logisticGP package vignette

Install R Package

```r
#devtools::install_github("Zmup2eSNntdt/logisticGP")
```

Load Library

```r
library(ddalpha)
```

```
## Loading required package: MASS

## Loading required package: class

## Loading required package: robustbase

## Warning: package 'robustbase' was built under R version 4.3.1

## Loading required package: sfsmisc

## Loading required package: geometry
```

```r
library(xgboost)
```

```
## Warning: package 'xgboost' was built under R version 4.3.1
```

```r
library(logisticGP)
library(ggpubr)
```

```
## Loading required package: ggplot2

## Warning: package 'ggplot2' was built under R version 4.3.1
```

```r
library(latex2exp)
library(gridExtra)
library(reshape2)
```

Introduction

This is an introduction to `logisticGP` package.

Given a response-covariate pair $(y, \mathbf{x}^{\mathrm{T}}) \in \mathbb{R} \times \mathbb{R}^p$, Conditional density estimation (CDE) aims to find the density function of y conditioned on the $\mathbf{x}^{\mathrm{T}}$ slice, denoted by $f(y \mid \mathbf{x}^{\mathrm{T}})$. In Bayesian paradigm, we assume prior knowledge on f and subsequently find posterior estimates of f given the data.

In [our article], we focus on developing a computationally tractable technique to model the conditional density using Logistic Gaussian Process (LGP) prior. The main idea behind this formulation is to use the triangular basis to approximate the Gaussian process (GP) using a pre-fixed regular grid, as discussed in Maatouk and Bay (2017). The logistic density transform was introduced by Leonard, 1978 and we utilize the foundation to model the conditional density of spatially varying response in the presence of a high dimensional covariate space.

Model

Let us denote $\mathcal{S} = \{1, 2, \dots, \mathrm{K}\}$ be the set of K locations which is assumed to be fixed throughout this article. Call $y_{is} \in (0,1), (i = 1, 2, \dots, n,\ \mathrm{s} \in \mathcal{S})$ denote the response (FA measurement) corresponding to i^{th} individual at the s^{th} location and $\mathbf{X}$ be a $n \times p$ design matrix where the i^{th} row $\mathbf{x}_i^{\mathrm{T}} = (x_{i1}, x_{i2}, \dots x_{ip})$ represent the covariate vector for the i^{th} individual. Furthermore, the rows of $\mathbf{X}$ are normalized such that $\max_{i \in \{1,2,\dots,n\}} \|\mathbf{x}_i^{\mathrm{T}}\|_2 = 1$, where $\|\cdot\|_2$ denote the ℓ_2-norm. Let $\beta(\mathrm{s})$ be the p–dimensional vector that varies spatially for each $\mathrm{s} \in \mathcal{S}$, such that $\|\beta(\mathrm{s})\|_2 = 1$. For any fixed $\mathrm{s} \in \mathcal{S}$, define the following map $\mathbf{x}_{\mathrm{o}} \to w_{\mathbf{x}_{\mathrm{o}},\mathrm{s}} := [\mathbf{x}_{\mathrm{o}}^{\mathrm{T}}\beta(\mathrm{s}) + 1]/2$. One can see that $w_{\mathbf{x}_{\mathrm{o}},\mathrm{s}} \in [0,1]$, which easily follows from $\left|x_{\mathrm{o}}^{\mathrm{T}}\beta(\mathrm{s})\right| \le \|x_{\mathrm{o}}^{\mathrm{T}}\|_2\|\beta(\mathrm{s})\|_2 \le 1$. Define $\Theta := \left\{(\xi, \tau, \beta) : \xi, \tau \in \mathbb{R}^{(\mathrm{N}+1)^2}, \beta \in \mathbb{R}^{p\mathrm{K}}\right\}$, given a covariate $(\mathbf{X} = \mathbf{x}_{\mathrm{o}}^{\mathrm{T}})$ and location $(\mathrm{S} = \mathrm{s})$, the conditional density of response (y) is modeled using

$$f_\theta(y \mid \mathbf{X} = \mathbf{x}_{\mathrm{o}}^{\mathrm{T}}, \mathrm{S} = \mathrm{s}) = \exp\left[g_1\left(y, w_{\mathbf{x}_{\mathrm{o}},\mathrm{s}}\right) + g_2(y, \mathrm{s}) - \Phi_\theta\left(\mathbf{x}_{\mathrm{o}}, \mathrm{s}\right)\right]$$

where, $\Phi_\theta\left(\mathbf{x}_{\mathrm{o}}, \mathrm{s}\right) = \log \int_0^1 \exp\left[g_1\left(y, w_{\mathbf{x}_{\mathrm{o}},\mathrm{s}}\right) + g_2(y, \mathrm{s})\right] dy$ and $g_1(\cdot),\ g_2(\cdot) : [0,1]^2 \to \mathbb{R}$ are unknown functions, such that $\{g_1(z_1, z_2) = \sum_{ij=0}^{\mathrm{N}} \xi_{ij} h_i(z_1) h_j(z_2)\}$ and $\{g_2(z_1, z_2) = \sum_{ij=0}^{\mathrm{N}} \tau_{ij} h_i(z_1) h_j(z_2)$ for any $(z_1, z_2) \in [0,1]^2\}$ and some $\xi, \tau \in \mathbb{R}^{(\mathrm{N}+1)^2}$.

Example

Data Generation and Initialization

```
n1 <- 200 ## number of individual
p1 <- 5 ## number of co-variates
K1 <- 20 ## number of locations

n2 <- 0.2 * n1 ## test set
RNGkind(sample.kind = "Rejection")
set.seed(403) ## setting seed
index.sample <- sample(1:n1,size=n2,replace = F) ## random indices for test set
## define beta0(s)
beta0_func <- function(j,x) {
  if(j==1)
    return(x^2+1) ## beta0_1(x)
  if(j==2)
    return((1-x)^2) ## beta0_2(x)
  if(j==3)
    return(4*x*(1-x)) ## beta0_3(x)
```

```
  if(j==4)
    return(-1 + 2*(x-0.75)^2) ## beta0_4(x)
  if(j==5)
    return(1.5 + 4*sin(x-0.5)) ## beta0_5(x)
  if(j==6)
    return(cos(x+2) + 0.25 * (x-0.5)^4 ) ## beta0_6(x)
  if(j==7)
    return(log(x+1)- 4*x^2) ## beta0_7(x)
  else
    return("wrong input")
}

beta0.true <- matrix(0,nr=p1,nc=K1) ## generate beta_0.true
for(j in 1:p1){
  beta0.true[j,] <- (matrix(beta0_func(j, seq(0,1,length.out = K1)),nr=1))
}

X1 <- matrix(runif(n1*p1,-5,5),nc=p1) ## generate covariates

## generate and normalize covariates
X1 <- apply(X1,MARGIN = 2,FUN = function(x)(x-mean(x)))
max_norm<- max(sqrt(rowSums(X1*X1)))
X2 <- X1/max_norm

## normalize beta_0.true
beta <- beta0.true
beta0.true <- t(t(beta)/sqrt(colSums(beta * beta)))

## generate y
W_0 <- (kronecker(diag(ncol(beta)),X2) %*% matrix(as.vector(beta0.true),nc=1) + 1)/2
W_1 <- 2*(W_0-0.5) #Centralize the probability
y_vec <- numeric(nrow(X2) * ncol(beta0.true))
y1 <- matrix(0,nr=n1,nc=K1)
for (j in 1:K1) {
  for(i in 1:n1){
    y_vec[(j-1)*nrow(X2) + i] <- ifelse(runif(1)<=1/(1+exp(W_1[(j-1)*nrow(X2) + i])),
                                        rbeta(1,10*exp((j/ncol(beta0.true)-0.5)/2),4*j^{3/4}),
                                        rbeta(1,32*sin(W_0[(j-1)*nrow(X2) + i]),
                                              8*(j/ncol(beta0.true) +1)^{1/2}))
  }
}
y1 <- matrix(y_vec,ncol = ncol(beta0.true))

## define test & train set
test_knots <- seq(0,1, length.out = 51) ## location of knots
Nplus <- length(test_knots) ## number of knots

# index.sample = n1 + 50 ## if want to train on the whole data

X = X_train <- X2[-index.sample,]
X_test <- X2[index.sample,]
y = y_train <- y1[-index.sample,]
y_test <- y1[index.sample,]
```

Initiate parameters

```
beta_Sigma <- 1*Sigma_kron(tau=0.10,rho=0.10,
                           K=ncol(y), p=ncol(X)) ## Variance-Covariace matrix of pi(beta)
Gamma1 <- Matern_cov(test_knots, nu= 2.5,
                     sigma = 1,theta = 0.292) ## Var-Cov matrix on \xi and \tau
CHOL1 <- t(chol(Gamma1))

xi <- matrix(CHOL1%*%rnorm(Nplus^2),nc=Nplus,byrow = T)
beta <- matrix(as.vector(mvtnorm::rmvnorm(1,mean = rep(0, ncol(X)*ncol(y)))),
               nc=ncol(y))
beta <- t(t(beta)/sqrt(colSums(beta * beta))) #normalize \beta
tau <- matrix(CHOL1%*%rnorm(Nplus^2),nc=Nplus,byrow = T)
h_loc <- hBasis(seq(0,(K1-1),by=1)/(K1-1),
                test_knots) # calculate the basis function
```

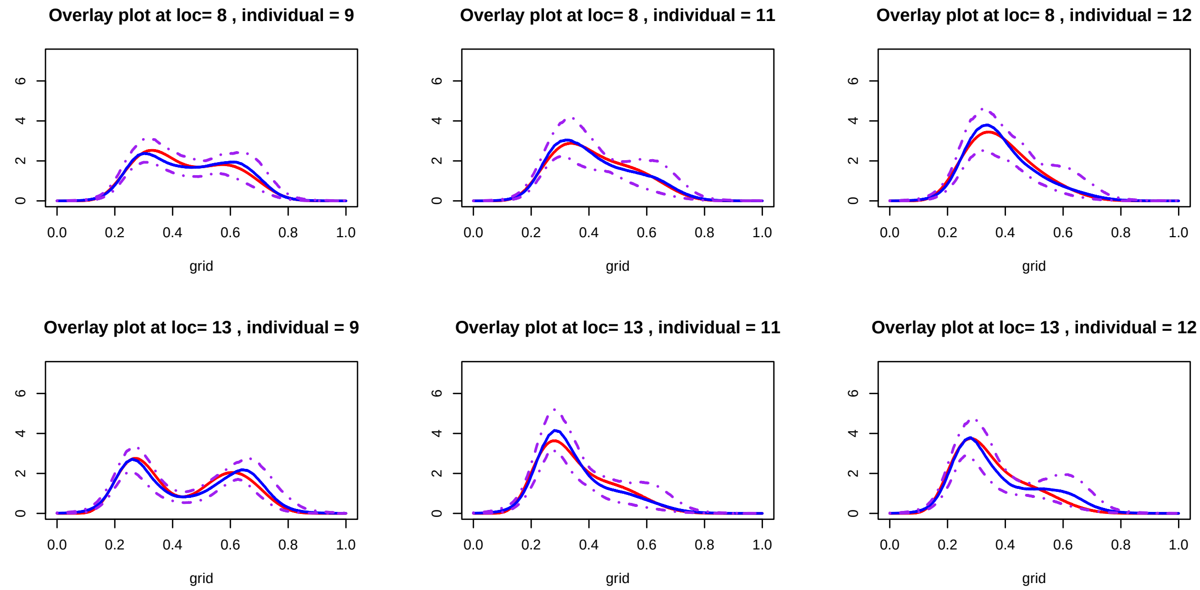
Get updates using MCMC sampler

```
nmcmc <- 10000 ## number of MCMC sample
burnin <- 10000## number of burnin sample
thining <- 10
run1<- get_updates(xi=xi,
                   beta = beta,
                   tau=tau,
                   CHOL1 = CHOL1,
                   h_loc = h_loc,
                   X = X,
                   y = y,
                   test_knots = test_knots,
                   verbose = F,
                   burnin = burnin,
                   nmcmc = nmcmc,
                   thining = thining)
## obtain the posterior samples
XI_mat <- run1$XI_mat.out
TAU_mat <- run1$TAU_mat.out
BETA_mat <- run1$BETA_mat.out
```

Plotting CDE

```
n <- nrow(X) #no. of individuals
K <- ncol(y) #no. of Location
p <- ncol(X) #no. of covariates

grid <- seq(0,1,length.out = 10001) ## setting up density domain
par(mfrow=c(2,3))
location.1 <- sort(sample(1:K,2,
                          replace = F)) ## spatial-locations where density required
density_mat <- matrix(0,nr=length(grid),
                      nc=length(location.1)) ## initiate matrix to store density
density_mat.true <- density_mat
ind.index <- c(9,11,12) ## Random individuals for plots
X_new <- matrix(X_test[ind.index,],nc=p) ## covariates of selected individuals
```

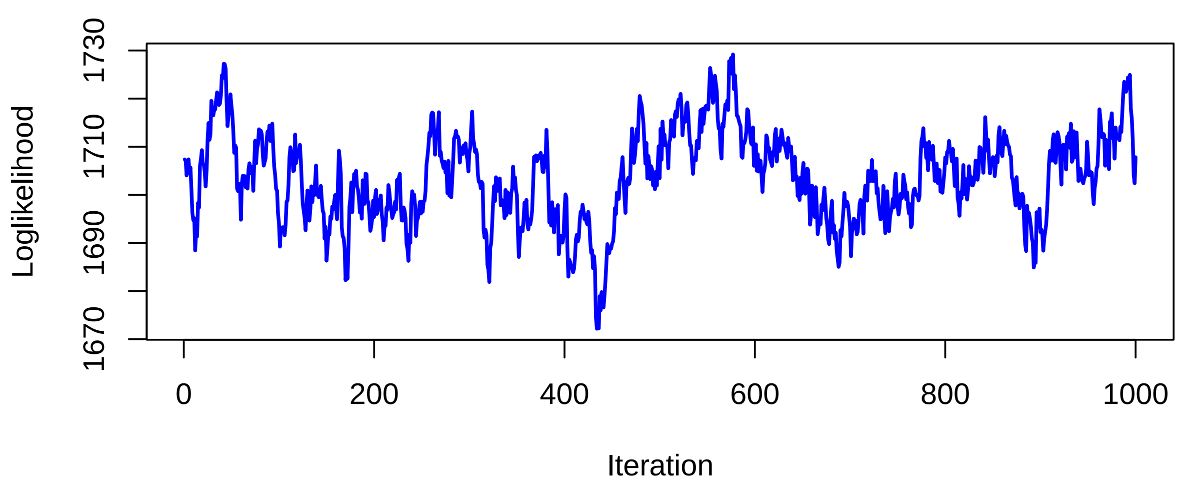
```
for(i in 1:length(location.1))
{
  beta0.true.1 <- beta0.true[,location.1[i]]
  a.vec <- as.numeric((X_new%*%beta0.true.1+1)/2)
  a1.vec <- (a.vec-0.5)*2
  density.array <- PostFun_loc(XI_mat, grid, X_new,
                               BETA_mat, TAU_mat, ## call Posterior density estimate
                              location = location.1[i],
                              test_knots = test_knots)
  for(j in 1:nrow(X_new)){
    a <- a.vec[j]
    a1 <- a1.vec[j]
    density.true <- dbeta(grid,
                          10*exp((location.1[i]/ncol(beta0.true) - 0.5)/2),
                          4*location.1[i]^{3/4})*1/(1+exp(a1)) +
      dbeta(grid,32*sin(a),
            8*(location.1[i]/ncol(beta0.true)+1)^{1/2})*1/(1+exp(-a1))

    density <- density.array[,,j]
    density_q2 <- apply(density,1,function(x) {quantile(x,0.50)}) ## estimated density
    density_q2 <- density_q2/sum(density_q2*(grid[2]-grid[1])) ## normalize density
    ## calculate quantiles at each grid position for density
    density_q1 <- apply(density,1,function(x) {quantile(x,0.025)})
    density_q3 <- apply(density,1,function(x) {quantile(x,0.975)})
    max_lim <- min(max(density.true,density_q2),10^3)
    min_lim <- min(density.true,density_q2)
    plot(grid, density.true,ylab = "",ylim= c(0, 7.3),
         type = "l",col="red",lwd=2,lty=1, ## plot true density
         main = paste("Overlay plot at loc=",
                      location.1[i],", individual =",ind.index[j]))
    lines(grid, density_q2,type = "l",
          col="blue",lwd=2,lty=1) ## plot estimated density
    lines(grid, density_q1,type = "l",
          col="purple",lwd=2,lty=4) ## plot quantiles
    lines(grid, density_q3,type = "l",
          col="purple",lwd=2,lty=4)
  }
}
```



Model Diagnostics

- Plot log-likelihood of the estimated density.

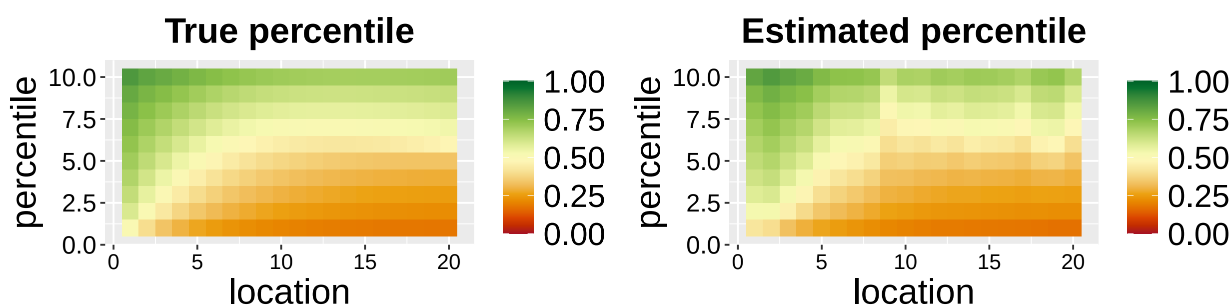
```
par(mfrow=c(1,1))
plot(run1$LOG_Like.out,type='l',col='blue',
     lwd=2,ylab='Loglikelihood',xlab='Iteration')
```



- Compare theoretical percentiles with estimated percentiles

```r
X_pred <- X_test[c(1,2),] ## Calculate percentile for individual #1 & #2
n <- nrow(X_pred)
Niter <- nmcmc/thining
Median_mat <- array(0,dim = c(n,K,Niter))
u <- seq(0.05,0.95,by=0.10) ## percentile
b <- rep(0,length(u))
x.grid <- seq(0,1,length.out = 100001)
Median_mat.loc <- array(0,dim = c(n,K,length(u)))
Median_mat.loc.th <- array(0,dim = c(n,K,length(u)))

for(j in 1: length(u)){
  for(i in 1:Niter){
    xi <- XI_mat[,,i]
    tau <- (TAU_mat[,,i])
    beta <- as.matrix(BETA_mat[, , i])
    Median_mat[,,i] <- get_quantile(xi = xi,tau = tau,
                                    beta = beta, ## calculate percentile
                                    test_knots = test_knots, #based on each posterior sample
                                    prob = u[j],X_pred = X_pred)
    #if(i%%100==0) print(c(i,j))
  }
  Median_mat.loc[,,j] <- apply(Median_mat,MARGIN = c(1,2), mean) ## find median (estimate) of percentile
}

##Calculate true percentiles

for (k in 1:n) {
  for(i in 1:K){
    beta0.true.1 <- beta0.true[,i]
    a <- as.numeric((X_pred[k,]%*%beta0.true.1 + 1)/2)
    a1 <- (a-0.5)*2
    A <- pbeta(x.grid,10*exp((i/K - 0.5)/2),4*i^{3/4})*1/(1+exp(a1)) +
      pbeta(x.grid,32*sin(a),8*(i/K+1)^{1/2})*1/(1+exp(-a1))

    for(j in 1:length(u)){b[j] <- (x.grid[min(which(A>u[j]))])}
    Median_mat.loc.th[k,i,] <- b
  }
  #print(k)
}

A <- melt(Median_mat.loc[1,,])
names(A) <- c('location','percentile','value')
B <- melt(Median_mat.loc.th[1,,])
names(B) <- c('location','percentile','value')
#A$percentile = B$percentile = u

My_Theme2 <-  theme(axis.text.x=element_text(size = 12,colour = "black"),
  axis.text.y = element_text(size = 14,colour = "black"),
  axis.title.y = element_text(size = 20),
  axis.title.x = element_text(size = 20),
  plot.title = element_text(size=20,hjust = 0.5, face="bold"),
  legend.title = element_blank(), legend.text = element_text(size = 18))

p11 <- ggplot(A, aes(x = location, y = percentile, fill = value)) +
  geom_tile() + scale_fill_gradientn(colors = hcl.colors(20, "RdYlGn"), limits=c(0,1)) +
  coord_fixed() +
  labs(title = 'Estimated percentile') +
  My_Theme2 +
```

```
  theme(plot.title = element_text(hjust=0.5))

p22 <- ggplot(B, aes(x = location, y = percentile, fill = value)) +
  geom_tile() +
  scale_fill_gradientn(colors = hcl.colors(20, "RdYlGn"), limits=c(0,1)) +
  coord_fixed() +
  labs(title = 'True percentile') +
  My_Theme2 +
  theme(plot.title = element_text(hjust=0.5))

gridExtra::grid.arrange(p22,p11,ncol=2)
```



Application to real Data

fitting the model

```
set.seed(1616)
Covariates <- read.table("Covariates.txt")
Response <- read.table("Response.txt")
X <- lapply(Covariates[2:214,], function(x) as.numeric(as.character(x)))
X <- matrix(unlist(X),nr=213)
y <- matrix(unlist(Response),nr=213)

max_norm<- max(sqrt(rowSums(X*X)))
X2 <- X/max_norm
y1 <- y
n1 <- nrow(X)
n2 <- 0.2 * n1 ## test set
RNGkind(sample.kind = "Rejection")
set.seed(12)
index.sample <- sample(1:n1,size=n2,replace = F)
X = X_train <- X2[-index.sample,]
```

```
X_test <- X2[index.sample,]
y = y_train <- y1[-index.sample,]
y_test <- y1[index.sample,]

test_knots <- seq(0,1, length.out = 51)
Nplus <- length(test_knots)
K1 <- ncol(y)

beta_Sigma <- 1*Sigma_kron(tau=0.10,rho=0.10, K=ncol(y), p=ncol(X))

Gamma1 <- Matern_cov(test_knots, nu= 2.5, sigma = 1,theta = 0.292)
CHOL1 <- t(chol(Gamma1))

xi <- matrix(CHOL1%*%rnorm(Nplus^2),nc=Nplus,byrow = T)

beta <- matrix(as.vector(mvtnorm::rmvnorm(1,mean = rep(0, ncol(X)*ncol(y)))),
               nc=ncol(y))
beta <- t(t(beta)/sqrt(colSums(beta * beta)))
tau <- matrix(CHOL1%*%rnorm(Nplus^2),nc=Nplus,byrow = T)

h_loc <- hBasis(seq(0,(K1-1),by=1)/(K1-1),test_knots)
```

Define MCMC parameters and get updates

```
nmcmc <- 5000
burnin <- 5000
thining <- 5
run1 <- readRDS("./real_data_analysis.RDS")
XI_mat <- run1$XI_mat.out
TAU_mat <- run1$TAU_mat.out
BETA_mat <- run1$BETA_mat.out
```

```
nmcmc <- 5000
burnin <- 5000
thining <- 5
run1<- get_updates(xi=xi,
                   beta = beta,
                   tau=tau,
                   CHOL1 = CHOL1,
                   h_loc=h_loc,
                   X=X2,
                   y=y1,
                   test_knots = test_knots,
                   verbose = F,
                   burnin = burnin,
                   nmcmc = nmcmc,
                   thining = thining)

XI_mat <- run1$XI_mat.out
TAU_mat <- run1$TAU_mat.out
BETA_mat <- run1$BETA_mat.out
```

plotting real data

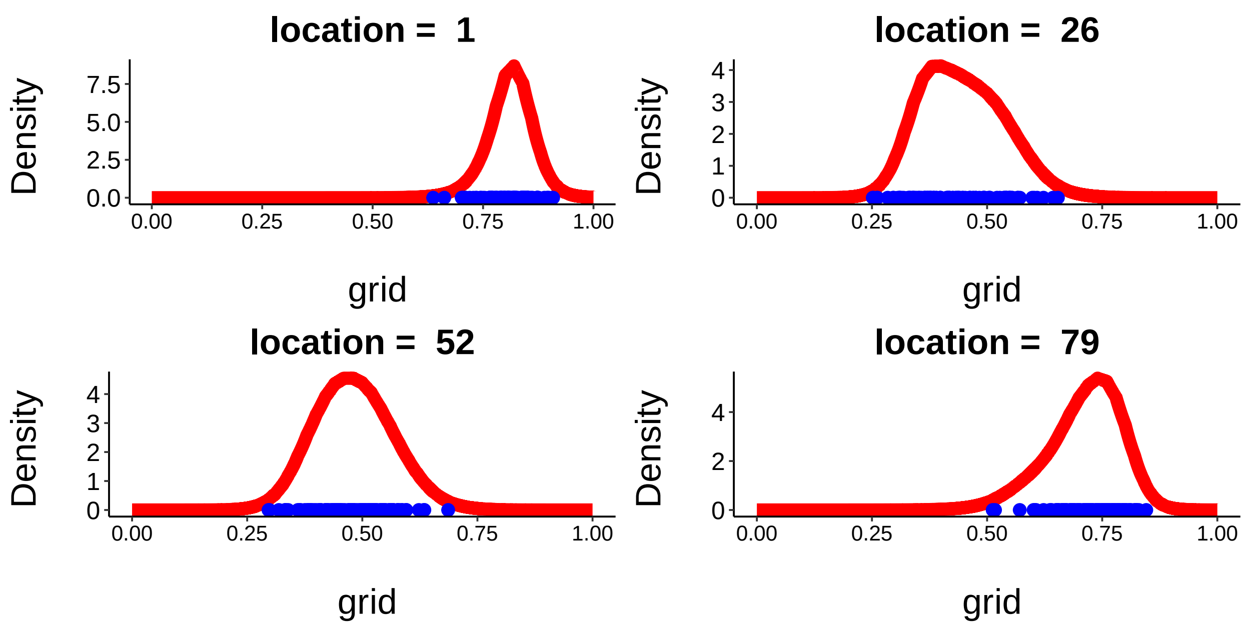
Fit the model.

```r
XI_mat <- run1$XI_mat.out[,,501:1000]
TAU_mat <- run1$TAU_mat.out[,,501:1000]
BETA_mat <- run1$BETA_mat.out[,,501:1000]

n <- nrow(X) #no. of individuals
K <- ncol(y) #no. of Location
p <- ncol(X) #no. of covariates

set.seed(738)
grid <- seq(0,1,length.out = 10001)
location.1 <- c(1,26,52,79)
density_mat <- matrix(0,nr=length(grid),nc=length(location.1))
density_mat.true <- density_mat
density_mat.NNKCDE <- density_mat
ind.index <- sort(sample(1:nrow(X2),100,replace = F))
X_new <- matrix(X2[ind.index,],nc=p)
for(i in 1:length(location.1))
{
  density.array<- PostFun_loc(XI_mat, grid, X_new, BETA_mat, TAU_mat,
                              location = location.1[i],
                              test_knots = test_knots)
  for(j in 1:nrow(X_new)){
    density <- density.array[,,j]
    density_q2 <- apply(density,1,function(x) {mean(x)})
    density_q2 <- density_q2/sum(density_q2*(grid[2]-grid[1]))
    density_mat[,i] <- density_mat[,i] + density_q2
    rm(density)
  }
  density_mat[,i] <- density_mat[,i]/nrow(X_new)
  rm(density.array)
}
```

Plot CDE for an individual.

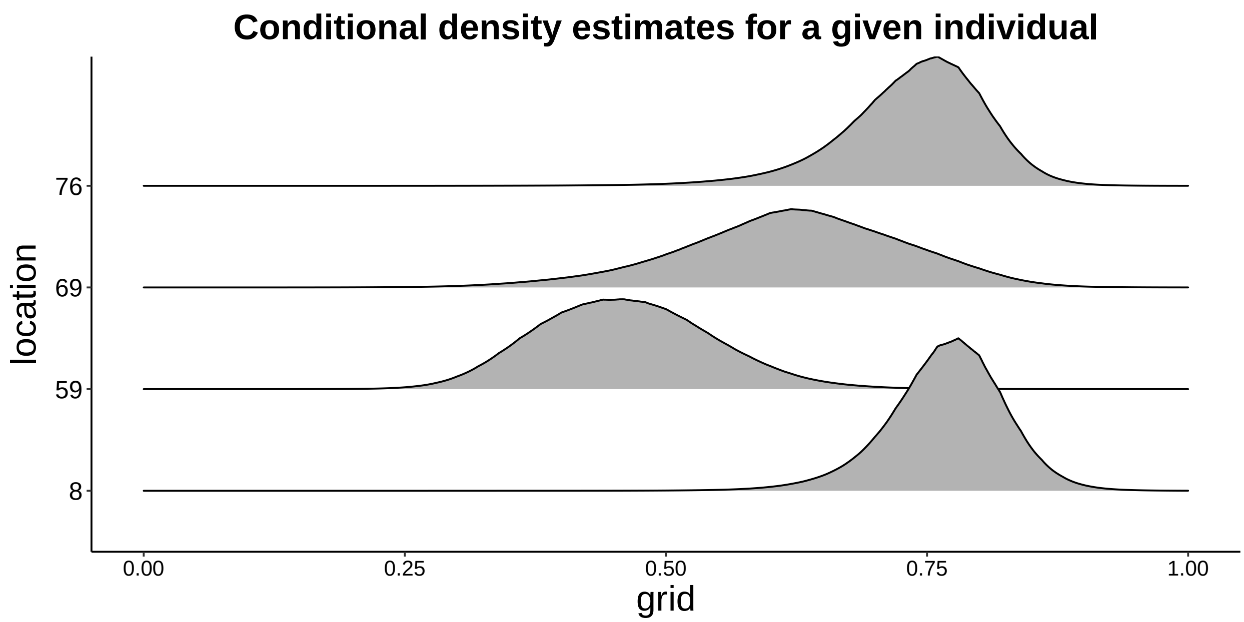
```r
My_Theme2 <-  theme(axis.text.x=element_text(size = 12,colour = "black"),
  axis.text.y = element_text(size = 14,colour = "black"),
  axis.title.y = element_text(size = 20),
  axis.title.x = element_text(size = 20),
  plot.title = element_text(size=20,hjust = 0.5, face="bold"),
  legend.title = element_blank(), legend.text = element_text(size = 18))

dat1 <- data.frame(grid,density_mat)
dat2 <- data.frame(y1[ind.index,location.1])


g1 <- ggplot(dat1,aes(x=grid,y=density_mat[,1])) +
  geom_line(lwd=3.5,col="red") + xlab("\n grid") + ylab("Density \n") +
  ggtitle(paste("location = ",location.1[1])) +
    theme_classic() +  My_Theme2 +
    geom_point(data = dat2, aes(x=y1[ind.index,location.1[1]],y=0),
               col="blue",size=3)

g2 <- ggplot(dat1,aes(x=grid,y=density_mat[,2])) +
  geom_line(lwd=3.5,col="red") + xlab("\n grid") + ylab("Density \n") +
  ggtitle(paste("location = ",location.1[2])) +
    theme_classic() +  My_Theme2 +
    geom_point(data = dat2, aes(x=y1[ind.index,location.1[2]],y=0),
               col="blue",size=3)
```

```r
g3 <- ggplot(dat1,aes(x=grid,y=density_mat[,3])) +
  geom_line(lwd=3.5,col="red") + xlab("\n grid") + ylab("Density \n") +
  ggtitle(paste("location = ",location.1[3])) +
    theme_classic() +  My_Theme2 +
    geom_point(data = dat2, aes(x=y1[ind.index,location.1[3]],y=0),
               col="blue",size=3)

g4 <- ggplot(dat1,aes(x=grid,y=density_mat[,4])) +
  geom_line(lwd=3.5,col="red") + xlab("\n grid") + ylab("Density \n") +
  ggtitle(paste("location = ",location.1[4])) +
    theme_classic() +  My_Theme2 +
    geom_point(data = dat2, aes(x=y1[ind.index,location.1[4]],y=0),
               col="blue",size=3)

ggarrange(g1,g2,g3,g4, ncol=2, nrow = 2)
```



Ridge plot for an individual at some randomly selected location

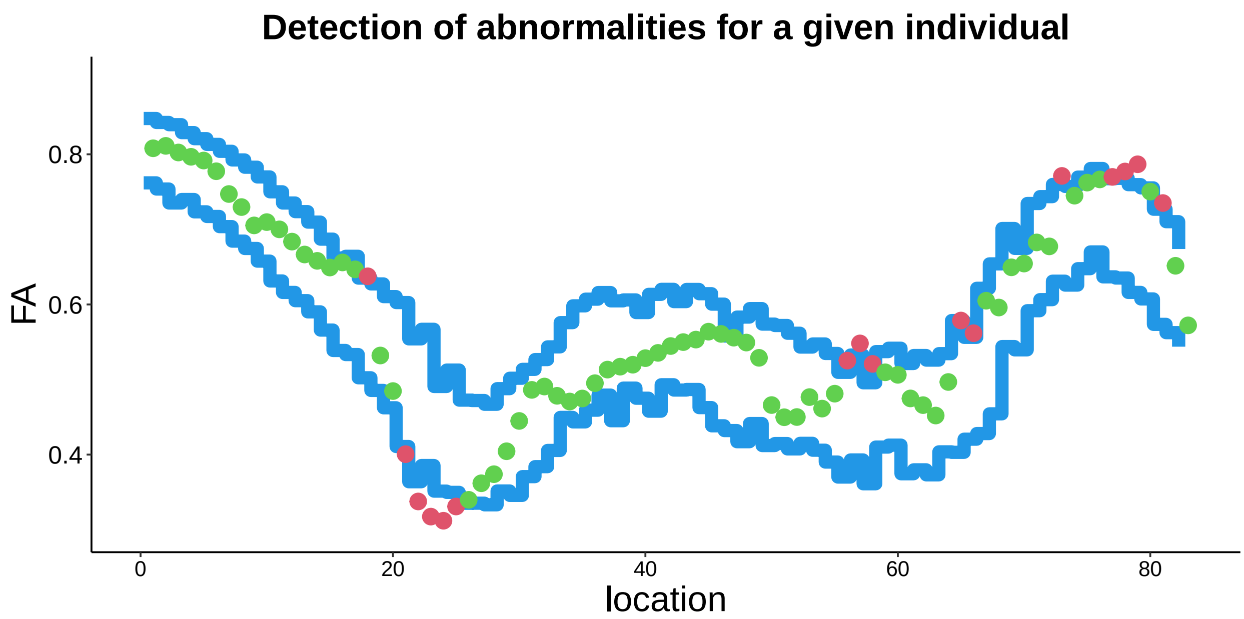
```r
source('density_ridge.R')

ggplot(data = density.df1, aes(x=grid, y=variable, height = value, group= variable)) +
  geom_density_ridges(stat = 'identity',scale=1.5) + theme_classic() + My_Theme2 +
  labs(title = 'Conditional density estimates for a given individual',
       y = 'location')
```



We plot 20^{th} and 80^{th} percentile for an individual at different locations and detect if there are observations outside the normal range.

```
source('conf_ind.R')
My_Theme2 <- theme(axis.text.x=element_text(size = 12,colour = "black"),
  axis.text.y = element_text(size = 14,colour = "black"),
  axis.title.y = element_text(size = 20),
  axis.title.x = element_text(size = 20),
  plot.title = element_text(size=20,hjust = 0.5, face="bold"),
  legend.title = element_blank(), legend.text = element_text(size = 18),
  legend.position = 'none')
ggplot(data.patient)+geom_step(aes(x=location-0.75,y=step1),size=3.5,col=4) +
  geom_step(aes(x=location-0.75,y=step2),size=3.5,col=4) + ylim(c(0.3,0.9)) +
  geom_point(aes(x=location,y=obs,col=col),size=4) +
  scale_color_manual(values = c(2,3)) +
  theme_classic() +
  My_Theme2 +
  labs(title = "Detection of abnormalities for a given individual",
       y=TeX('FA'),x='location')
```

```
## Warning: Using ‘size‘ aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use ‘linewidth‘ instead.
## This warning is displayed once every 8 hours.
## Call ‘lifecycle::last_lifecycle_warnings()‘ to see where this warning was
## generated.
```


Detection of abnormalities for a given individual
FA
0.8
0.6
0.4
0
20
40
60
80
location