**An Illustration for the multi-variate folded normal distribution**

2023-10-06

# **Initialization**

To initialize the program, the following packages are required:

|  |  |
| --- | --- |
| Package | Comment |
| MASS | *kde2d()* |
| Rcpp | *cppFunction()* |
| mvtnorm | *dmvnorm()* |

source("utils.R")

library(MASS)

library(mvtnorm)

**R**

# 

# **A Simple Walk through**

In this section we will illustrate the two-dimensional case of the folded normal distribution.

## Simulation Data Generation

**R**

set.seed(123)

n <- 100

u1 <- 4

u2 <- 6

sig1 <- 1

sig2 <- 2

rho <- 0.2

mean <- c(u1, u2)

sigma2 <- matrix(c(

sig1^2, rho \* sig1 \* sig2,

rho \* sig1 \* sig2, sig2^2),

2, 2)

dat <- mvrnorm(n, mean, sigma2)

## 

## BFGS Optimization

We use Cholsky decomposition to initialize the parameters.

**R**

covmat <- cov(dat)

init <- c(mean(dat[, 1]), mean(dat[, 2]), chol(covmat)[c(1, 3, 4)])

inputx <- abs(dat)

## The following is the result of the optimization.

result <- optim(init, loglik.G2cholesky, method = "BFGS")

print(result)

*## $par*

*## [1] 4.1273896 6.1666814 0.9701374 0.4121426 1.7639570*

*##*

*## $value*

*## [1] 337.4436*

*##*

*## $counts*

*## function gradient*

*## 35 9*

*##*

*## $convergence*

*## [1] 0*

*##*

*## $message*

*## NULL*

## The following is the result of the optimization.

*## Estimations*

print(result$par)

*## [1] 4.1273896 6.1666814 0.9701374 0.4121426 1.7639570*

*## Covariance Matrix*

est\_helper.G2(result$par, method = "chole")[["sigma2"]]

*## [,1] [,2]*

*## [1,] 0.9411666 0.3998349*

*## [2,] 0.3998349 3.2814058*

# 

# **2d FN MLE simulation**

One could change the settings to the following value and try again.

* n = 20,30,40,50,60,70,80,90,100;
* mu = (2.5,2.5),(5,5),(7.5,7.5),(10,10),(12.5,12.5).

**R**

set.seed(123456)

simu\_n <- 1000

dim\_p <- 2

result\_df <- data.frame()

n <- 20

mu <- c(2.5, 2.5)

ss <- matrix(c(25, 5, 5, 25), 2, 2)

lower\_idx <- f\_lower\_idx(dim\_p)

**for** (i **in** seq\_len(simu\_n)) {

dat <- mvrnorm(n, mu, ss)

inputx <- abs(dat)

sss <- chol(cov(dat))

init <- c(

mean(dat[, 1]), mean(dat[, 2]),

sss[lower\_idx]

)

fit <- optim(init, loglik.G2cholesky, method = "BFGS", hessian = TRUE)

fisher\_info <- solve(fit$hessian)

prop\_sigma <- sqrt(diag(fisher\_info))

prop\_sigma <- diag(prop\_sigma)

a <- diag(prop\_sigma)

prop\_sigma <- a

upper <- fit$par + 1.96 \* prop\_sigma

lower <- fit$par - 1.96 \* prop\_sigma

true\_para <- c(mu, chol(ss)[lower\_idx])

p <- c()

**for** (k **in** 1:5) {

p[k] <- (lower[k] <= true\_para[k] & true\_para[k] <= upper[k])

}

result\_df <- rbind(result\_df, p)

}

*## calculate coverage rate of parameters ##*

*# Be sure to handle NA's before the*

*# coverage rate calculation*

result\_df[is.na(result\_df)] <- FALSE

p <- apply(result\_df, 2, mean)

p

*## FALSE. TRUE. TRUE..1 TRUE..2 TRUE..3*

*## 0.733 0.723 0.756 0.691 0.550*

round(p, 2)

*## FALSE. TRUE. TRUE..1 TRUE..2 TRUE..3*

*## 0.73 0.72 0.76 0.69 0.55*

Here:

* ***n***: samples size
* ***simu\_n***: simulation times

The coverage rate of parameters are:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| n | simu\_n | mu1 | mu2 | sigma11 | sigma21 | sigma22 |
| 20 | 1000 | 0.73 | 0.72 | 0.76 | 0.69 | 0.55 |
| 100 | 100 | 0.63 | 0.76 | 0.76 | 0.71 | 0.73 |

# **4d FN MLE simulation**

We should point out that the speed of dim = 4 is much slower than dim = 2.

**R**

set.seed(123456)

simu\_n <- 1000

dim\_p <- 4

result\_df <- data.frame()

n <- 20

mu <- c(2.5, 2.5, 2.5, 2.5)

ss <- matrix(5, 4, 4)

diag(ss) <- 25

lower\_idx <- f\_lower\_idx(dim\_p)

**for** (i **in** seq\_len(simu\_n)) {

dat <- mvrnorm(n, mu, ss)

inputx <- abs(dat)

sss <- chol(cov(dat))

init <- c(

mean(dat[, 1]), mean(dat[, 2]), mean(dat[, 3]), mean(dat[, 4]),

sss[lower\_idx]

)

fit <- optim(init, loglik.G2cholesky, method = "BFGS", hessian = TRUE)

fisher\_info <- solve(fit$hessian)

prop\_sigma <- sqrt(diag(fisher\_info))

prop\_sigma <- diag(prop\_sigma)

a <- diag(prop\_sigma)

prop\_sigma <- a

upper <- fit$par + 1.96 \* prop\_sigma

lower <- fit$par - 1.96 \* prop\_sigma

true\_para <- c(mu, chol(ss)[lower\_idx])

*#c(lower[1], upper[1], lower[2], upper[2], (lower[3]),*

*# upper[3], (lower[4]), (upper[4]), (lower[5]), (upper[5]))*

p <- rep(0., 14)

**for** (k **in** seq\_len(14)) {

p[k] <- (lower[k] <= true\_para[k] & true\_para[k] <= upper[k])

}

result\_df <- rbind(result\_df, p)

}

*## calculate coverage rate of parameters ##*

*# Be sure to handle NA's before the*

*# coverage rate calculation*

result\_df[is.na(result\_df)] <- FALSE

p <- apply(result\_df, 2, mean)

round(p, 2)

*## X1 X1.1 X1.2 X0 X1.3 X1.4 X0.1 X0.2 X1.5 X1.6 X1.7 X0.3 X1.8 X0.4*

*## 0.72 0.70 0.72 0.71 0.75 0.69 0.70 0.70 0.58 0.59 0.58 0.39 0.47 0.17*

Here the coverage rate of parameters are (n = 20, simu\_n = 1000) vs (n = 100, simu\_n = 100).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| n | simu\_n | mu1 | mu2 | mu3 | mu4 | sigma11 | sigma21 | sigma22 | sigma31 | sigma32 | sigma33 | sigma41 | sigma42 | sigma43 | sigma44 |
| 20 | 1000 | 0.72 | 0.70 | 0.72 | 0.71 | 0.75 | 0.69 | 0.70 | 0.70 | 0.58 | 0.59 | 0.58 | 0.39 | 0.47 | 0.17 |
| 100 | 100 | 0.65 | 0.65 | 0.65 | 0.61 | 0.73 | 0.7 | 0.68 | 0.77 | 0.71 | 0.6 | 0.62 | 0.69 | 0.64 | 0.57 |

# 

⚠ **NOTE**: It is noticable the number of parameters is 14, which is much larger than the number of parameters in the 2d case. Therefore, the number of observations n should be larger than dim=2’s to get a reasonable coverage rate.

# **Real data example**

We use the bmi.nz data in the VGAM package as an example. It is the body mass indexes and ages from an approximate random sample of 700 New Zealand adults.

**R**

source("utils.R")

library(MASS)

library(ggplot2)

library("shape")

library("MASS")

*## R package VGAM bmi data*

data <- VGAM::bmi.nz

*## For users' convinience, we provide the tab separated data file as well*

*## data <- read.csv("bmi.csv", header = TRUE, sep = " ")[, c(2, 3)]*

colnames(data) <- c("age", "bmi")

*# kernel density estimate ##*

kde\_estimation <- kde2d(data[, 1], data[, 2])

length(kde\_estimation$x)

*## [1] 25*

dim(kde\_estimation$z)

*## [1] 25 25*

*## estimate mle ##*

dat <- data.frame(data$age, data$bmi)

dat <- as.matrix(data)

inputx <- dat

sss <- chol(cov(dat))

init <- c(

mean(dat[, 1]), mean(dat[, 2]),

sss[c(1, 3, 4)]

)

fit <- optim(init, loglik.G2cholesky, hessian = T)

muest <- fit$par[c(1, 2)]

sigma <- matrix(c(fit$par[3], 0, fit$par[4], fit$par[5]), 2, 2)

fisher\_info <- solve(fit$hessian)

prop\_sigma <- sqrt(diag(fisher\_info))

prop\_sigma <- diag(prop\_sigma)

a <- diag(prop\_sigma)

prop\_sigma <- a

sigmaest <- t(sigma) %\*% sigma

x <- seq(min(data$age), max(data$age), length.out = 25)

y <- seq(min(data$bmi), max(data$bmi), length.out = 25)

mu1 <- muest[1]

mu2 <- muest[2]

summary(data)

*## age bmi*

*## Min. :18.31 Min. :15.22*

*## 1st Qu.:32.94 1st Qu.:23.51*

*## Median :41.57 Median :26.10*

*## Mean :43.73 Mean :26.68*

*## 3rd Qu.:53.08 3rd Qu.:29.25*

*## Max. :85.06 Max. :58.46*

sgm1 <- sqrt(sigmaest[1, 1])

sgm2 <- sqrt(sigmaest[2, 2])

rou <- sigmaest[1, 2] / (sgm1 \* sgm2)

f <- **function**(x, y) {

(1.0 / (2.0 \* pi \* sgm1 \* sgm2 \* sqrt(1 - rou^2))

) \* exp((-1.0 / (2.0 \* (1 - rou^2))) \* ((((x - mu1)^2) /

(sgm1^2)) - (2 \* rou \* (x - mu1) \* (y - mu2) / (sgm1 \* sgm2)) + (((y - mu2)^2) / sgm2^2)))

}

f1 <- **function**(x, y) {

(1.0 / (2.0 \* pi \* sgm1 \* sgm2 \* sqrt(1 - rou^2))

) \* (exp((-1.0 / (2.0 \* (1 - rou^2))) \* ((((x - mu1)^2) / (sgm1^2)) -

(2 \* rou \* (x - mu1) \* (y - mu2) / (sgm1 \* sgm2)) + (((y - mu2)^2) / sgm2^2))) +

exp((-1.0 / (2.0 \* (1 - rou^2))) \* ((((x + mu1)^2) / (sgm1^2)) -

(2 \* rou \* (x + mu1) \* (y - mu2) / (sgm1 \* sgm2)) + (((y - mu2)^2) / sgm2^2)))

+ exp((-1.0 / (2.0 \* (1 - rou^2))) \* ((((x - mu1)^2) / (sgm1^2)) -

(2 \* rou \* (x - mu1) \* (y + mu2) / (sgm1 \* sgm2)) + (((y + mu2)^2) / sgm2^2))) +

exp((-1.0 / (2.0 \* (1 - rou^2))) \* ((((x + mu1)^2) / (sgm1^2)) - (2 \* rou \* (x + mu1) \* (y + mu2) /

(sgm1 \* sgm2)) + (((y + mu2)^2) / sgm2^2))))

}

*# generate pdf of folded normal*

z <- outer(x, y, f1)

*# generate the figure(s)*

png("figure/combined\_plot.png", width = 18, height = 8, units = "in", res = 300)

layout(matrix(c(1, 2), nrow = 1))

par(mgp = c(3, 2, 5))

persp(x, y, z, theta = 60, phi = 10, expand = 0.6, r = 180, ltheta = 0, shade = 0.5,

ticktype = "detailed", xlab = "Age", ylab = "Body Mass Index", zlab = "Density",

col = "lightblue", main = "", cex.axis = 1.25, cex.lab = 1.75)

par(mgp = c(3, 2, 5))

persp(kde\_estimation$x, kde\_estimation$y, kde\_estimation$z, theta = 60, phi = 10,

expand = 0.6, r = 180, ltheta = 0, shade = 0.5,

ticktype = "detailed", xlab = "Age", ylab = "Body Mass Index",

zlab = "Density", col = "lightgray", main = "", cex.axis = 1.25, cex.lab = 1.75)

dev.off()

Check the figures as follows:

* The left figure is the estimated density surface of the proposed MLE.
* The right figure is the estimated density surface of the kernel density estimation.

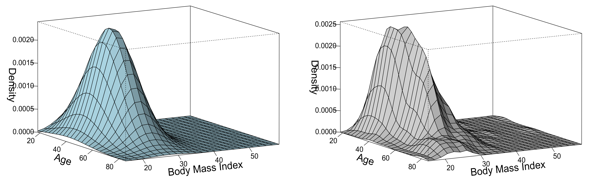


Figure 1 Density graphs of 2d folded normal. Left: MLE, Right: KDE

# **Notice**

⚠ **NOTE**: In utils.R, the loglik.G2() and loglik.G2cholesky() functions use the **global** varibale inputx, which stores the data in a matrix format. Therefore, the user should be careful when using these two functions. Especially, the user should make sure that: - the inputx is updated before calling these two functions; - parrallel computing does not work properly with these two functions, i.e. be sure to run the demo code in a sequential way.