A Relationship Between Orthogonal Regression And The Coefficient Of Determination Under Rotation Of Data Sets: Supplemental Materials

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Abstract

Supplemental materials (*Figure 3 data* & *Rotation R Code for Revision1*) for the publication, "A Relationship Between Orthogonal Regression and the Coefficient of Determination Under Rotation of Data Sets," by Gregory S. Rhoads, **Eric S. Marland**, Jose A. Sanqui, Michael J. Bossé, and W. Bauldry.

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# These are the codes that generate the plots in Figure 3 of the paper.

# This function calculates the value of Q-squared
Q2 <-function(x,y)
{
  library(MethComp)
  # Calculate the centroid of the data
  centx <- mean(x)
  centy <- mean(y)
  lam <- 1.0

  # Calculate the slope by Deming package in MethComp
  # This is a check on the other two methods to make sure
  # we get the same answer as the package value
  bopt <- Deming(x, y, vr=lam)[[2]]
  b0opt <- centy-bopt*centx
  dopt <- y - (b0opt+bopt*x)
  xopt <- x + 1/lam*bopt*dopt/(1+1/lam*bopt^2)
  yopt <- y - dopt/(1+1/lam*bopt^2)
  ssopt <- sum( (x-xopt)^2 + 1/lam*(y-yopt)^2 )


  # Proposed comparison slope
  # Also calculate the sum of squares
  b1 <- -1/bopt*lam
  b0 <- centy-b1*centx # set value of b0
  d <- y - (b0+b1*x)
  xh <- x + 1/lam*b1*d/(1+1/lam*b1^2)
  yh <- y - d/(1+1/lam*b1^2)
  sscomp <- sum( (x-xh)^2 + 1/lam*(y-yh)^2 )


  # official calculation of Q
  Q <- 1 - (ssopt/sscomp)
  return(Q)
}

# This code considers 2 data sets - the first has 1000 points and the
second
# has 10 points.  Both of these data sets have a Q-squared value of
0.8206713

# The code creates a scatterplot of the two data sets and then plots the
value
# of R-squared as each data set is rotated about its centroid.  There are
# 10000 angles of rotation from 0 to pi/2 (since the value of R-squared
is
# periodic, the plot is periodic with period pi/2).  One can see the two
# graphs are the same up to a horizontal rotation.

x1 <-c(
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-4.362206463,  -4.122017236,   3.324016168,   1.479061897,  -5.981858025,
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-10.667589846,  -2.199833794, -10.083178941,  -3.225286164,
1.216441840,
-1.198396805, -13.704390680, -10.042343487,   4.351119363, -11.063625187,
-6.943528083, -10.672838364,  -1.909776994,   0.290003538,  -0.599791530,
-10.294830891,  -1.433981675,  -5.158154837,  -3.604129976,
3.150338827,
-0.849210118,   4.053316200,   1.175326173,   0.839680409,  -8.092018894,
1.548206944, -11.336065928,   6.441887754,   1.065318982,   1.652311305,
0.024567859,  -9.773689392, -14.253904739,   0.150867398,  -3.424083462,
-12.673376084,  -6.897383494,  -6.972744564,   4.956074112,  -
3.075202675,
0.766369780,  -2.696639359, -15.406713950,   5.948829687,   3.474049640)

x2<-c(9.38842044, 9.41009631, 6.13350886, 5.79630747, 8.78032310,
5.37301021,
        6.28339816, 3.24112479, 9.71991573, 20)

y2<-c(-7.158380, -13.320740,  -4.164128,  -5.235486, -14.342440,
1.289806,
      -5.715725, -7.375107,  -3.654835, 12.519535)

#  check the values of Q to make sure they are both 0.8206713

print(Q2(x1, y1))
print(Q2(x2, y2))


Niter <- 2                   # the 2 data sets
Niterations <- 100000        # the number of angles between 0 and pi/2
R <- numeric(Niterations)    # the R^2 values for each angle of rotation
angle <- numeric(Niterations) # the angle of rotation.  Saved for the
plot
minangle <- numeric(Niter)
minR2value <- numeric(Niter)
maxangle <- numeric(Niter)
maxR2value <- numeric(Niter)
maxderivative <- numeric(Niter)

# make scatterplots of the data values

plot(x1, y1, xlim=c(0, 10), ylim=c(-20, 20), xlab='x', ylab='y')
plot(x2, y2, xlim=c(0, 25), ylim=c(-20, 20), xlab='x', ylab='y')
```

```
#  Now rotate the data around the centroid and calculate the R^2 value
for
#     each rotation.  Store that value and plot the R^2 value as a
function of
#     rotation angle. If i=1, we consider the data set with 10000 points,
if i=2,
#     we consider the data set with 10 points.

for (i in 1:2){

  if (i == 1){
    #  Translate the first data set so the centroid is 0.
    xmean <- mean(x1)
    ymean <- mean(y1)
    x <- x1 - xmean
    y <- y1 - ymean
  } else if (i == 2){
    #  Translate the second data set so the centroid is 0.
    xmean <- mean(x2)
    ymean <- mean(y2)
    x <- x2 - xmean
    y <- y2 - ymean
  }


  for (j in 1:Niterations){
    angle[j] <- j/Niterations * pi/2.0
    xt <- cos(angle[j])*x - sin(angle[j])*y
    yt <- sin(angle[j])*x + cos(angle[j])*y
    R[j] <- cor(xt,yt)^2
}

  plot(angle, R, xlim=c(0, 1.6), ylim=c(0, 1), xlab='angle', ylab='R-
squared value')
}
```

```
Q2 <-function(x,y)
{
  library(MethComp)
  # Calculate the centroid of the data
  centx <- mean(x)
  centy <- mean(y)
  lam <- 1.0

  # Calculate the slope by Deming package in MethComp
  # This is a check on the other two methods to make sure
  # we get the same answer as the package value
  bopt <- Deming(x, y, vr=lam)[[2]]
  b0opt <- centy-bopt*centx
  dopt <- y - (b0opt+bopt*x)
  xopt <- x + 1/lam*bopt*dopt/(1+1/lam*bopt^2)
  yopt <- y - dopt/(1+1/lam*bopt^2)
  ssopt <- sum( (x-xopt)^2 + 1/lam*(y-yopt)^2 )


  # Proposed comparison slope
  # Also calculate the sum of squares
  b1 <- -1/bopt*lam
  b0 <- centy-b1*centx # set value of b0
  d <- y - (b0+b1*x)
  xh <- x + 1/lam*b1*d/(1+1/lam*b1^2)
  yh <- y - d/(1+1/lam*b1^2)
  sscomp <- sum( (x-xh)^2 + 1/lam*(y-yh)^2 )


  # official calculation of Q
  Q <- 1 - (ssopt/sscomp)
  return(Q)
}


# These data sets all have Q = 0.7

x1<-c(9.5388103, 6.6515706, 5.2759388, 9.4317805, 0.7935329, 1.0665410,
      6.1517730, 9.6005346, 7.2360382, 20)
y1<-c(0.9154004, -2.2450810, -2.0975256, 13.1722065,  6.1003400, -
3.3684675,
      11.0381757,  3.9906343, 0.8668084, 12.422735)
#(x1,y1) is Data Set 1 used in Figure 1a in the Rotation paper
x2<-c(7.600377, 1.978002, 7.229740, 4.862896, 7.745258, 7.690310,
6.971579,
      2.637068, 4.193724, 20)
y2<-c(-12.0054001,  3.9684054, -6.3496456, -3.8531945, -3.1506936,
0.2927867,
      -0.8112592, -6.5683334, 3.6315538, 11.35770465)
x3<-c(3.791484, 8.867788, 8.026258, 1.818301, 2.137551, 1.689739,
8.805128,
      2.055237, 1.717903, 20)
y3<-c(-4.186807, -9.021588, -4.171665, -5.090640, -2.447193,  4.988260,
      -4.207612, -8.575323, -5.638246, 10.00566298)
```

```
x4<-c(7.673671, 4.571537, 2.470910, 5.285842, 8.682613, 6.211939,
8.371959,
     1.747533, 4.985990, 20)
y4<-c(-11.6155633, -1.8179629, -6.8795721, -2.7372764, -2.7703824, -
0.6348984,
     -7.2191548,-1.7636753, -9.3273300, 6.09109914)
x5<-c(6.9191473, 0.9695953, 0.5669041, 7.2773368, 0.4809697, 8.0060446,
     5.6657512, 7.8714489, 9.2133091, 20)
y5<-c(-3.79126724, -2.16360975, -5.31559767, -4.13001172,  6.72841753,
     -0.01992244, -7.53218534, -2.48123582, -2.18766031, 12.72532643)
#(x5,y5) is Data Set 3 used in Figure1c in the rotation paper

# These data sets all have Q = 0.9

x1 <-c(5.763246, 6.287920, 7.336722, 6.682707, 4.528821, 5.322331,
9.319445,
       7.480564, 9.314869, 20)
y1 <-c(-6.641493,  -7.284916,  -8.676793,  -6.892503,  -9.785372,
1.457690,
       -3.693516,  -4.342233, -16.915876, 15.361597)
x2<-c(3.597624, 1.230082, 8.013625, 6.174664, 1.352494, 2.103500,
1.856918,
      9.548380, 9.229362, 20)
y2<-c(-4.695678,  -5.239988,  -8.038837,  -2.898970,  -2.076787,  -
3.951345,
      -3.503952,  -7.895826, -13.696331, 31.140772)
#(x2,y2) is Data Set 2 used in Figure1b in the rotation paper
x3 <-c(1.248854, 2.583930, 9.520510, 5.554796, 4.292270, 7.343227,
3.831285,
       4.943790, 2.741467, 20)
y3 <-c(1.7544716,  -5.0089915, -13.4749902,   0.8065788,  -7.7156718,-
9.6930938,
       -8.6635424,   1.8212712, 0.3552457, 28.181317)
x4 <-c(9.207210, 8.676869, 7.229433, 8.223267, 6.296429, 6.212920,
8.122089,
       3.217325, 1.332194, 20)
y4 <-c(-9.2231435,-8.0710845,-12.1840090,-13.1389584,-0.6600742,-
2.6573070,
       -1.2316607,  -3.9198290, -2.6377542, 23.547340)
#x5<-c(0.7695457, 6.0163024, 4.4737159, 4.0596842, 7.3274447, 2.8274228,
 #     5.1400239, 9.5929732, 1.5157290, 20)
#y5<-c(-5.330598,  -3.445811,  -4.248221,  -3.911983, -12.035504,
 #     -2.568957,  -4.905784,  -8.702279, 4.546078, 28.205795)
#  check the values of Q to make sure they are all the same

print(Q2(x1, y1))
print(Q2(x2, y2))
print(Q2(x3, y3))
print(Q2(x4, y4))
print(Q2(x5, y5))

Niter <- 5
Niterations <- 100000
R <- numeric(Niterations)
```

```
slope <- numeric(Niter)
percentarea <- numeric(Niter)
Q <- numeric(Niter)
R2 <- numeric(Niter)
angle <- numeric(Niterations)
minangle <- numeric(Niter)
minR2value <- numeric(Niter)
maxangle <- numeric(Niter)
maxR2value <- numeric(Niter)
maxderivative <- numeric(Niter)

for (i in 1:5){

# initialize minimum R2 value and angle which yields the minimum value

  minangle[i] <- 0.0
  minR2value[i] <- 1.0
  maxangle[i] <- 0.0
  maxR2value[i] <- 0.0

  if (i == 1){
    #  Compute the centroid and translate the data so the centroid is 0.
    xmean <- mean(x1)
    ymean <- mean(y1)
    x <- x1 - xmean
    y <- y1 - ymean
  } else if (i == 2){
    #  Compute the centroid and translate the data so the centroid is 0.
    xmean <- mean(x2)
    ymean <- mean(y2)
    x <- x2 - xmean
    y <- y2 - ymean
  } else if (i == 3){
    #  Compute the centroid and translate the data so the centroid is 0.
    xmean <- mean(x3)
    ymean <- mean(y3)
    x <- x3 - xmean
    y <- y3 - ymean
  } else if (i == 4){
    #  Compute the centroid and translate the data so the centroid is 0.
    xmean <- mean(x4)
    ymean <- mean(y4)
    x <- x4 - xmean
    y <- y4 - ymean
  } else if (i == 5){
    #  Compute the centroid and translate the data so the centroid is 0.
    xmean <- mean(x5)
    ymean <- mean(y5)
    x <- x5 - xmean
    y <- y5 - ymean
  }
#  loop through angles between 0 and Pi/2 to find the rotation angle 
which
#  gives the R2 value closest to 0
```

```
  xmean <- mean(x5)
  ymean <- mean(y5)
  x <- x5 - xmean
  y <- y5 - ymean


  for (j in 1:Niterations){
    angle[j] <- j/Niterations * pi/2.0
    xt <- cos(angle[j])*x - sin(angle[j])*y
    yt <- sin(angle[j])*x + cos(angle[j])*y
    R[j] <- cor(xt,yt)^2
    if (abs(R[j]) < minR2value[i]) {
      minR2value[i] <- R[j]
      minangle[i] <- angle[j]
    }
    if (abs(R[j]) > maxR2value[i]) {
      maxR2value[i] <- R[j]
      maxangle[i] <- angle[j]
    }
} #j loop end

# Now you have the angle that gives the largest and smallest R^2 values
# and the largest and smallest R^2 values

  maxderivative[i] <- 0.0
  deltaangle <- 1/Niterations * pi/2.0
  summ <- R[1]
  for (j in 2:(Niterations-1)){
    summ <- summ + 2*R[j]
    derivest <- (R[j] - R[j-1]) / (angle[j] - angle[j-1])
    if (abs(derivest) > maxderivative[i]) {
      maxderivative[i] <- abs(derivest)
    }
  }
  summ <- deltaangle/2 * (summ + R[Niterations])
  print("maxR2value")
  print(maxR2value[i])
  percentarea[i] <- summ /(pi/2*maxR2value[i])
#   percentarea[i] <- summ /(pi/2)
  print("percentarea")
  print(percentarea[i])
  plot(angle, R, xlim=c(0, 1.6), ylim=c(0, 1), xlab='angle', ylab='R-
squared value')
}

library(ggplot2)
df2<-data.frame(angle,R)
#Plot of R^2g vs log(lambda) for the paper
ggplot(df2,aes(angle,R))+
  geom_line()+
  labs(x = expression(theta),
       y = expression(R[theta]^2))+
```

```
      # title=expression(paste("                    ",R[angle]^2,"  vs
",theta))+
  xlim(0,1.6)+
    ylim(0,1)+
  geom_hline(yintercept=Q2(x1,y1),linetype="dashed")+
  scale_x_continuous(breaks  = c(seq(0, pi/2, pi/4)),
                     labels = c("0", "\u03c0/4", "\u03c0/2"))

# this is (x5,y5) for Q = 0.7
x3<-c(6.9191473, 0.9695953, 0.5669041, 7.2773368, 0.4809697, 8.0060446,
      5.6657512, 7.8714489, 9.2133091, 20)
y3<-c(-3.79126724, -2.16360975, -5.31559767, -4.13001172,  6.72841753,
      -0.01992244, -7.53218534, -2.48123582, -2.18766031, 12.72532643)


df <- data.frame(x3,y3)

#Plot of simulated data for the paper
ggplot(df,aes(x3,y3))+
  geom_point()+
  labs(title="           Scatterplot for Data Set 3")





#plot(slope,minangle,xlim=c(0,2),ylim=c(0,1.57),xlab='slope',ylab='angle
R2=0')
#plot(R2,minangle,xlim=c(0,1),ylim=c(0,1.57),xlab='R2',ylab='angle R2=0')

# Output -
#[1] "maxR2value"
#[1] 0.2899408
#[1] "percentarea"
#1] 0.2899408
#[1] "percentarea"
#[1] 0.5426885
#[1] "maxR2value"
#[1] 0.2899408
#[1] "percentarea"
#[1] 0.5426866
#[1] "maxR2value"
#[1] 0.2899408
#[1] "percentarea"
#[1] 0.5426866
#[1] "maxR2value"
#[1] 0.2899408
#[1] "percentarea"
#[1] 0.5426867
```