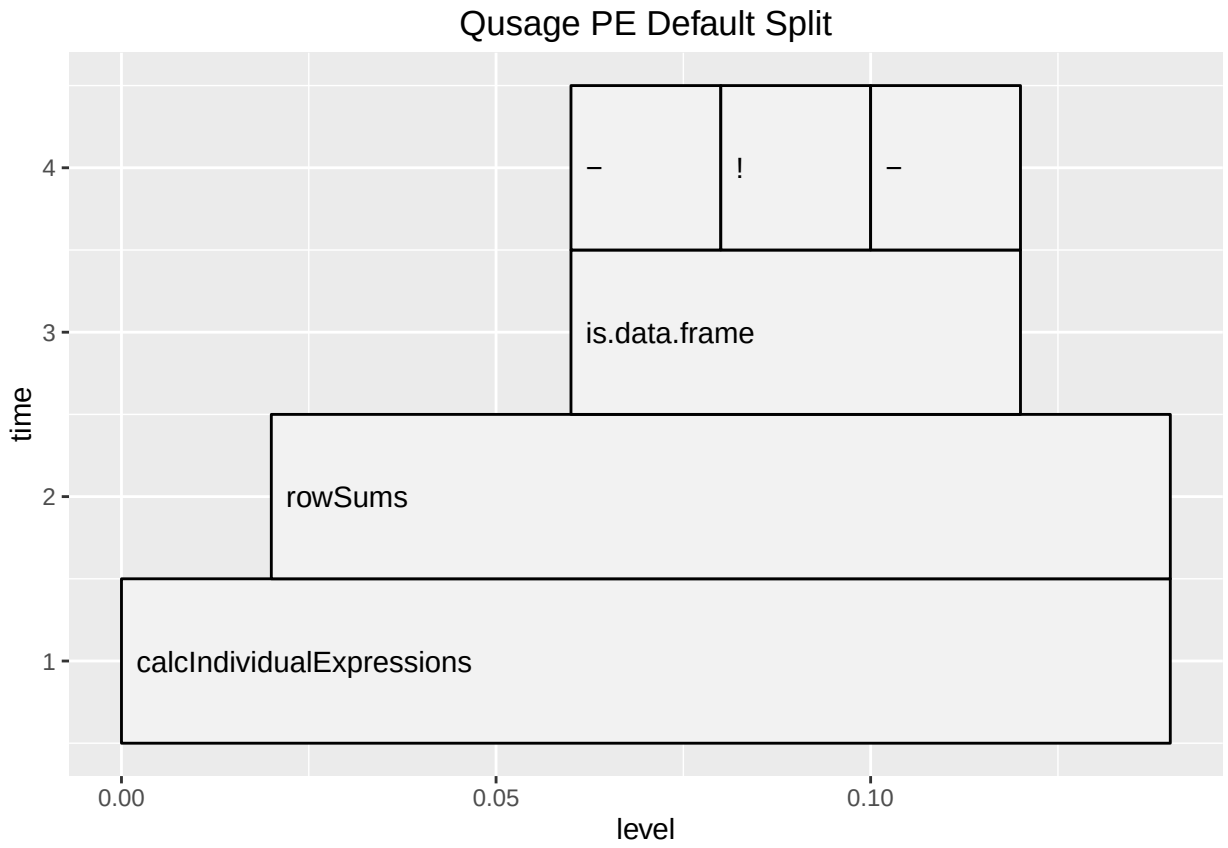
```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



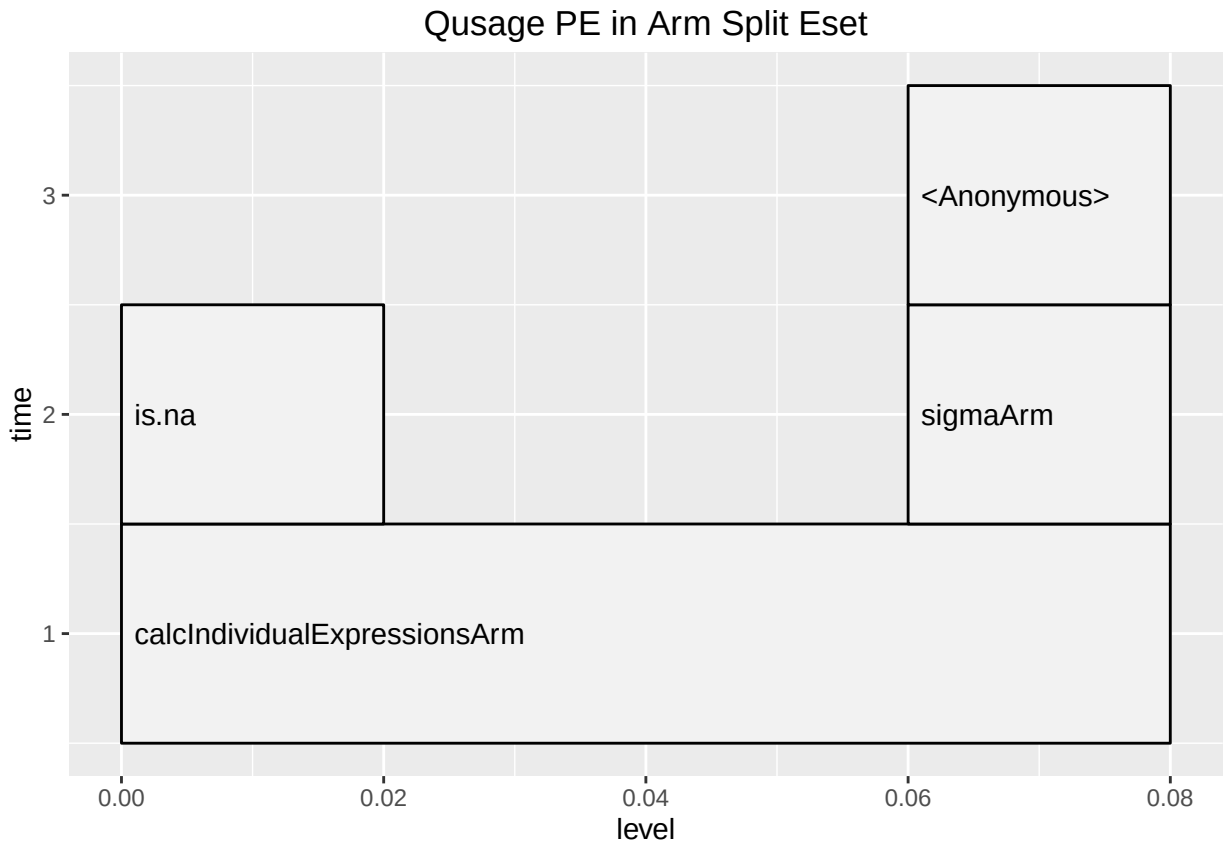

```
microbenchmark(
 original<-calcIndividualExpressions(eset.1,eset.2,paired=TRUE),
 cpp<-calcIndividualExpressionsC(eset.1,eset.2,paired=TRUE),
 arm<-calcIndividualExpressionsArm(eset.1,eset.2,paired=TRUE))
```

```
## Unit: milliseconds
##                                                                  expr
##  original <- calcIndividualExpressions(eset.1, eset.2, paired = TRUE)
##      cpp <- calcIndividualExpressionsC(eset.1, eset.2, paired = TRUE)
##    arm <- calcIndividualExpressionsArm(eset.1, eset.2, paired = TRUE)
##        min        lq      mean    median        uq      max neval cld
##  139.70778 146.67344 157.91105 150.28262 154.61108 226.5829   100   c
##  122.72607 128.48925 137.49920 131.95793 135.33833 222.9347   100  b
##   87.19454  89.87242  97.70817  93.50934  97.20076 164.5031   100 a
```

```
#showing profiles
library(profr)
library(ggplot2)

yy<-profr(calcIndividualExpressions(eset.1,eset.2,paired=TRUE))
ggplot(yy) + labs(title="Qusage PE Default Split")
```




```
tt<-profr(calcIndividualExpressionsArm(eset.1,eset.2,paired=TRUE))
ggplot(tt)+ labs(title="Qusage PE in Arm Split Eset")
```



5 Non-paired end the eset.1, eset.2 split by label

This simulates how makeComparison will compare a split eset with label split

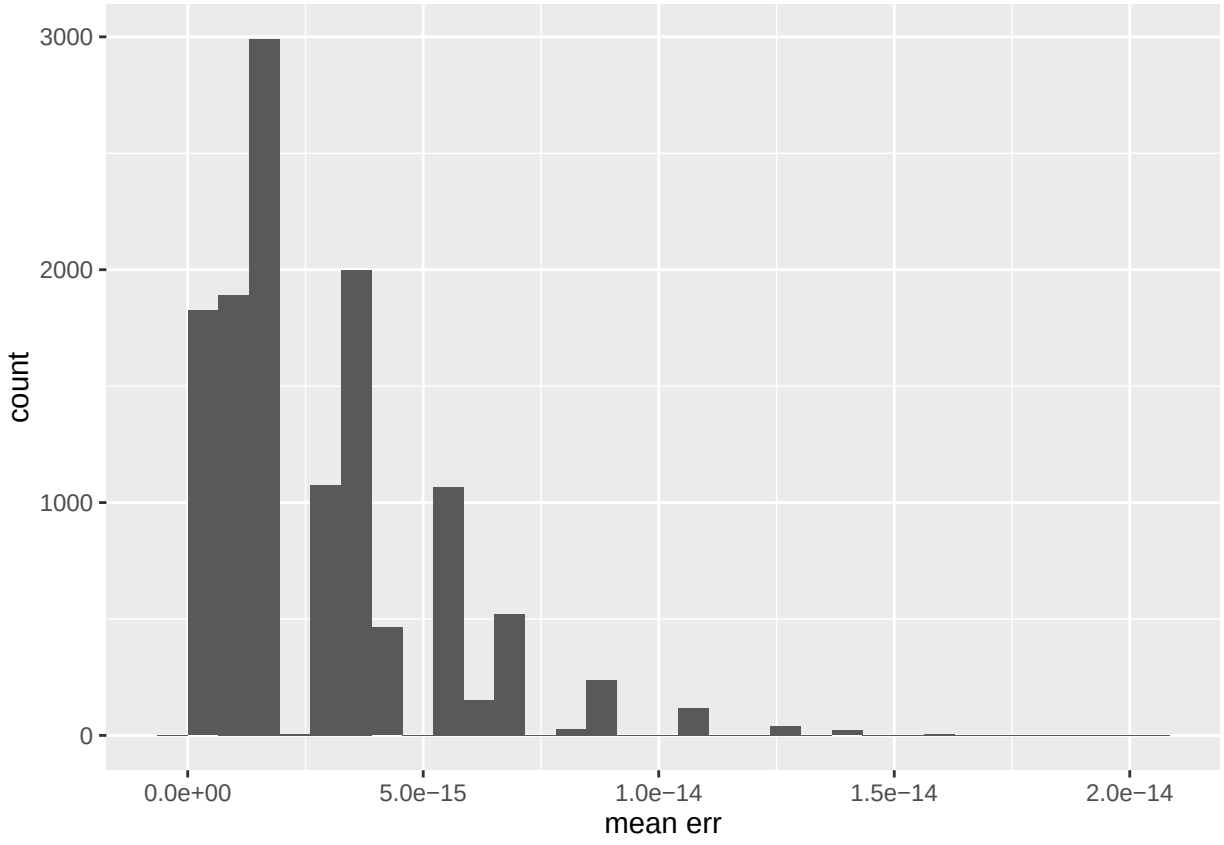
```
library(microbenchmark)
library(profr)
library(ggplot2)
library(Rcpp)
eset.1<-system.file("extdata","eset.1.RData",package="speedSage")
eset.2<-system.file("extdata","eset.2.RData",package="speedSage")
ncol(eset.1)
```

```
## NULL
```

```
load(eset.1)
load(eset.2)
sourceCpp(file="/home/anthonycolombo/Documents/qusage/qusage_repos/qusage_speed/R/sigmasCpp.cpp")
sourceCpp(file="/home/anthonycolombo/Documents/qusage/qusage_repos/qusage_speed/R/sigmaArm.cpp")
original<-calcIndividualExpressions(eset.1,eset.2,paired=FALSE)
cpp<-calcIndividualExpressionsC(eset.1,eset.2,paired=FALSE)
arm<-calcIndividualExpressionsArm(eset.1,eset.2,paired=FALSE)
e1<-(abs(original[[1]]-arm[[1]]))
e2<-(abs(original[[2]]-arm[[2]]))
e3<-(abs(original[[3]]-arm[[3]]))
```

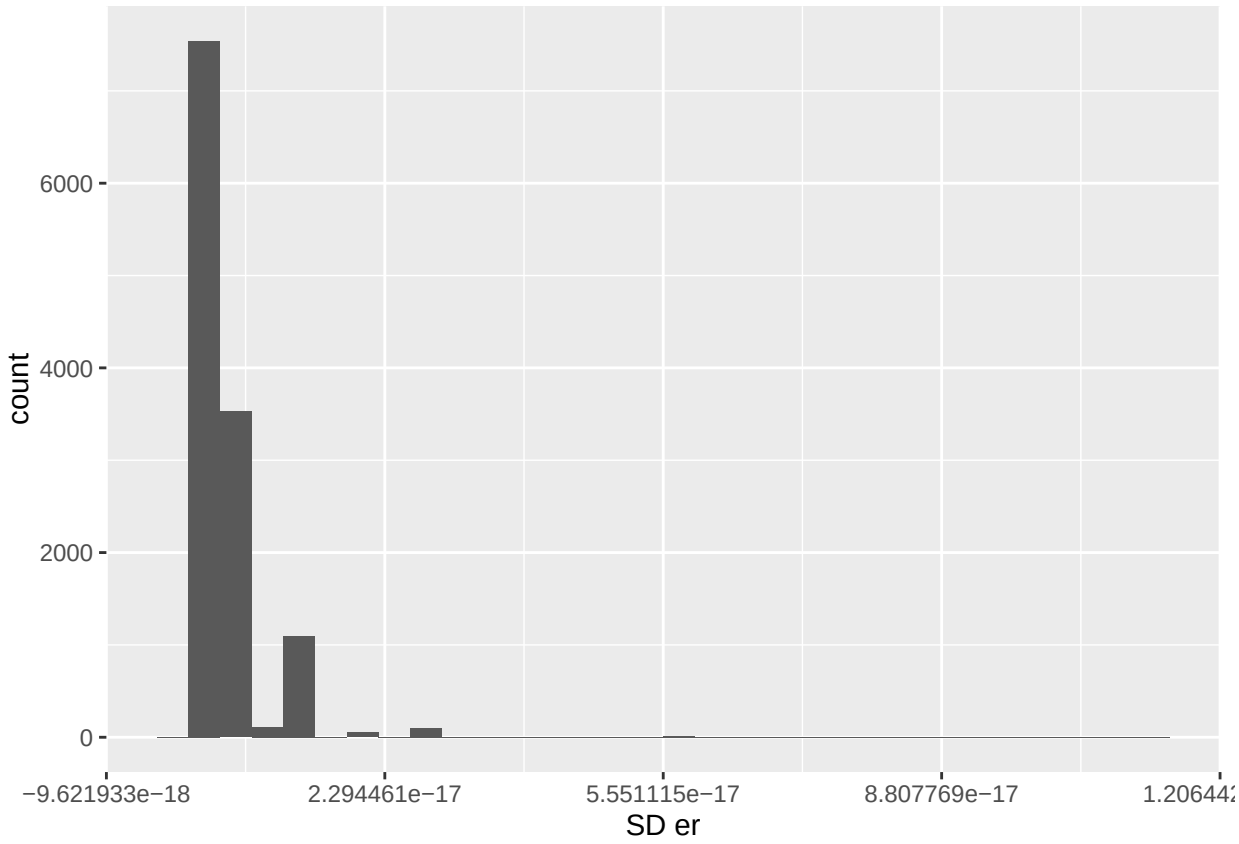
```
e4<-(abs(original[[4]]-arm[[4]]))
qplot(as.vector(e1), xlab="mean err")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



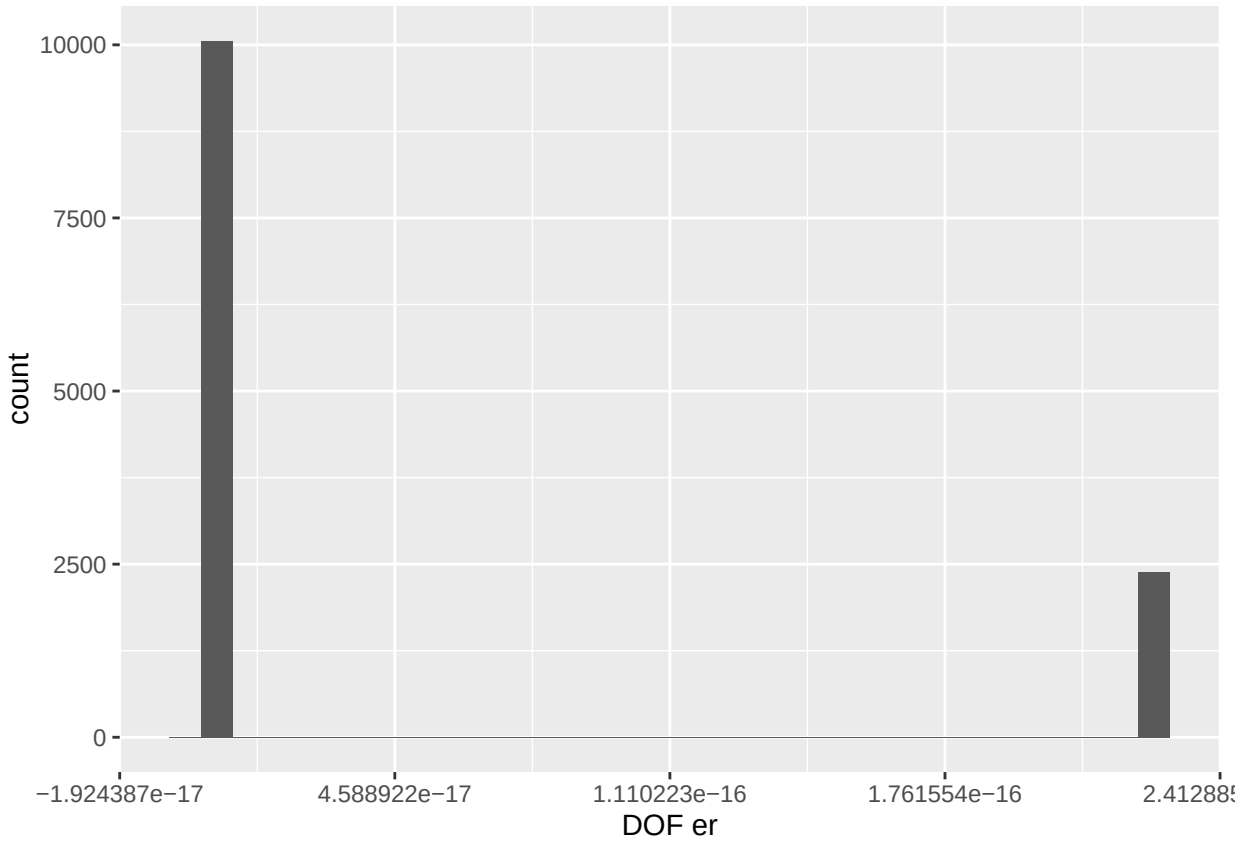

```
qplot(as.vector(e2), xlab="SD er")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



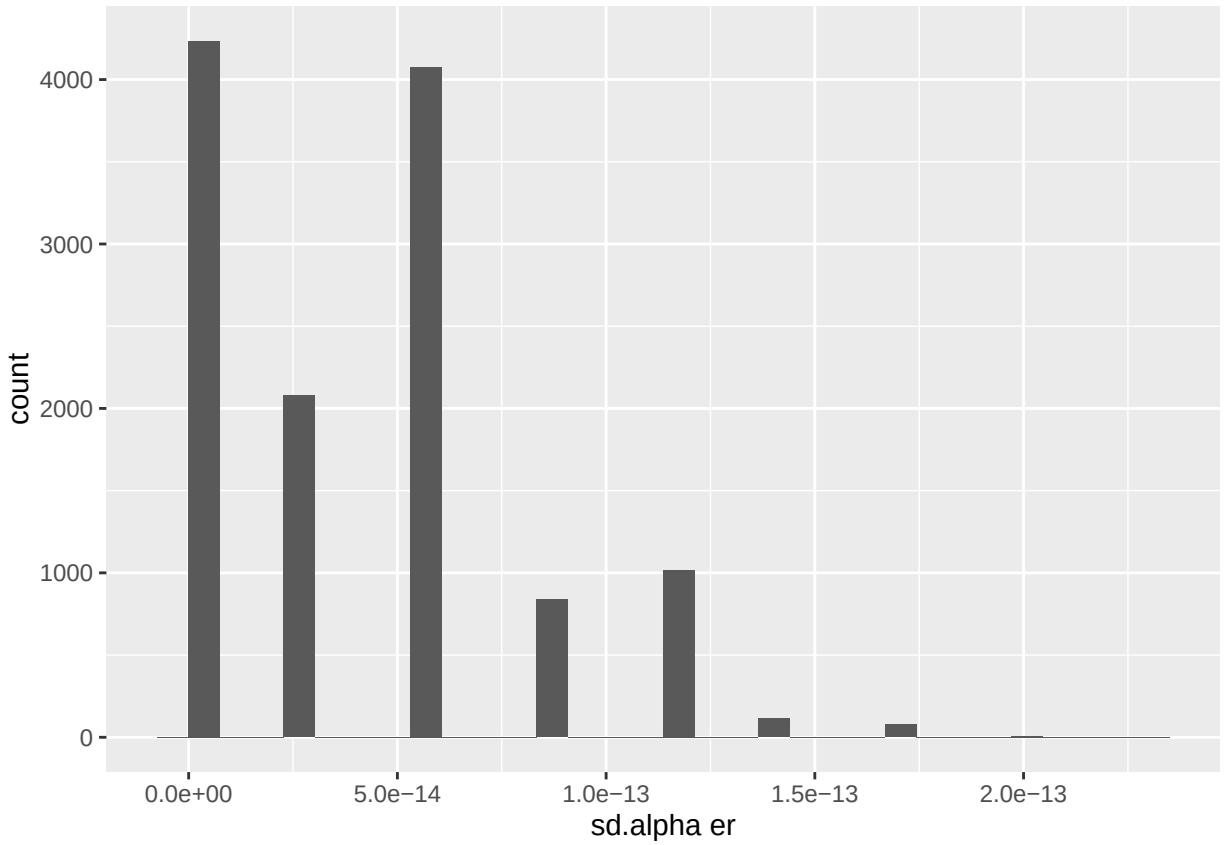

```
qplot(as.vector(e3), xlab="DOF er")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```




```
qplot(as.vector(e4), xlab="sd.alpha er")
```

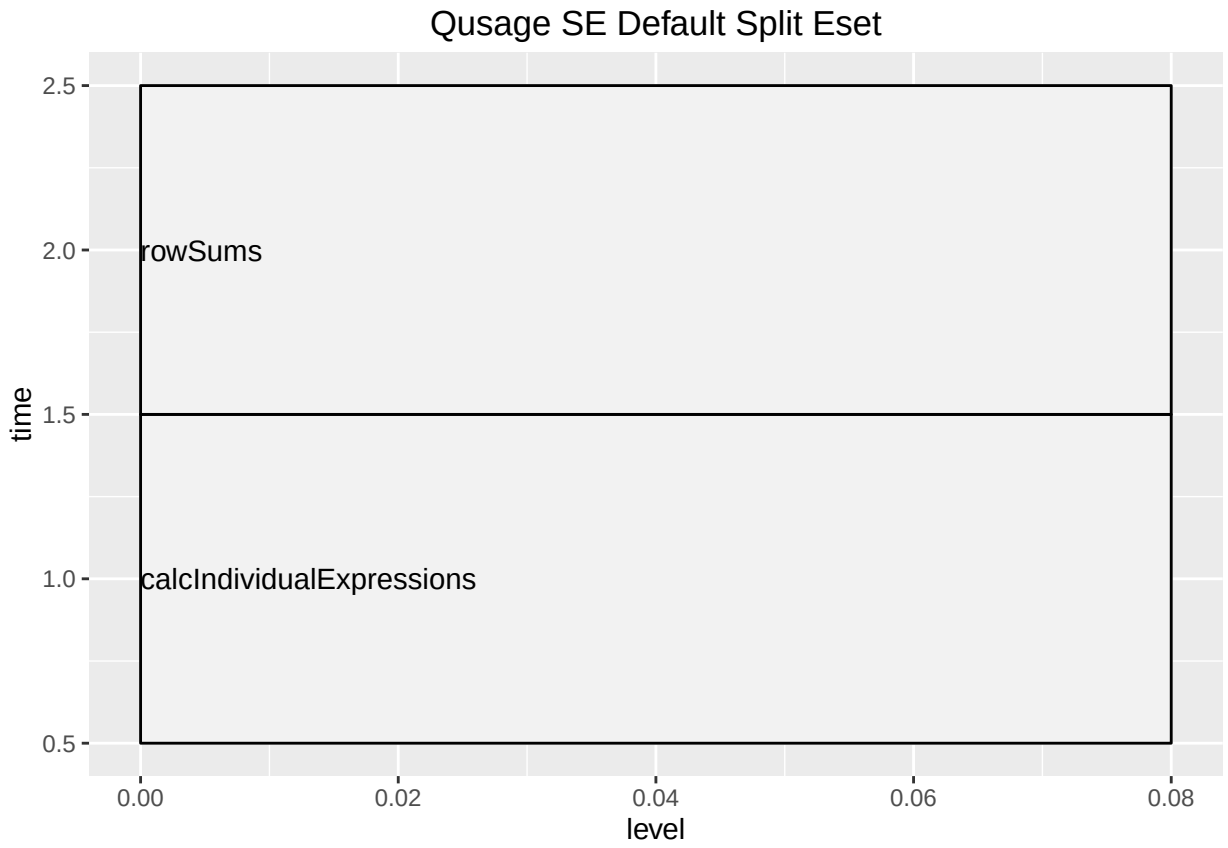
```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



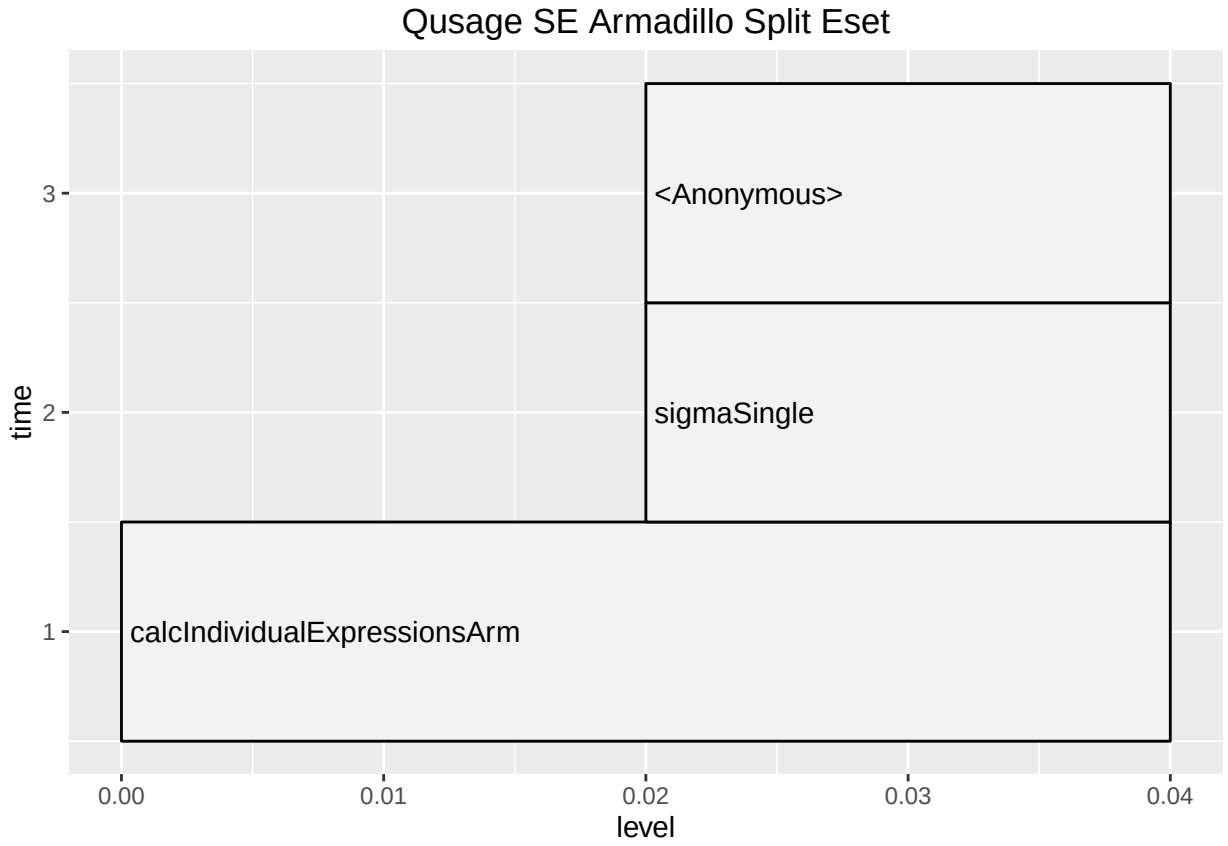

```
microbenchmark(
 original<-calcIndividualExpressions(eset.1,eset.2,paired=FALSE),
 cpp<-calcIndividualExpressionsC(eset.1,eset.2,paired=FALSE),
 arm<-calcIndividualExpressionsArm(eset.1,eset.2,paired=FALSE))
```

```
## Unit: milliseconds
##                                                                  expr
##  original <- calcIndividualExpressions(eset.1, eset.2, paired = FALSE)
##      cpp <- calcIndividualExpressionsC(eset.1, eset.2, paired = FALSE)
##    arm <- calcIndividualExpressionsArm(eset.1, eset.2, paired = FALSE)
##       min       lq     mean   median       uq       max neval cld
##  90.96663 93.85508 97.40574 95.87249 98.34231 160.33290   100   c
##  63.17562 64.45020 67.30091 65.72186 68.10181 128.28527   100  b
##  42.44482 44.86955 46.91926 46.24674 48.56804  63.23528   100 a
```

```
x<-profr(calcIndividualExpressions(eset.1,eset.2,paired=FALSE))
y<-profr(calcIndividualExpressionsArm(eset.1,eset.2,paired=FALSE))
ggplot(x) + labs(title="Qusage SE Default Split Eset")
```




```
ggplot(y) + labs(title="Qusage SE Armadillo Split Eset")
```


Qusage SE Armadillo Split Eset
time
3
2
1
<Anonymous>
sigmaSingle
calcIndividualExpressionsArm
0.00
0.01
0.02
0.03
0.04
level