Computational Statistics - STAT 575 - Exam #1

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Problem 1

Part (1) (10 points)

Use accept-reject algorithm to generate a truncate standard Normal distribution, with density

$$f(x) \propto e^{-x^2/2} I(x > 2).$$

Consider the proposed distribution $g(x) = 2e^{-2(x-2)} I(x > 2)$.

Part (a)

$\boxed{\text{Sample from } g \text{ using inverse-transform method.}}$

First, we must find the cdf G of g. One way to derive G is to notice that g is the density of the shifted exponential, i.e., if $S \sim \exp(\lambda = -2)$, then $X = 2 + S$ has a cdf

$$\begin{aligned}
G(x) &= P(X \leq x) && (1)\\
&= P(2 + S \leq x) && (2)\\
&= P(S \leq x - 2) && (3)\\
&= F_S(x - 2) && (4)\\
&= \qquad = I(x > 2)(1 - \exp(-2(x-2))). && (5)
\end{aligned}$$

As a quick proof that G is the cdf of g, note that $dG/dx = g$.

Alternatively, the cdf G is defined as

$$\begin{aligned}
G(x) &= \int_{-\infty}^{x} g(s) ds && (6)\\
&= I(x > 2) \int_{2}^{x} 2e^{-2(s-2)} ds && (7)\\
&= I(x > 2) e^4 \int_{2}^{x} 2e^{-2s} ds && (8)\\
&= -I(x > 2) e^4 \int_{2}^{x} (-2) e^{-2s} ds && (9)\\
&= -I(x > 2) e^4 \left(e^{-2s} \Big|_2^x \right) && (10)\\
&= -I(x > 2) e^4 \left(e^{-2x} - e^{-4} \right) && (11)\\
&= I(x > 2)(1 - e^4 e^{-2x}) && (12)\\
&= I(x > 2)(1 - e^{-2(x-2)}), && (13)
\end{aligned}$$

which obtains the same result. Either way, we solve for x in

$$\begin{aligned}
u &= G(x) \\
u &= 1 - e^{-2(x-2)} \\
1 - u &= e^{-2(x-2)} \\
\log(1-u) &= -2(x-2) \\
-\frac{1}{2}\log(1-u) &= x - 2,
\end{aligned}$$

and thus

$$x = -\frac{1}{2}\log(1-u) + 2$$

where u is drawn from UNIF$(0,1)$. That is, if $U \sim$ UNIF$(0,1)$ then

$$X = -\frac{1}{2}\log(1-U) + 2$$

is a random variable whose density is g.

Part (b)

Use accept-reject algorithm to generate a sample of 10000 from f. Choose a c so that $f(y)/[cg(y)] \leq 1$. Verify the generated sample via a plot of the true normalized density, and a histogram of the generated values.

We wish to find a c such that $f(y)/[cg(y)] \leq 1$.

However, we do not need f, we only need the kernel of f, which has already been given.

So, ideally, we find the smallest c that satisifes the inequality

$$\frac{k(y)}{g(y)} \leq 1$$

where k is the kernel of f, which is given by $c = \max\{k(y)/g(y)\}$. We may solve this analytically by finding

$$y^* = \arg\max_y k(y)/g(y)$$

and then let $c = k(y^*)/g(y^*)$.

First, we let

$$h(y) = k(y)/g(y) = \frac{e^{-y^2/2}}{2e^{-2(y-2)}}.$$

We can find the value that maximizes h by finding the value that maximizes $\log h$, which is given by

$$\log h(y) = \log \frac{e^{-y^2/2}}{2e^{-2(y-2)}} = -\frac{1}{2}y^2 + 2(y-2).$$

The value y^* that maximizes $\log h$ satisfies

$$\left.\frac{d\log h}{dy}\right|_{y=y^*} = -y^* + 2 = 0,$$

which means $y^* = 2$ maximizes $\log h$ and thus

$$\begin{aligned}
c = h(2) &= \frac{k(2)}{g(2)} && (14) \\
&= \frac{1}{2e^2}. && (15)
\end{aligned}$$

Thus, we sample y from g and u from $\text{UNIF}(0,1)$ and accept the sample as being drawn from f if

$$u \leq \frac{k(y)}{g(y)} = e^{-(y-2)^2/2}.$$

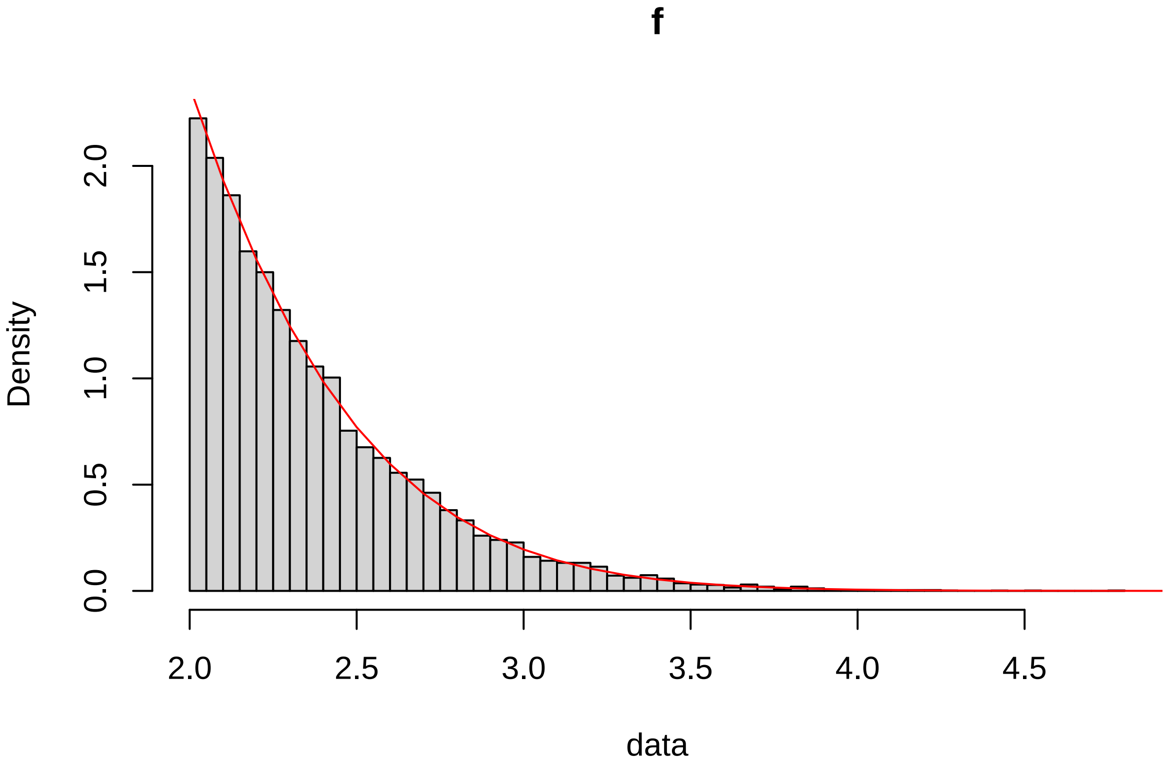
Here is the code that implements our sampling method for f using acceptance-rejection sampling:

```r
# the proposed density we can easily sample from
g <- function(y)
{
  2*exp(-2*(y-2))
}

# inverse transform method for sampling from g
rg <- function(n)
{
  -0.5*log(1-runif(n))+2
}

rf <- function(n)
{
  data <- vector(length=n)
  for (i in 1:n)
  {
    repeat
    {
      y <- rg(1)
      u <- runif(1)
      if (runif(1) <= exp(-(y-2)^2/2))
      {
        data[i] <- y
        break
      }
    }
  }
  data
}

k <- function(y)
{
  exp(-y^2/2)
}

f <- function(y)
{
  # normalizing constant
  Z <- 17.5358
  Z*k(y)
}
```

To verify the sampling method, we drawn $n = 10000$ samples from f and plot its histogram along with a plot of its density function f.

```r
data <- rf(10000)
ys <- seq(2,10,by=.1)
```

```
hist(data,freq=F,breaks=50,main="f")
lines(x=ys,f(ys),col="red")
```



The histogram seems compatible with the pdf f.

NOTE TO Dr. Q: On the in-class portion, I forgot to plug the value that I found that maximizes h back into h to find c. Maybe my brain is just getting too old!

Problem 2 (5 points)

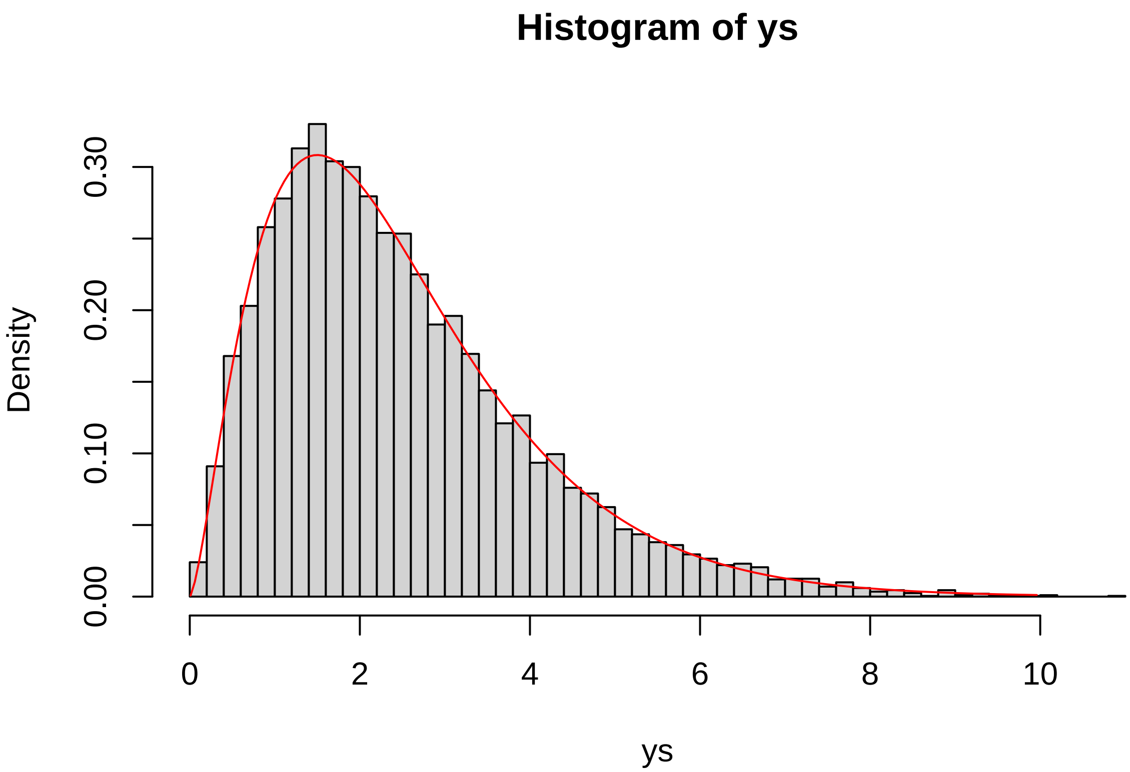
Implement your accept-reject algorithm to get a sample of 10000 from Gamma$(2.5, 1)$. Verify that your method works via a plot of the true normalized density, and a histogram of the generated values.

This is not the approach you were looking for, but on the test I did poorly on this section.

Be that as it may, here is essentially my answer on the test, except that the solution is so slow that I decreased c so that, at the extreme tail of the distribution, $f(y)/cg(y) > 1$.

```
alpha <- 2.5
n <- 10000
c <- 10
a <- floor(alpha)
b <- a / alpha

ys <- vector(length=n)
for (i in 1:n)
{
  repeat
  {
```

```r
    y <- rgamma(n=1,shape=a,scale=b)
    u <- runif(1)
    P <- dgamma(y,shape=alpha,scale=1) / (c*dgamma(y,shape=a,scale=b))
    if (u < P)
    {
      ys[i] <- y
      break
    }
  }
}

hist(ys,freq=F,breaks=50)
lines(x=seq(.01,10,by=.05),y=dgamma(seq(.01,10,by=.05),shape=alpha,scale=1),col="red")
```



Problem 3 (30 points)

Considers 197 animals randomly divided into four categories (four phenotypes) as follows: $X = (x1, x2, x3, x4)^T$ with cell probabilities $(1/2+\theta/4, (1-\theta)/4, (1-\theta)/4, \theta/4)^T$. We observe $X = (125, 18, 20, 34)^T$.

Part (a)

Hand code your algorithm using Newton-Ralphson to find the maximum likelihood estimator of θ directly from the observed likelihood. Compare your result with what you get using the built-in optim() function in R.

In part 1 of the exam, the log-likelihood given the data was determined to be

$$\ell(\theta|\vec{x}) = x_1 \log\left(\frac{1}{2} + \frac{\theta}{4}\right) + x_2 \log\left(\frac{1-\theta}{4}\right) + x_3 \log\left(\frac{1-\theta}{4}\right) + x_4 \log\left(\frac{\theta}{4}\right).$$

We derived the updating equation for the MLE of θ to be

$$\theta^{(t+1)} = \theta^{(t)} - \frac{d\ell/d\theta}{d^2\ell/d\theta^2}$$

where

$$\frac{d\ell}{d\theta} = \frac{x_1}{\theta+2} + \frac{x_2}{\theta-1} + \frac{x_3}{\theta-1} + \frac{x_4}{\theta}$$

and

$$\frac{d^2\ell}{d\theta^2} = -\frac{x_1}{(\theta+2)^2} - \frac{x_2}{(\theta-1)^2} - \frac{x_3}{(\theta-1)^2} - \frac{x_4}{\theta^2}.$$

Instead of taking the time to simplify this expression, we will just substitute these derivations into the updating equation in the following R code:

```r
l1 <- function(theta,x)
{
  x[1]/(theta+2) + (x[2]+x[3])/(theta-1) + x[4]/theta
}

l2 <- function(theta,x)
{
  -x[1]/(theta+2)^2 - (x[2]+x[3])/(theta-1)^2 - x[4]/theta^2
}

theta_mle <- function(x, start = 0.5, eps = 1e-6)
{
  i <- 0
  theta0 <- start
  theta1 <- NULL
  repeat
  {
    theta1 <- theta0 - l1(theta0,x) / l2(theta0,x)
    if (abs(theta1-theta0) < eps) { break }
    theta0 <- theta1
    i <- i + 1
  }
  list(mle=theta1,iterations=i)
}
```

We invoke the updating equations on the given data to estimate θ with the following R code:

```r
# observed data
x <-c(125, 18, 20, 34)
sol <- theta_mle(x=x, start=0.5, eps=1e-6)
mle <- sol$mle
mle_iterations <- sol$iterations
```

We see that the MLE converges to a solution around 0.6268215 after 3. We compare this result with the built-in procedure, optim:

```r
# the function to maximize, the log-likelihood function
loglike <- function(theta)
{
  x[1]*log(0.5+theta/4) + x[2]*log(0.25*(1-theta)) + x[3]*log(0.25*(1-theta)) + x[4]*log(0.25*theta)
}

# since optim finds the value that minimizes the function, we provide it with
# the negative of the log-likelihood.
optim(0.5,function(theta) { -loglike(theta) },lower=0.1,upper=0.9,method="L-BFGS-B")$par
```

```
## [1] 0.626821
```

The value optim found is approximately the same. It was fussy with explicitly providing upper and lower bounds. This warrants further investigation, but for another time.

Part (b)

Implement the E-M algorithm to find the the maximum likelihood estimator of θ with the "augmented" data with missing information $Z = y_2$. Compare your result with part (a).

We split the first category into two,

$$\vec{y} = (y_1, y_2, y_3, y_4, y_5)^T$$

with cell probabilities $(1/2, \theta/4, (1-\theta)/4, (1-\theta)/4, \theta/4)^T$.

So, y_1 and y_2 are *unobserved*. The pdf is given by

$$f(\vec{y}|\theta) \propto \prod_{i=1}^{5} \pi_i(\theta)^{y_i}$$

where

$$\vec{\pi}(\theta) = (1/2, \theta/4, (1-\theta)/4, (1-\theta)/4, \theta/4)^T.$$

Thus, the complete log-likelihood is given by

$$\log f(\vec{y}|\theta) = \sum_{i=1}^{5} y_i \log \pi_i(\theta)$$

which may be written as

$$\log f(\vec{y}|\theta) = k(\vec{y}) + y_2 \log(\theta) + y_3 \log(1-\theta) + y_4 \log(1-\theta) + y_5 \log \theta.$$

E-step

The function we seek to maximize Q is thus given by

$$Q(\theta|\theta^{(t)}) = E_{Z|\vec{x},\theta^{(t)}}(\log f(\vec{y}|\theta)),$$

which is given by

$$Q(\theta|\theta^{(t)}) = E_{Z|\vec{x},|\theta^{(t)}}\left(y_2 \log(\theta) + y_3 \log(1-\theta) + y_4 \log(1-\theta) + y_5 \log \theta\right)$$

which by the property of linearity of expectations is equivalent to

$$\begin{aligned} Q(\theta|\theta^{(t)}) = {} & E_{Z|\vec{x},|\theta^{(t)}}(y_2) \log(\theta) + E_{Z|\vec{x},|\theta^{(t)}}(y_3) \log(1-\theta) + \\ & E_{Z|\vec{x},|\theta^{(t)}}(y_4) \log(1-\theta) + E_{Z|\vec{x},|\theta^{(t)}}(y_5) \log \theta. \end{aligned} \tag{16}$$

Note that y_3, y_4, and y_5 are respectively observed to be x_2,x_3,x_4 and thus, for instance,

$$E_{Z|\vec{x}}(y_3) = x_2.$$

The missing data $Z = y_2$ is distributed

$$Z|(\vec{x}, \theta^{(t)}) \sim \mathrm{BIN}(\mathrm{x}_1, \frac{^{(\mathrm{t})}}{2 + \ ^{(\mathrm{t})}}).$$

and thus

$$E_{Z|\vec{x},|\theta^{(t)}}(y_2) = \frac{x_1\theta^{(t)}}{2+\theta^{(t)}}.$$

Putting it all together, we may rewrite Q as

$$Q(\theta|\theta^{(t)}) = \frac{x_1\theta^{(t)}}{2+\theta^{(t)}}\log(\theta) + x_2\log(1-\theta) + x_3\log(1-\theta) + x_4\log\theta.$$

M-step

In the M-step, we seek

$$\theta^{(t+1)} = \arg\max_\theta Q(\theta|\theta^{(t)}),$$

which can be found by solving

$$\left.\frac{dQ(\theta|\theta^{(t)})}{d\theta}\right|_{\theta=\theta^{(t+1)}} = 0.$$

Since the final solution is a little noisy when we leave $\vec{x}$ symbolic, we are going to finish the solution with the observed values of $\vec{x}$. So,

$$\frac{dQ}{d\theta} = \frac{125\theta^{(t)}}{2+\theta^{(t)}} - \frac{38}{1-\theta} - \frac{34}{\theta} = 0$$

has the solution, when we replace θ with $\theta^{(t+1)}$,

$$\theta^{(t+1)} = \frac{159\theta^{(t)} + 68}{197\theta^{(t)} + 144}.$$

Iterating update equation until some stopping condition that signifies convergence may then be done. We denote the converged solution of the EM algorithm by

$$\hat{\theta}_{\mathrm{EM}} = \lim_n \theta^{(t)}.$$

We implement the EM algorithm in the following R code:

```r
theta0 <- .5
theta1 <- NULL
i <- 1
repeat
{
  theta1 <- (159*theta0 + 68)/(197*theta0 + 144)
  cat("theta[",i,"] = ", theta1,"\n")
  if (abs(theta1-theta0) < 1e-6) { break }
  theta0 <- theta1
  i <- i + 1
}
```

```
## theta[ 1 ] =  0.6082474
## theta[ 2 ] =  0.6243211
## theta[ 3 ] =  0.6264889
## theta[ 4 ] =  0.6267773
## theta[ 5 ] =  0.6268156
## theta[ 6 ] =  0.6268207
## theta[ 7 ] =  0.6268214
```

```
print(theta1)
```

```
## [1] 0.6268214
```

We see the standard MLE $\hat{\theta}_{\text{mle}}$ and $\hat{\theta}_{\text{EM}}$ both obtain the same solution up to 6 decimal places when using the same starting value and stopping condition. However, $\hat{\theta}_{\text{EM}}$ required more iterations before convergence, which was expected given that the EM algorithm is of linear order while the MLE using Newton-raphson is of quadratic order. However, the EM algorithm does have the benefit of a less complex updating equation.

Part (c)

Find the standard error of the MLE using either a numerical calculation of the inverse of the observed fisher's information, i.e $[-l''(\theta)]^{-1}$, or using Louis' Method.

We already have the second derivative of the log-likelihood, so we choose to use the observed Fisher information evaluated at $\theta = \theta_{\text{mle}}$.

```
obs_fisher <- -l2(mle,x)
var_mle <- 1 / obs_fisher
sqrt(var_mle)
```

```
## [1] 0.05146735
```

We see that an estimate of standard error of the MLE is $\text{sd}(\hat{\theta}_{\text{mle}}) = 0.0514673$.

Problem 4 (10 points)

Consider the density $f(x) \propto 3e^{-0.5(x+2)^2} + 7e^{-0.5(x-2)^2}$ (problems 6, Homework 1).

Part (a)

Compute the exact normalizing constant, both in closed form using π (pencil and paper), and also to 5 decimal places (by evaluating the exact version in R).

It is given that

$$f(x) \propto \ker(x)$$

i.e., $f(x) = C\ker(x)$, where

$$\mathrm{ker(x) = 3e^{-0.5(x+2)^2} + 7e^{-0.5(x-2)^2}}$$

and C is the normalizing constant that satisfies the equation

$$\int_{-\infty}^{\infty} \frac{1}{C} \ker(x) dx = 1.$$

Solving for C yields the result

$$C = \int_{-\infty}^{\infty} 3e^{-0.5(x+2)^2} dx + \int_{-\infty}^{\infty} 7e^{-0.5(x-2)^2} dx.$$

Each mode of the bimodal distribution resembles a normal distribution with $\sigma = 1$. We may rewrite the above to

$$C = 3\sqrt{2\pi}\int_{-\infty}^{\infty}\frac{e^{-0.5(x+2)^2}}{\sqrt{2\pi}}dx + 7\sqrt{2\pi}\int_{-\infty}^{\infty}\frac{e^{-0.5(x-2)^2}}{\sqrt{2\pi}}dx$$

which is equivalent to

$$C = 3\sqrt{2\pi}\int_{-\infty}^{\infty}\phi(x+2)dx + 7\sqrt{2\pi}\int_{-\infty}^{\infty}\phi(x-2)dx.$$

Since ϕ is a pdf, each integral evaluates to 1, and thus

$$C = 3\sqrt{2\pi} + 7\sqrt{2\pi} = 10\sqrt{2\pi}$$

is the normalizing constant, which is 25.06628 to 5 decimal places.

Using R's numerical integrator, we get the result:

```
C <- 10*sqrt(2*pi)
ker <- function(x) { 3*exp(-0.5*(x+2)^2) + 7*exp(-0.5*(x-2)^2) }
res <- integrate(ker,lower = -Inf, upper = Inf)
print(res)
```

```
## 25.06628 with absolute error < 4e-05
```

Part (b)

Approximate this integral with a Simpson's rule to three decimal places. What is the effective range and number of subintervals required?

Simpson's rule is implemented by the following R code. Note that we did not bother to optimize it.

```
# simpson : numerical integrator applying simpson's rule to n subintervals
# over the range (a,b).
#
# arguments;
#   f : the function to integrate
#   a : the lower-bound
#   b : the upper-bound. (a,b) together discrete the range.
#   n : the number of subintervals to partition the range
#
# we evenly partition the range into n subintervals of size (b-a)/n
# and apply simson's rule to each subinterval. then, we accumulate these
# values and return the result.
simpson <- function(f, a, b, n)
  {
    h <- (b-a)/n
    s <- 0
    x <- a
    for (i in 1:(n/2))
    {
      s <- s + f(x) + 4 * f(x+h) + f(x+2*h)
      x <- x + 2*h
    }
    s*h/3
}
```

To test effective range and subintervals, we decided to make a program that exhaustively searches for the minimum range and number of subintervals over a discrete set of points. In particular, we search for a range of the form $(-r, r)$ that is symmetric and an even n. It is not perfect, but it seems like a reasonable way to estimate these requirements.

Here is the R code:

```
R <- NULL
N <- NULL
found <- F
for (r in 1:200)
{
  for (n in 1:100)
  {
    res <- simpson(ker,-r/10,r/10,2*n)
    if (abs(res - C) < 0.001)
    {
      R <- r/10
      N <- 2*n
      cat("r = +-", R, ", n = ", N, ", C = ", res, "\n")
      found <- T
      break
    }
  }
  if (found) { break }
}
```

```
## r = +- 5.9 , n =  16 , C =  25.06603
```

The minimum range $(-r, r)$, $r > 0$, when divided into n subintervals, that is the same as the true value $10\sqrt{2\pi}$ to 3 decimal places is given by $r = 5.9$ and $n = 16$.