Simulated ROC

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Contents

Preface and Assignment

In this document I have used Rmarkdown and SAS to LaTeX to create a pdf document file containing a description of the theory used in this problem with the code and output for the analysis using Rmarkdown with RStudio and SAS. I do not expect you to be able to reproduce a document of this type but I do want you to be able to preform the analysis with simulated data. The R and SAS code are found in the pdf document. You should be able to copy this material for use in R or RStudio and SAS. Generate you own simulation by controlling the separation between the population means, c_0 and c_1. What conclusion can you reach?

Theory

Receiver Operating Characteristics Curve (ROC)

In this section, assume that the random variable Y is continuous and that the test is said to be positive if $Y \geq c$, for some c. For example, let Y denote the PSA levels that is commonly used to indicate potential problems with the prostrate gland when Y is "large". The binary test given in the previous section can be constructed for any value of c. That is, the test is positive if $Y \geq c$ and is negative if $Y < c$, from which we have

$$\begin{aligned} \text{FPF}(c) &= \Pr[Y \geq c \mid D = 0] \\ \text{TPF}(c) &= \Pr[Y \geq c \mid D = 1]. \end{aligned}$$

The receiver operating characteristic curve (ROC) for a test using the random variable Y is defined as

$$ROC(\cdot) = \{(\text{FPF}(c), \text{TPF}(c)), c \in (-\infty, \infty)\} \tag{1}$$

or

$$ROC(\cdot) = \{(t, ROC(t)), t \in (0, 1)\}. \tag{2}$$

Some of the properties for the ROC include:

1. The ROC curve is invariant to strictly (monotone) increasing transformations of Y
2. Let $S_D = 1 - F_Y(y \mid D = 1)$ and $S_{\bar{D}} = 1 - F_Y(y \mid D = 0)$ denote the survivor functions of Y for the diseased and non-diseased populations given by

$$S_D(y) = \Pr[Y \geq y \mid D = 1]$$

$$S_{\bar{D}}(y) = \Pr[Y \geq y \mid D = 0]$$

then

$$ROC(t) = S_D(S_{\bar{D}}^{-1}(t)), t \in (0, 1).$$

3. $$\frac{\partial ROC(t)}{\partial t} = \frac{f_D(S_{\bar{D}}^{-1}(t))}{f_{\bar{D}}(S_D^{-1}(t))}$$

where f_D denotes the probability density for Y in the diseased population ($D = 1$) and $f_{\bar{D}}$ denotes the probability density for Y in the healthy population ($D = 0$).

4. The area under the ROC curve (AUC) is

$$\begin{aligned} AUC &= \Pr[Y_D > Y_{\bar{D}}] \quad (3) \\ &= \int ROC(t)dt. \quad (4) \end{aligned}$$

5. (Special Case - Parametric Binormal Form) Suppose that $Y_D \sim N(\mu_D, \sigma_D^2)$ and $Y_{\bar{D}} \sim N(\mu_{\bar{D}}, \sigma_{\bar{D}}^2)$ then

$$ROC(t) = \Phi(a + b\Phi^{-1}(t))$$

and

$$AUC = \Phi(\frac{a}{\sqrt{1 + b^2}})$$

where $a = \frac{\mu_D - \mu_{\bar{D}}}{\sigma_D}$, $b = \frac{\sigma_{\bar{D}}}{\sigma_D}$ and Φ is the standard normal c.d.f.

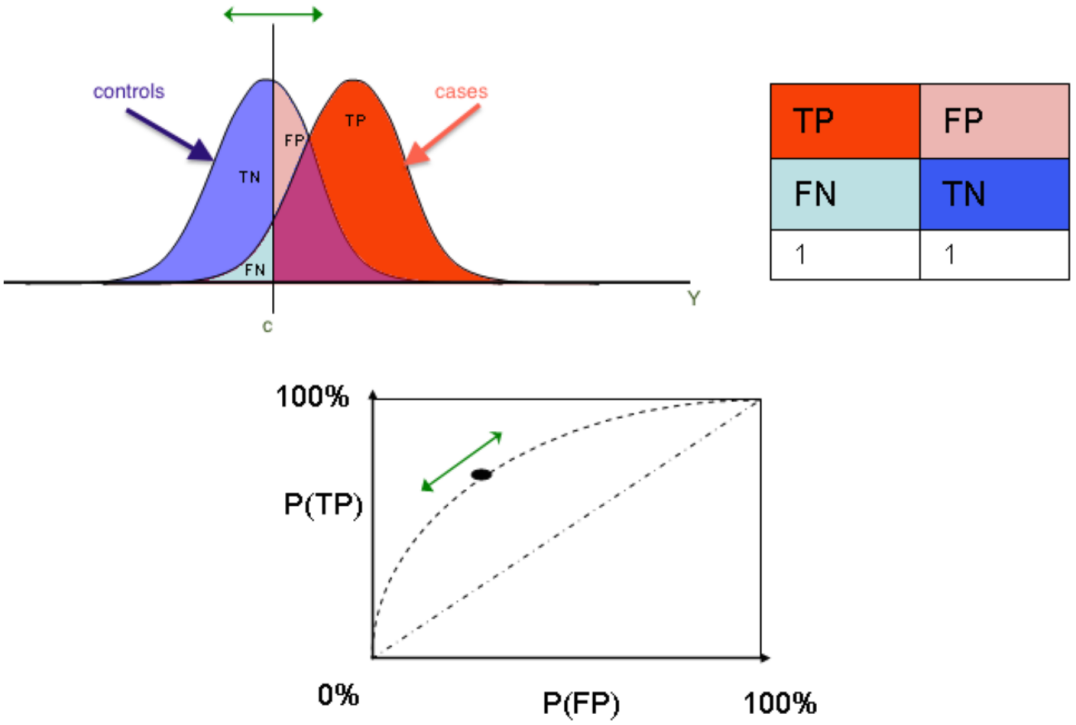


Figure 1: ROC Basics

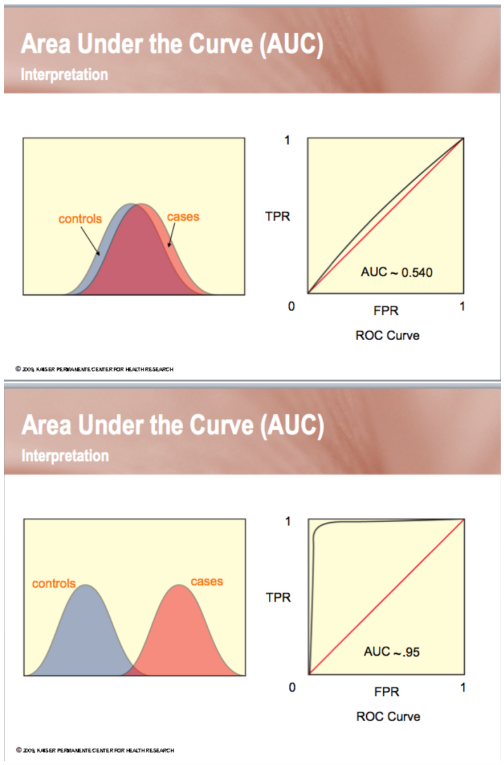


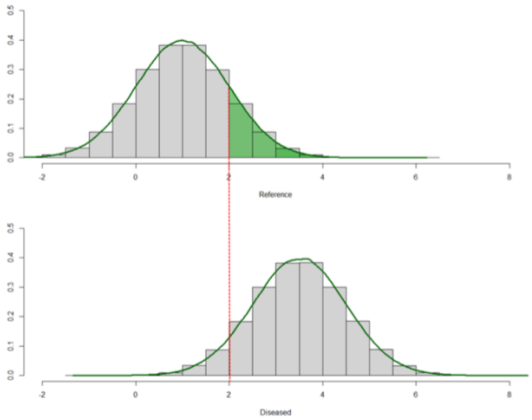
Figure 2: Area Under the Curve - AUC

Placement Values

A useful concept that is related to the ROC and AUC is a value called the Placement score.

Placement Values

- Cai(2002) defines $PV_D = S_{\bar{D}}(Y_D)$.



- The ROC is equivalent to the cdf of PV_D.

$$\begin{aligned} P[PV_D \leq t|\boldsymbol{X}] &= P[S_{\bar{D}\boldsymbol{X}}(Y_D) \leq t|\boldsymbol{X}] \\ &= P[Y_D \geq [S^{-1}_{\bar{D}\boldsymbol{X}}(t)|\boldsymbol{X}] \\ &= ROC_{\boldsymbol{X}}(t). \end{aligned}$$

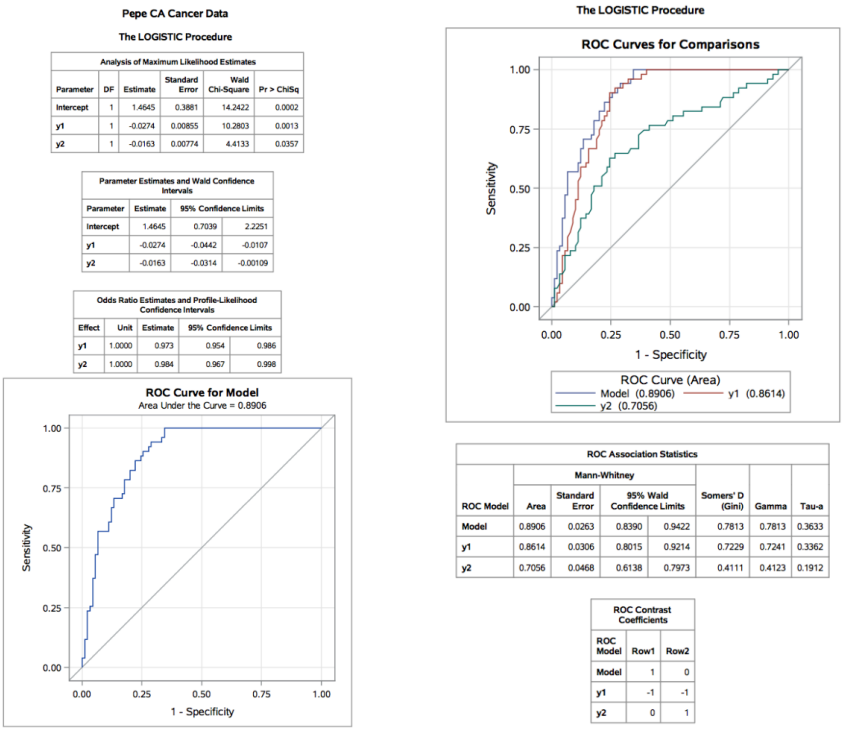
Figure 3:

SAS – Example

The SAS code is,

```
proc logistic data=temp plots(only)=roc;;
  model d=y1 y2 / scale=none
                          clparm=wald
                          clodds=pl
                          rsquare;
 roc 'y1' y1;
 roc 'y2' y2;
   roccontrast reference('y1') / estimate e;
run;
```

Figure contains the SAS output.



Pepe CA Cancer Data

The LOGISTIC Procedure

Analysis of Maximum Likelihood Estimates

Parameter	DF	Estimate	Standard Error	Wald Chi-Square	Pr > ChiSq
Intercept	1	1.4645	0.3881	14.2422	0.0002
y1	1	-0.0274	0.00855	10.2803	0.0013
y2	1	-0.0163	0.00774	4.4133	0.0357

Parameter Estimates and Wald Confidence Intervals

Parameter	Estimate	95% Confidence Limits	
Intercept	1.4645	0.7039	2.2251
y1	-0.0274	-0.0442	-0.0107
y2	-0.0163	-0.0314	-0.00109

Odds Ratio Estimates and Profile-Likelihood Confidence Intervals

Effect	Unit	Estimate	95% Confidence Limits	
y1	1.0000	0.973	0.954	0.986
y2	1.0000	0.984	0.967	0.998

ROC Curve for Model

Area Under the Curve = 0.8906

Sensitivity

1 - Specificity

The LOGISTIC Procedure

ROC Curves for Comparisons

Sensitivity

1 - Specificity

ROC Curve (Area)

Model (0.8906) y1 (0.8614) y2 (0.7056)

ROC Association Statistics

ROC Model	Mann-Whitney Area	Standard Error	95% Wald Confidence Limits		Somers' D (Gini)	Gamma	Tau-a
Model	0.8906	0.0263	0.8390	0.9422	0.7813	0.7813	0.3633
y1	0.8614	0.0306	0.8015	0.9214	0.7229	0.7241	0.3362
y2	0.7056	0.0468	0.6138	0.7973	0.4111	0.4123	0.1912

ROC Contrast Coefficients

ROC Model	Row1	Row2
Model	1	0
y1	-1	-1
y2	0	1

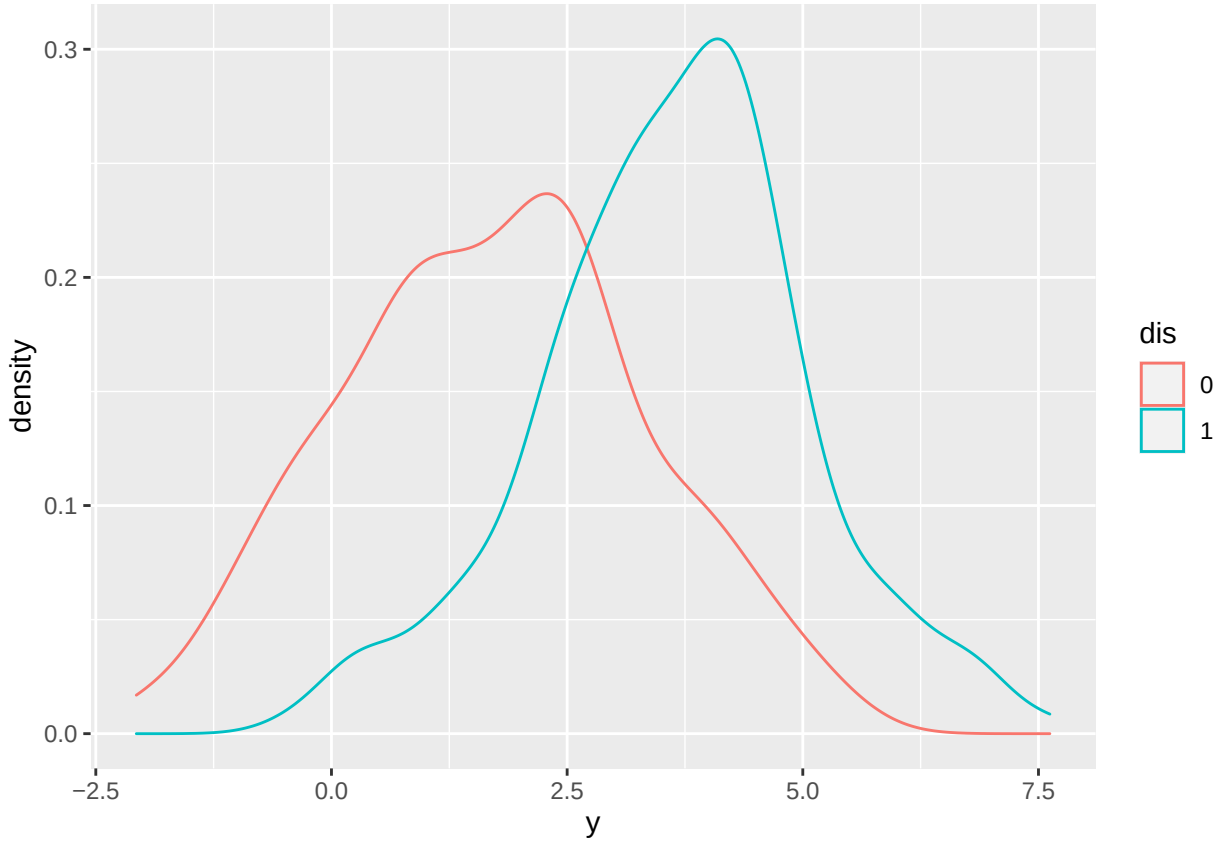
R

Set seed for the simulation

```
  # clear the environment and set seed
rm(list = ls())
set.seed(12345)
```

Function to generate normal data. For dis=0 (“Control”) and dis=1 (“Disease”). The separation between the two groups is controlled by one’s choice of c0, c1, sd_e0, and sd_e1. n0 and n1 are the sample sizes for the groups.

```r
library(ggplot2)

gen_Norm_data = function(c0,sd_e0,n0,c1,sd_e1,n1){
  eps0 = rnorm(n0,0,sd_e0)
  eps1 = rnorm(n1,0,sd_e1)
  y0 = c0 + eps0
  y1 = c1 + eps1

  data.frame(y = c(y0, y1),
             dis = as.factor(c(rep(0,n0), rep(1,n1))))
}
dat1 = gen_Norm_data(1.5,1.5,200,3.5,1.5,200)

#plot density functions
ggplot(dat1, aes(color = dis, y)) + geom_density()
```



Create discrete variables for Y

```r
y=dat1[,1]
summary(y)
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##  -2.071   1.395   2.737   2.672   4.024   7.621
```

```r
case=dat1[,2]
```

Create binary table with cutoff y $>$ 2.5

```
high_y = y > 2.5
tex1 = table(case,high_y)
addmargins(tex1)
```

```
##      high_y
## case  FALSE TRUE Sum
##   0     137   63 200
##   1      40  160 200
##   Sum   177  223 400
```

```
prop.out = prop.table(tex1,1)
specificity = prop.out[1,1]
sensitivity = prop.out[2,2]
prop.out
```

```
##     high_y
## case FALSE  TRUE
##    0 0.685 0.315
##    1 0.200 0.800
```

```
sensitivity
```

```
## [1] 0.8
```

```
specificity
```

```
## [1] 0.685
```

```
TPR = sensitivity
FPR = 1 - specificity
TPR
```

```
## [1] 0.8
```

```
FPR
```

```
## [1] 0.315
```

Create binary table with cutoff y > 3.0

```
high_y = y > 3.0
tex1 = table(case,high_y)
addmargins(tex1)
```

```
##      high_y
## case  FALSE TRUE Sum
##   0     161   39 200
##   1      60  140 200
##   Sum   221  179 400
```

```
prop.out = prop.table(tex1,1)
specificity = prop.out[1,1]
sensitivity = prop.out[2,2]
prop.out
```

```
##     high_y
## case FALSE  TRUE
##    0 0.805 0.195
##    1 0.300 0.700
```

```
sensitivity
```

```
## [1] 0.7
```

```
specificity
```

```
## [1] 0.805
```

```
TPR = sensitivity
FPR = 1 - specificity
TPR
```

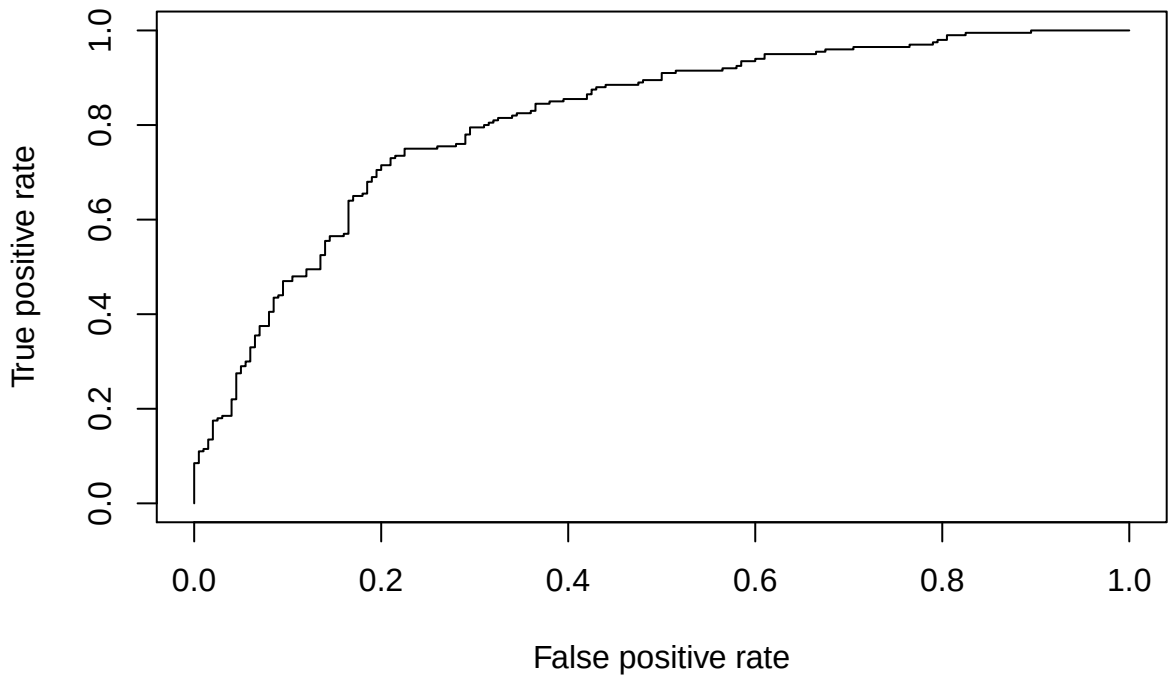
```
## [1] 0.7
```

```
FPR
```

```
## [1] 0.195
```

Instead of creating a table at each cutoff point one can construct a ROC plot for a continuous variable Y. Which is constructing using the pairs (TPR, FPR) at each cutoff point (in R). Sometimes (as in SAS) this curve is smoothed.

```
library(ROCR)
pred = prediction(y,case)
perf=performance(pred, "tpr", "fpr")
plot(perf)
```



SAS

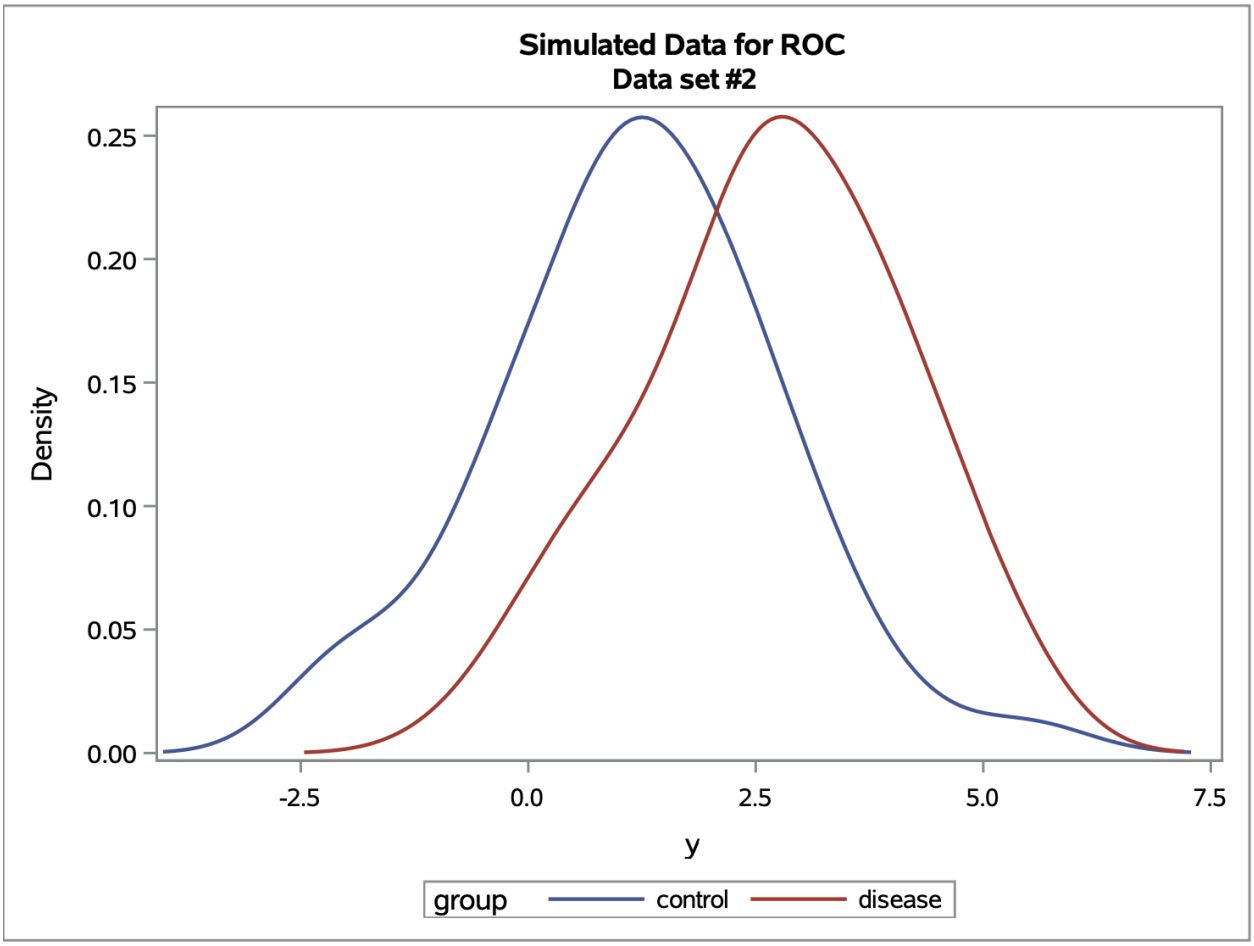
Code

```
libname LDATA '/home/jacktubbs/my_shared_file_links/jacktubbs/myfolders/Titanic/';
options center nodate pagesize=100 ls=80;
/* Simplified LaTeX output that uses plain LaTeX tables */
ods tagsets.simplelatex file="/home/jacktubbs/my_shared_file_links
/jacktubbs/LaTeX/ROC_sim.tex"
```

```
stylesheet="/home/jacktubbs/my_shared_file_links
/jacktubbs/LaTeX/sas.sty"(url="sas");

/*
The above will create a new file that can be inputed into LaTeX
(simple.tex) and the new style needed by LaTex (sas.sty).

The following example can be found at

http://support.sas.com/rnd/base/ods/odsmarkup/latex.html

*/
ods graphics on;

title1 'Simulated Data for ROC';
* Run Macro;
%macro binorm(dsn, title);
title2 &title;
data a;set &dsn;
  seed=12345;
  do i = 1 to n0;
   group='control';
   y = c0 + rand("Normal", 0, sd_e0);
   output;
  end;
  do i = 1 to n1;
   group='disease';
   y = c1 + rand("Normal", 0, sd_e1);
   output;
  end;
run;

data a; set a; y_cut = (y > cutoff); run;

proc sgplot data=a;
density y /type=kernel group=group;
run;

proc freq; table group*y_cut/ nopercent nocol outpct out=b ; run;
data c; set b;
if group = 'disease' and y_cut = '1' then sensitivity = pct_row;
if group = 'control' and y_cut = '0' then specificity = pct_row;
keep sensitivity specificity;
run;
proc print data=c; var sensitivity specificity; run;

proc logistic data=a plots(only)=roc ;
class group ;
model group(event='disease')=y;
run;
%mend binorm;

*Run data genration;
data parms1; c0=1.5; sd_e0=1.5; n0=100; c1=2.0; sd_e1=1.5; n1=100; cutoff = 3.0;
run;
data parms2; c0=1.5; sd_e0=1.5; n0=100; c1=2.5; sd_e1=1.5; n1=100; cutoff = 3.0;
run;
data parms3; c0=1.5; sd_e0=1.5; n0=100; c1=3.0; sd_e1=1.5; n1=100; cutoff = 3.0;
run;
```

```
data parms4; c0=1.5; sd_e0=1.5; n0=100; c1=3.5; sd_e1=1.5; n1=100; cutoff = 3.0;
run;

*%binorm(parms1,'Data set #1');
%binorm(parms2,'Data set #2');
*%binorm(parms3,'Data set #3');
*%binorm(parms4,'Data set #4');
quit;
```

Output



Simulated Data for ROC
Data set #2
The FREQ Procedure

Table of group by y_cut			
group	y_cut		
	0	1	Total
control	86 86.00	14 14.00	100
disease	60 60.00	40 40.00	100
Total	146	54	200

Simulated Data for ROC
Data set #2

Obs	sensitivity	specificity
1	.	86
2	.	.
3	.	.
4	40	.

Simulated Data for ROC

Data set #2

The LOGISTIC Procedure

Model Information	
Data Set	WORK.A
Response Variable	group
Number of Response Levels	2
Model	binary logit
Optimization Technique	Fisher's scoring

Number of Observations Read	200
Number of Observations Used	200

Response Profile		
Ordered Value	group	Total Frequency
1	control	100
2	disease	100

Model Fit Statistics		
Criterion	Intercept Only	Intercept and Covariates
AIC	279.259	255.599
SC	282.557	262.196
-2 Log L	277.259	251.599

Testing Global Null Hypothesis: BETA=0			
Test	Chi-Square	DF	Pr > ChiSq
Likelihood Ratio	25.6598	1	<.0001
Score	24.2216	1	<.0001
Wald	21.7853	1	<.0001

Analysis of Maximum Likelihood Estimates					
Parameter	DF	Estimate	Standard Error	Wald Chi-Square	Pr > ChiSq
Intercept	1	−0.9345	0.2504	13.9281	0.0002
y	1	0.4804	0.1029	21.7853	<.0001

Odds Ratio Estimates			
Effect	Point Estimate	95% Wald Confidence Limits	
y	1.617	1.321	1.978

Association of Predicted Probabilities and Observed Responses			
Percent Concordant	70.2	Somers' D	0.405
Percent Discordant	29.8	Gamma	0.405
Percent Tied	0.0	Tau-a	0.203
Pairs	10000	c	0.702