

Supplementary material to:

Estimating meaningful thresholds for multi-item questionnaires using item response theory

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1. Item parameters for simulation

Item	Discrimination	Difficulty		
	a	b_1	b_2	b_3
1	1.30	-1.60	-0.80	0.40
2	1.96	-2.00	-0.80	0.10
3	0.98	-1.30	-0.40	0.40
4	1.63	-1.30	-0.40	0.70
5	2.28	-1.00	0.00	1.00
6	2.28	-0.80	0.00	1.10
7	1.96	-0.70	0.40	1.60
8	1.63	-0.80	0.40	1.30
9	1.30	-0.30	0.80	1.80
10	0.98	-0.20	0.80	1.60
<i>Mean</i>	1.63	-1.00	0.00	1.00

2. Simulation syntax (R-code)

```
library(mirt)
library(lavaan)
library(e1071)
library(ggplot2)
library(psych)
library(pROC)

##### Create set of item parameters

N <- 1000           # simulated sample size
nitems <- 10         # number of items
ncat <- 4            # number of response categories per item

a <- c(0.6,0.6,0.8,0.8,1,1,1.2,1.2,1.4,1.4)
b2 <- (a-1)*2
bc <- (a-1)/2

set.seed(12345)

a <- sample(a)
b1 <- b2 - 1 + sample(bc)
b3 <- b2 + 1 + sample(bc)

# Adjust a to get the desired reliability

a1 <- a*1.63        # Creates reliability of ~0.85

cf.simb <- data.frame(a1,b1,b2,b3)
round(cf.simb, 3)
round(colMeans(cf.simb), 3)

( mean.b <- mean(as.matrix(cf.simb[,-1])) )
( sd.b <- sd(as.matrix(cf.simb[,-1])) )

# Transform b-parameters to d-parameters
# difficulty (b) = easiness (d) / -a

cf.sim1 <- cf.simb

colnames(cf.sim1) <- c("a1","d1","d2","d3")

cf.sim1$d1 <- -cf.simb$b1*a1
cf.sim1$d2 <- -cf.simb$b2*a1
```

```

cf.sim1$d3 <- -cf.simb$b3*a1
round(cf.sim1, 3)                      # displays the item parameters
round(colMeans(cf.sim1), 3)

# Simulate dataset using 'mirt'

a1 <- as.matrix(cf.sim1[ , 1])
d1 <- as.matrix(cf.sim1[ , -1])

# Check reliability
# Create dataset with theta = N(0,1)

Y <- rnorm(N*10, 0, 1)
Y <- (Y-mean(Y))/sd(Y)      # set mean = 0 and SD = 1
theta.org <- as.matrix( Y )

dat <- simdata(a1, d1, N*10, itemtype="graded", Theta=theta.org)
dat <- as.data.frame(dat)

alpha(dat)$total$raw_alpha

#####
# Calculate the true expected test score (ETS) corresponding to theta=0
# from the item parameters

( apars <- cf.simb[,1] )      # a parameters
( bpars <- cf.simb[,2:4] )    # b parameters

p1 <- numeric(nitems)      # probability of X = 1
p2 <- numeric(nitems)      # probability of X = 2
p3 <- numeric(nitems)      # probability of X = 3
eis <- numeric(nitems)     # expected item score

th = 0                      # theta of threshold

# p1p = probability of X >= 1
# p2p = probability of X >= 2

for(j in 1:nitems)  {
( p1p <- exp(apars[j]*(th-bpars[j,1]))/(1+exp(apars[j]*(th-bpars[j,1]))) )
( p2p <- exp(apars[j]*(th-bpars[j,2]))/(1+exp(apars[j]*(th-bpars[j,2]))) )
( p3[j]  <- exp(apars[j]*(th-bpars[j,3]))/(1+exp(apars[j]*(th-bpars[j,3]))) )
( p2[j] <- p2p-p3[j] )
( p1[j] <- p1p-p2p )
( eis[j] <- p1[j]*1 + p2[j]*2 + p3[j]*3 )
}

```

```

}

round(cbind(p1,p2,p3,eis),3)

sum(eis)      # Expected test score

#####
##### Actual simulations

## Set parameters and numbers (of subjects and samples)

par.mn.sim <- c(-1.4, -0.7, 0, 0.7, 1.4)
par.sd.sim <- c(1, 1.5, 2)
par.rel.state <- c(0.5, 0.7, 0.9)

nr=100      # set number of times each combination must be repeated

npc <- length(par.mn.sim) * length(par.sd.sim) * length(par.rel.state)
npc          # total number of combinations
ns <- npc * nr
ns          # total number of simulated samples

## Variables to hold the results

mn.sim.par    <- as.numeric(rep(NA, ns))
sd.sim.par    <- as.numeric(rep(NA, ns))
rel.state.par <- as.numeric(rep(NA, ns))
mn.sum        <- as.numeric(rep(NA, ns))
sd.sum        <- as.numeric(rep(NA, ns))
flor          <- as.numeric(rep(NA, ns))
ceil          <- as.numeric(rep(NA, ns))
skew.sum      <- as.numeric(rep(NA, ns))
kurt.sum      <- as.numeric(rep(NA, ns))
mn.sim        <- as.numeric(rep(NA, ns))
sd.sim        <- as.numeric(rep(NA, ns))
prev.tru      <- as.numeric(rep(NA, ns)) # thtrue prevalence
prev.obs      <- as.numeric(rep(NA, ns)) # observed prevalence
alpha         <- as.numeric(rep(NA, ns)) # Cronbach's alpha
cor.state.sum <- as.numeric(rep(NA, ns)) # point biserial correlation
rel.state     <- as.numeric(rep(NA, ns)) # state reliability
thr.rocy     <- as.numeric(rep(NA, ns)) # threshold based on ROC (Youden)
thr.pred     <- as.numeric(rep(NA, ns)) # threshold based on predictive modeling
thr.adj      <- as.numeric(rep(NA, ns)) # threshold based on adjusted pred.
modeling

```

```

thr.thet.pls <- as.numeric(rep(NA, ns)) # theta thr based on plausible PVs
thr.ets.pls <- as.numeric(rep(NA, ns)) # threshold based on old IRT method
thr.thet.irt <- as.numeric(rep(NA, ns)) # theta thr based on new IRT method
thr.ets.irt <- as.numeric(rep(NA, ns)) # threshold based on new IRT method
cfa.check <- logical(ns) # Check admissibility of CFA solution

set.seed(1234)
index <- 0

for(k1 in 1:length(par.mn.sim)) {
  for(k2 in 1:length(par.sd.sim)) {
    for(k3 in 1: length(par.rel.state)) {
      for(k4 in 1:nr) {

        index <- (k1-1)*length(par.sd.sim)*length(par.rel.state)*nr +
          (k2-1)*length(par.rel.state)*nr +
          (k3-1)*nr + k4

        print(index)

        ( mn.sim.par[index] <- par.mn.sim[k1] )
        ( sd.sim.par[index] <- par.sd.sim[k2] )
        ( rel.state.par[index] <- par.rel.state[k3] )

        Y <- rnorm(N, 0, 1)
        theta.org <- as.matrix( Y )
        theta.sim <- theta.org*par.sd.sim[k2] + par.mn.sim[k1] # transform theta.sim

        ( mn.sim[index] <- mean(theta.sim) )
        ( sd.sim[index] <- sd(theta.sim) )

        dat <- simdata(a1, d1, N, itemtype="graded", Theta=theta.sim)
        dat <- as.data.frame(dat)

        sumscore <- rowSums(dat)

        ( alpha[index] <- alpha(dat)$total$raw_alpha )
        ( mn.sum[index] <- mean(sumscore) )
        ( sd.sum[index] <- sd(sumscore) )
        ( flor[index] <- table(sumscore)[1] / length(sumscore) )
        ( ceil[index] <- table(sumscore)[length(table(sumscore))] / length(sumscore) )
        ( skew.sum[index] <- skewness(sumscore, type=2) )
        ( kurt.sum[index] <- kurtosis(sumscore, type=2) )

      # Perceived trait
    }
  }
}

```

```

( rel.st <- par.rel.state[k3] )      # reliability of the 'perceived trait'

sd.error <- sqrt(((1-rel.st)/rel.st)*sd(theta.sim)^2)
theta.err <- theta.sim + rnorm(N, 0, sd.error)

var(theta.sim)/var(theta.err)  # check reliability of perceived trait

mean(theta.sim)
sd(theta.sim)
mean(theta.err)
sd(theta.err)

# true prevalence
state <- numeric(N)
state[theta.sim > 0] <- 1
( prev.tru[index] <- mean(state) )

# observed prevalence
state <- numeric(N)
state[theta.err > 0] <- 1
( prev.obs[index] <- p <- mean(state) )

## Point biserial correlation
( cor.state.sum[index] <- cor(state, sumscore) )

#### old IRT method - plausible values

cap <- capture.output( mod <- mirt(data=dat, model=1,
                                       itemtype="graded", TOL=.001) )

# plausible values

n.pls <- 10

fs.mod <- fscores(mod, plausible.draws = n.pls)

theta.thr      <- numeric(n.pls)
exp.testscore <- numeric(n.pls)

for (i in 1:n.pls)  {
  theta.thr[i] <- quantile(fs.mod[[i]], prob=(1-p))
  Theta <- as.matrix( theta.thr[i] )
  exp.testscore[i]  <- expected.test(mod, Theta)
}

```

```

( thr.thet.pls[index] <- mean(theta.thr) )
( thr.ets.pls[index] <- mean(exp.testscore) )

# Estimate reliability of diagnosis: CFA analysis

datw <- data.frame(dat, state)

model <- '
F1 =~ Item_1+Item_2+Item_3+Item_4+Item_5+Item_6+
Item_7+Item_8+Item_9+Item_10+state
'

fit <- cfa(model, data=datw, ordered=T, std.lv=T)

( cfa.check[index] <- lavInspect(fit, what="post.check") )

# Estimate state reliability
pe <- parameterEstimates(fit, rsquare=T)
( rel.state[index] <- pe$est[pe$lhs=="state" & pe$op=="r2"] )      # R-squared

rm(fit)

## ROC analysis

rocobj <- roc(state, sumscore, quiet = TRUE)
mic.roc <- coords(rocobj, x="best", input="threshold", ret="threshold",
best.method="youden", transpose = TRUE)
( thr.rocy[index] <- mic.roc[sample(length(mic.roc),1)] )

rm(rocobj)

## Predictive modeling method / adjusted predictive modeling method

mylogit <- glm(state ~ sumscore, family = "binomial")
C <- coef(mylogit)[1]                      # intercept coefficient C
B <- coef(mylogit)[2]                      # regression coefficient B
q <- log(p/(1-p))                         # q = logodds(pre)
( thr.pred[index] <- (q-C)/B )            # predictive modeling threshold

# Adjusted predictive modeling method
rf <- (0.8/rel.state[index] - 0.5) * sd.sum[index] * cor.state.sum[index]
( thr.adj[index] <- thr.pred[index] - rf * q )

rm(mylogit)

```

```

## New IRT method

cap <- capture.output( modw <- mirt(data=datw, model=1,
                                         itemtype="graded", TOL=.001) )

cf <- coef(modw, simplify=TRUE, IRTpars=TRUE)$items

( thr.thet.irt[index] <- Theta <- as.matrix( cf[nitems+1, 2] ) )
( thr.ets.irt[index] <- expected.test(modw, Theta, which.items = 1:10) )

rm(modw)

}

}

}

}

####

df <- data.frame(
mn.sim.par,
sd.sim.par,
rel.state.par,
mn.sum,
sd.sum,
flor,
ceil,
skew.sum,
kurt.sum,
mn.sim,
sd.sim,
prev.tru,
prev.obs,
alpha,
cor.state.sum,
rel.state,
thr.rocy,
thr.pred,
thr.adj,
thr.thet.pls,
thr.ets.pls,
thr.thet.irt,
thr.ets.irt,
cfa.check )

```

```

write.table(df, file = "E:/Simulation-results.txt", sep = " ", row.names = F,
col.names = T)

fix(df)

#####
##### Analysis of simulated data

df <- read.table(file.choose(), header=T)
## Read in: Simulation-results.txt

data.frame(names(df))
dim(df)

table(df$rel.state.par)
table(df$cfa.check)

#####
# SCATTERPLOTS

### Create sub-files

res <- df[df$rel.state.par==0.9, ]
nrow(res)

# threshold based on ROC Youden
ggplot(res,
aes(x=prev.obs, y=thr.rocy)) +
geom_point(shape=1, colour="grey50") + # Use open circles
geom_smooth(method="lm", se=FALSE,
formula = y ~ poly(x, 3),
size = 1) + # Defines regression line
dev.new(width=5, height=4) +
scale_x_continuous(limits=c(0.07, 0.93), breaks=c(0.2,0.4,0.6,0.8)) +
scale_y_continuous(limits=c(4, 26), breaks=c(5,10,15,20,25))

# threshold based on predictive modeling
ggplot(res,
aes(x=prev.obs, y=thr.pred)) +
geom_point(shape=1, colour="grey50") + # Use open circles
geom_smooth(method="lm", se=FALSE,
formula = y ~ poly(x, 3),
size = 1) + # Defines regression line

```

```

dev.new(width=5, height=4) +
scale_x_continuous(limits=c(0.07, 0.93), breaks=c(0.2,0.4,0.6,0.8)) +
scale_y_continuous(limits=c(4, 26), breaks=c(5,10,15,20,25))

# threshold based on (improved) adjusted predictive modeling
ggplot(res,
aes(x=prev.obs, y=thr.adj)) +
geom_point(shape=1, colour="grey50") + # Use open circles
geom_smooth(method="lm", se=FALSE,
formula = y ~ poly(x, 3),
size = 1) + # Defines regression line
dev.new(width=5, height=4) +
scale_x_continuous(limits=c(0.07, 0.93), breaks=c(0.2,0.4,0.6,0.8)) +
scale_y_continuous(limits=c(4, 26), breaks=c(5,10,15,20,25))

# threshold based on *-&*uantile of the plausible values
ggplot(res,
aes(x=prev.obs, y=thr.ets.pls)) +
geom_point(shape=1, colour="grey50") + # Use open circles
geom_smooth(method="lm", se=FALSE,
formula = y ~ poly(x, 3),
size = 1) + # Defines regression line
dev.new(width=5, height=4) +
scale_x_continuous(limits=c(0.07, 0.93), breaks=c(0.2,0.4,0.6,0.8)) +
scale_y_continuous(limits=c(4, 26), breaks=c(5,10,15,20,25))

# threshold based on IRT (Method Jakob)
ggplot(res,
aes(x=prev.obs, y=thr.ets.irt)) +
geom_point(shape=1, colour="grey50") + # Use open circles
geom_smooth(method="lm", se=FALSE,
formula = y ~ poly(x, 3),
size = 1) + # Defines regression line
dev.new(width=5, height=4) +
scale_x_continuous(limits=c(0.07, 0.93), breaks=c(0.2,0.4,0.6,0.8)) +
scale_y_continuous(limits=c(4, 26), breaks=c(5,10,15,20,25))

```

RESIDUALS ANALYSIS

```

true.ets.tru <- 15.139 # True test score threshold for theta = 0

# Create sub-files

res <- df[df$rel.state.par==0.5 & df$prev.obs<0.3,]
res <- df[df$rel.state.par==0.7 & df$prev.obs<0.3,]

```

```

res <- df[df$rel.state.par==0.9 & df$prev.obs<0.3,]

res <- df[df$rel.state.par==0.5 & df$prev.obs>=0.3 & df$prev.obs<0.5,]
res <- df[df$rel.state.par==0.7 & df$prev.obs>=0.3 & df$prev.obs<0.5,]
res <- df[df$rel.state.par==0.9 & df$prev.obs>=0.3 & df$prev.obs<0.5,]

res <- df[df$rel.state.par==0.5 & df$prev.obs>=0.5 & df$prev.obs<0.7,]
res <- df[df$rel.state.par==0.7 & df$prev.obs>=0.5 & df$prev.obs<0.7,]
res <- df[df$rel.state.par==0.9 & df$prev.obs>=0.5 & df$prev.obs<0.7,]

res <- df[df$rel.state.par==0.5 & df$prev.obs>=0.7,]
res <- df[df$rel.state.par==0.7 & df$prev.obs>=0.7,]
res <- df[df$rel.state.par==0.9 & df$prev.obs>=0.7,]

dim(res)

# Means and 95CI

# ROC-Y
round( mean(res$thr.rocy), 2)
hlp <- res$thr.rocy - true.ets.tru
round( bias <- mean(hlp), 2)                                # bias
# round( quantile(hlp, prob=c(0.025, 0.975)), 2)
round( MSR <- bias^2 + var(hlp),2)                            # MSR

# Pred
round( mean(res$thr.pred), 2)
hlp <- res$thr.pred - true.ets.tru
round( bias <- mean(hlp), 2)                                # bias
# round( quantile(hlp, prob=c(0.025, 0.975)), 2)
round( MSR <- bias^2 + var(hlp),2)                            # MSR

# Adjusted 2
round( mean(res$thr.adj,na.rm=T), 2)
hlp <- res$thr.adj - true.ets.tru
round( bias <- mean(hlp,na.rm=T), 2)                          # bias
# round( quantile(hlp, prob=c(0.025, 0.975)), 2)
round( MSR <- bias^2 + var(hlp,na.rm=T),2)                  # MSR

# PVs
round( mean(res$thr.ets.pls), 2)
hlp <- res$thr.ets.pls - true.ets.tru
round( bias <- mean(hlp), 2)                                # bias
# round( quantile(hlp, prob=c(0.025, 0.975)), 2)
round( MSR <- bias^2 + var(hlp),2)                            # MSR

```

```

# IRT
round( mean(res$thr.ets.irt), 2)
hlp <- res$thr.ets.irt - true.ets.tru
round( bias <- mean(hlp), 2 )                                # bias
# round( quantile(hlp, prob=c(0.025, 0.975)), 2 )
round( MSR <- bias^2 + var(hlp),2 )                           # MSR

#####
# TABLE 1 -- DESCRIPTIVES

data.frame(names(df))

round(mean(df$mn.sum),1)
round(min(df$mn.sum),1)
round(max(df$mn.sum),1)

round(mean(df$sd.sum),1)
round(min(df$sd.sum),1)
round(max(df$sd.sum),1)

round(mean(df$skew.sum),2)
round(min(df$skew.sum),2)
round(max(df$skew.sum),2)

round(mean(df$kurt.sum),2)
round(min(df$kurt.sum),2)
round(max(df$kurt.sum),2)

round(mean(df$flor),2)
round(min(df$flor),2)
round(max(df$flor),2)

round(mean(df$ceil),2)
round(min(df$ceil),2)
round(max(df$ceil),2)

round(mean(df$prev.obs),2)
round(min(df$prev.obs),2)
round(max(df$prev.obs),2)

```

3. Calculation of the true threshold in terms of the expected test score

In the article, we simulated datasets of a hypothetical questionnaire with 10 items with 4 response options (0, 1, 2, and 3) using the IRT-parameters given in the Appendix, and we defined the true threshold of interest in terms of the latent trait as theta $\theta = 0$. Here we calculate the corresponding expected test score of this threshold, based on the IRT-parameters.

The probability of item X_j scoring $\geq k$ (k is 1, 2 or 3) is given by:

$$\ln\left(\frac{P(X_j \geq k)}{(1 - P(X_j \geq k))}\right) = a_j(\theta - b_{jk})$$

where \ln represents the natural logarithm, P represents the probability, a_j represents the item discrimination parameter and b_{jk} represents the k^{th} difficulty parameter of item j .

The equation can be rewritten as:

$$P(X_j \geq k) = \frac{e^{a_j(\theta - b_{jk})}}{1 + e^{a_j(\theta - b_{jk})}}$$

where e represents the natural exponential function.

The probability of item X_j scoring $= k$ is given by:

$$P(X_j = k) = P(X_j \geq k) - P(X_j \geq k + 1)$$

This way, the probabilities of item X_j scoring 1 ($P(X_j = 1)$), 2 ($P(X_j = 2)$), or 3 ($P(X_j = 3)$) can be calculated. The expected score of item X_j then is:

$$P(X_j = 1) * 1 + P(X_j = 2) * 2 + P(X_j = 3) * 3$$

After calculating the expected item scores, the expected test (or scale) score, can be calculated by summing the expected item scores of the scale.

4. R-code for estimating a meaningful threshold using IRT

```
# INSTRUCTIONS  
# This code let you estimate an IRT based meaningful threshold in your data.  
# Part 1 provides the code for simulating a dataset for illustration.  
# Part 2 provides the actual code for estimation.  
# If you want to analyze your own data, go to part 2.  
  
library(mirt)  
  
##### PART 1: SIMULATE DATASET  
  
# Create set of item parameters  
  
N <- 1000 # simulated sample size  
nitems <- 10 # number of items  
ncat <- 4 # number of response categories per item  
  
a <- c(0.6,0.6,0.8,0.8,1,1,1.2,1.2,1.4,1.4)  
b2 <- (a-1)*2  
bc <- (a-1)/2  
  
set.seed(12345)  
  
a1 <- sample(a)  
b1 <- b2 - 1 + sample(bc)  
b3 <- b2 + 1 + sample(bc)  
  
cf.simb <- data.frame(a1,b1,b2,b3)  
round(cf.simb, 3)  
round(colMeans(cf.simb), 3)  
  
# Transform b-parameters to d-parameters  
# difficulty (b) = easiness (d) / -a  
  
cf.sim1 <- cf.simb  
  
colnames(cf.sim1) <- c("a1","d1","d2","d3")  
  
cf.sim1$d1 <- -cf.simb$b1*a1  
cf.sim1$d2 <- -cf.simb$b2*a1  
cf.sim1$d3 <- -cf.simb$b3*a1  
round(cf.sim1, 3) # displays the item parameters  
round(colMeans(cf.sim1), 3)
```

```

# Simulate dataset using 'mirt'

a1 <- as.matrix(cf.sim1[ , 1])
d1 <- as.matrix(cf.sim1[ , -1])
theta.sim <- as.matrix( rnorm(N, 0, 1) )

dat <- simdata(a1, d1, N, itemtype="graded", Theta=theta.sim)
dat <- as.data.frame(dat)

head(dat)

# Create dichotomous state (i.e., anchor) variable

( rel.st <- 0.5 )      # reliability of the 'perceived trait'
sd.error <- sqrt(((1-rel.st)/rel.st)*sd(theta.sim)^2)
theta.err <- theta.sim + rnorm(N, 0, sd.error)

# State variable and observed prevalence
state <- numeric(N)
state[theta.err > 0] <- 1      # Threshold at theta.sim = 0
( p <- mean(state) )          # State prevalence

# Create dataset with state variable

dat <- data.frame(dat, state)
head(dat)

org <- dat

#####
##### PART 2: ESTIMATION

### Read your own data

# The following code opens a windows dialogue box in which you can browse
# to your data file.
# Note that your datafile should contain the <nitems> items of your PROM
# and in the last column the dichotomous state (or anchor) variable.

org <- read.table(file.choose(), header=T)  # The file is named "org"

nitems = 10      # Provide the number of items in the scale

```

```

# The file is next copied to a file called "dat" which is the working file
dat <- org

# Fit a graded response model
mod <- mirt(data=dat, model=1, itemtype="graded", TOL=.001)

# Recover the item parameters from the model
( cf <- coef(mod, simplify=TRUE, IRTpars=TRUE)$items )

# Extract the b-parameter of the state variable
( thr.thet <- as.matrix( cf[nitems+1, 2] ) )

# And calculate the corresponding expected test score
expected.test(mod, thr.thet, which.items = 1:nitems)

rm(mod)

##### Empirical bootstrap to find the 95% CI

nboot      <- 1000          # number of bootstrap samples
threshold <- as.numeric(rep(NA, nboot))

start.time <- Sys.time()

for(i in 1:nboot) {

  print(i)

  dat <- org[sample(1:dim(dat)[1], dim(dat)[1], replace=TRUE),]

  cap <- capture.output( mod <- mirt(data=dat, model=1,
                                         itemtype="graded", TOL=.001) )

  cf <- coef(mod, simplify=TRUE, IRTpars=TRUE)$items

  ( thr.thet <- as.matrix( cf[nitems+1, 2] ) )
  ( threshold[i] <- expected.test(mod, thr.thet, which.items = 1:nitems) )

  rm(mod)
}

end.time <- Sys.time()
time.taken <- end.time - start.time
time.taken

```

```
# NOTE: If you click on the R Console you can see how much bootstrap samples
# have been processed.

### Bootstrap results

round(mean(threshold),1)
round(quantile(threshold, c(0.025, 0.975)),1)

# Show histogram
hist(threshold)
```