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# ROC curve, AUC and optimal cutoff value for norquetiapine

library(ROCR)
library(OptimalCutpoints)

q <- read.csv("C:/Rwork/ROC/ROC_new/qm_data_r1.csv", header = T)
with(q, table(y_pred, y_true)) # Confusion matrix : y_pred, y_true

# logistic regression model & prediction
q_model <- glm(y_true ~ pconc + mconc, data = q)
q_p <- predict(q_model, q, type = 'link')
hist(q_p)

q_pred <- prediction(q_p, q$y_true)
pred_table_1 <-table(q_p, q$y_true)
pred_table_1

pred_table_2 <- data.frame(value=q_p, y_true=q$y_true, y_pred=q$y_pred)

# Cutoff & Accuracy
eval <- performance(q_pred, "acc", "cutoff")
plot(eval)

# Identify best cutoff/accuracy point
max <- which.max(slot(eval, "y.values")[[1]])
acc <- slot(eval,"y.values")[[1]][max]
cut <- slot(eval,"x.values")[[1]][max]
print(c(Accuracy=acc, Cutoff=cut))


# Optimal cutoff1
prf <- performance(q_pred, measure = "tpr", x.measure = "fpr")
optid <- (1:length(prf@y.values[[1]][-1]))[((prf@x.values[[1]][-1])^2
                                            + (1-prf@y.values[[1]][-11])^2)
                                           ==min((prf@x.values[[1]][-1])^2
                                                 + (1-prf@y.values[[1]][-1])^2)]
x <- prf@x.values[[1]][-1][optid]; x # 1-Specificity
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y <- prf@y.values[[1]][-1][optid]; y # Sensitivity
optcut <- prf@alpha.values[[1]][-1][optid]
optcut <- round(optcut, 3)
optcut

# Optimal cutoff2 by OptimalCutpoints package
optimal.cutpoint.Youden <- optimal.cutpoints(X = "value", status = "y_true", tag.healthy = 0,
                                             methods = "Youden", data = pred_table_2, pop.prev = NULL,
                                             control = control.cutpoints(), ci.fit = FALSE, conf.level = 0.95,
                                             trace = FALSE)

summary(optimal.cutpoint.Youden)
plot(optimal.cutpoint.Youden)
```

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# ROC curve, AUC and optimal cutoff value for 9-hydroxyrisperidone

library(ROCR)
library(OptimalCutpoints)

r <- read.csv("C:/Rwork/ROC/ROC_new/rm_data_r1.csv", header = T)
with(r, table(y_pred, y_true)) # Confusion matrix - y_pred, y_true

# logistic regression model & prediction
r_model <- glm(y_true ~ pconc + mconc, data = r)
r_p <- predict(r_model, r, type = 'link')
hist(r_p)

r_pred <- prediction(r_p, r$y_true)
pred_table <-table(r_p, r$y_true)
pred_table

pred_table_2 <- data.frame(value=r_p, y_true=r$y_true, y_pred=r$y_pred)

# Cutoff & Accuracy
eval <- performance(r_pred, "acc", "cutoff")
plot(eval)

# Identify best cutoff/accuracy point
max <- which.max(slot(eval, "y.values")[[1]])
acc <- slot(eval,"y.values")[[1]][max]
cut <- slot(eval,"x.values")[[1]][max]
print(c(Accuracy=acc, Cutoff=cut))


# Optimal cutoff1
prf <- performance(r_pred, measure = "tpr", x.measure = "fpr")
optid <- (1:length(prf@y.values[[1]][-1]))[((prf@x.values[[1]][-1])^2
                                            + (1-prf@y.values[[1]][-11])^2)
                                           ==min((prf@x.values[[1]][-1])^2
                                                 + (1-prf@y.values[[1]][-1])^2)]
x <- prf@x.values[[1]][-1][optid]; x # 1-Specificity
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```
y <- prf@y.values[[1]][-1][optid]; y # Sensitivity
optcut <- prf@alpha.values[[1]][-1][optid]
optcut <- round(optcut, 3)


# Optimal cutoff2 by OptimalCutpoints package
optimal.cutpoint.Youden <- optimal.cutpoints(X = "value", status = "y_true", tag.healthy = 0,
                                               methods = "Youden", data = pred_table_2, pop.prev = NULL,
                                             control = control.cutpoints(), ci.fit = FALSE, conf.level = 0.95, trace
= FALSE)

summary(optimal.cutpoint.Youden)
plot(optimal.cutpoint.Youden)
```