Illustration

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2025-06-18

This R Markdown document includes the codes and figures in Section 2 and Section 3.

```
source("Scales.R")
source("Functions.R")
library(sensitivity)
library(cowplot)
library(ggplot2)
library(plotly)
```

Summary of Core Parameters

N— size of grid
M— the number of realization
x.sample— initial data.independent
y.sample— initial data.dependent
d— d-dimension of input variable
lb— lower bound - vector
ub— upper bound - vector
budget— the number of samples in GP experiment
n— the 1/2 number of samples in uniform exxperiment for sensitivity analysis
Sensitivity Analysis— Run Sobol' Analysis Using Saltelli's Scheme

```
N <- 1000
M <- 500
d <- 2
lb = c(-2, 0.8)
ub = c(2, 1.2)
n <- 1000
budget <- 100
```

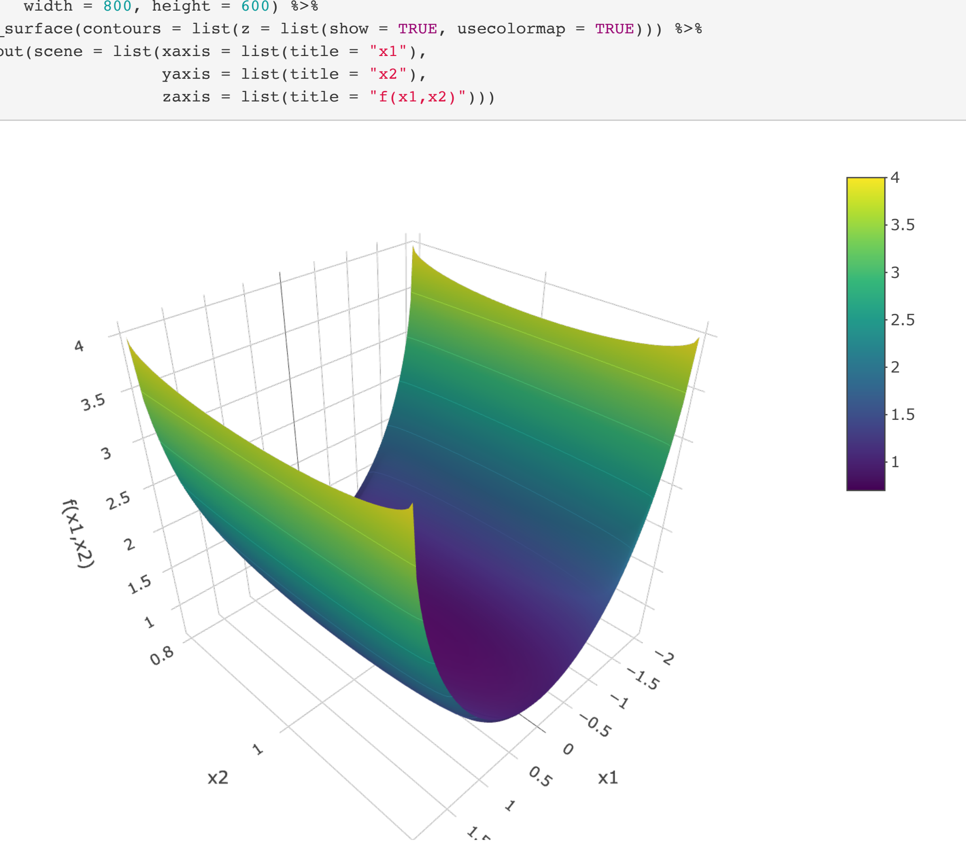
Function (Section 2)

$$y(x_1, x_2) = -0.3\sqrt{1-\frac{x_1^2}{4}} - 3\sqrt{1-\frac{(x_2-1)^2}{0.04}} + 4$$

```
quadratic_2D <- function(xx)
{
  x1 <- xx[1]
  x2 <- xx[2]

  y <- -sqrt(0.3^2 * (1 - x1^2/2^2)) - sqrt(1 - (x2 - 1)^2/0.2^2)*3 + 4

  return(y)
}
```

Plot Function (Figure 1(a) in Section 2)

```
x1_values <- seq(lb[1], ub[1], length.out = 100)
x2_values <- seq(lb[2], ub[2], length.out = 100)
grid <- expand.grid(x1 = x1_values, x2 = x2_values)
z_values <- numeric(nrow(grid))
for (i in 1:nrow(grid)) {
  tryCatch({
    z_values[i] <- quadratic_2D(c(grid$x1[i], grid$x2[i]))
  }, error = function(e) {
    z_values[i] <- NA
  }, warning = function(w) {
    z_values[i] <- NA
  })
}
grid$z <- z_values
grid <- grid[!is.na(grid$z), ]

plot_ly(x = x1_values, y = x2_values,
        z = matrix(grid$z, nrow = length(x1_values), byrow = FALSE),
        width = 800, height = 600) %>%
  add_surface(contours = list(z = list(show = TRUE, usecolormap = TRUE))) %>%
  layout(scene = list(xaxis = list(title = "x1"),
                      yaxis = list(title = "x2"),
                      zaxis = list(title = "f(x1,x2)")))
```



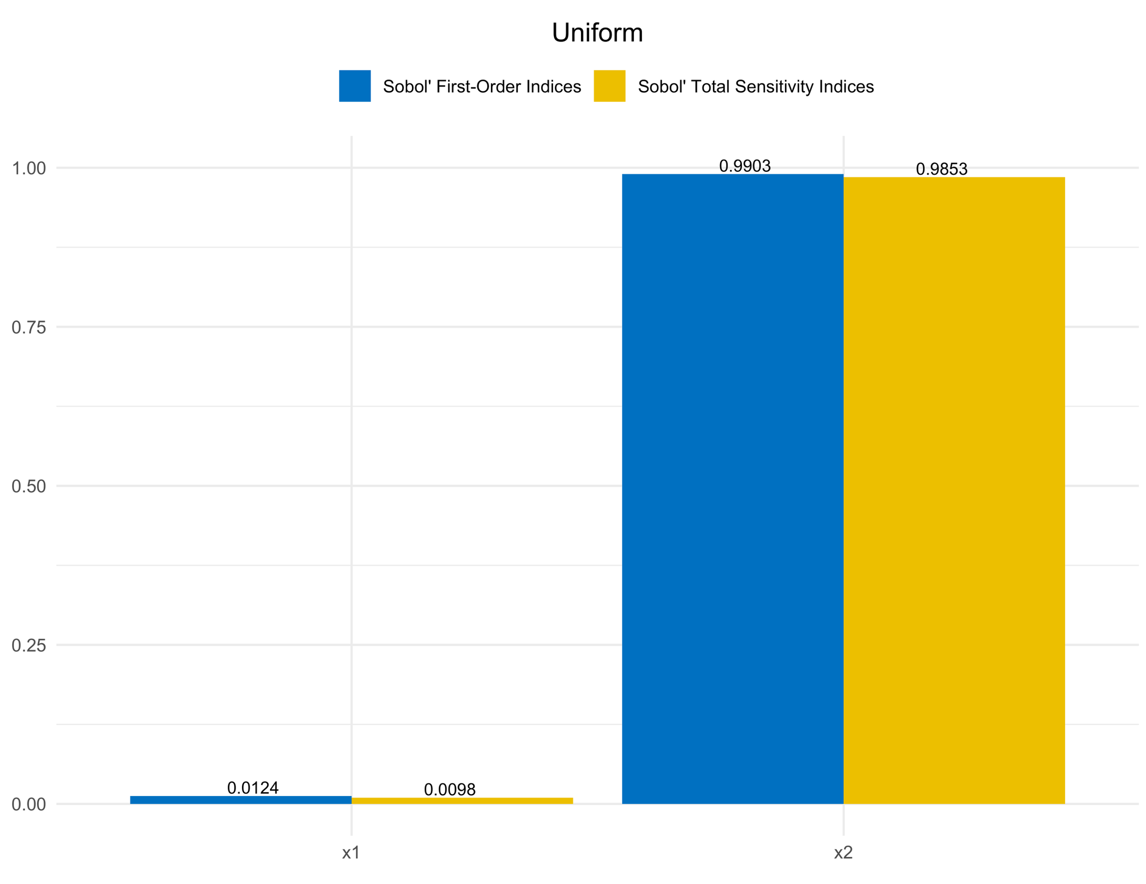
Sensativity Analysis

Uniform Experiment (Section 3)

```
set.seed(123)
X1 <- data.frame(x1 = runif(n, 0, 1), x2 = runif(n, 0, 1))
X1 <- scale_to_org(X1, lb, ub)

X2 <- data.frame(x1 = runif(n, 0, 1), x2 = runif(n, 0, 1))
X2 <- scale_to_org(X2, lb, ub)

sobol_result <- sobolSalt(model = NULL, X1, X2, scheme="A", nboot = 100)
sobol_result <- tell(sobol_result, y = apply(sobol_result$X, 1, quadratic_2D))
```

Plot Sensativity Analysis Result for Uniform Experiment (Figure 2(a) in Section 3)

```
ss_effects <- c(sobol_result$S$original, sobol_result$T$original)
sens <- data.frame(X=rep(c('x1','x2'), 2), value = ss_effects,
                   group = rep(c("Sobol' First-Order Indices",
                                 "Sobol' Total Sensitivity Indices"), each=2))

p_uniform <- ggplot(sens, aes(x = X, y = value)) +
  geom_col(aes(fill = group), position = "dodge") +
  geom_text(aes(label = sprintf("%.4f", value)), position = position_dodge2(width = 0.8),
            vjust = -0.2, size = 3) +
  geom_point(data = subset(sens, group == "First"),
             position = position_dodge(width = 0.8), size = 4) +
  geom_point(data = subset(sens, group == "Total"),
             position = position_dodge(width = 0.8), size = 4) +
  scale_color_manual(values = c("#0073C2FF", "#EFC000FF"), name = " ") +
  scale_fill_manual(values = c("#0073C2FF", "#EFC000FF"), name = " ") +
  scale_y_continuous(limits = c(0, 1)) +
  labs(title = "Uniform", x=NULL, y=NULL) +
  theme_minimal() +
  theme(plot.title = element_text(hjust = 0.5),
        legend.position = "top",
        axis.text = element_text(size = 9))
print(p_uniform)
```



Decision Uncertainty Experiment (Section 3)

```
set.seed(321)
x.sample <- randomLHS(budget, d)
x.sample <- scale_to_org(x.sample, lb, ub)
y.sample <- apply(x.sample, 1, quadratic_2D)
result_gp <- gp_opts_unconstraint(x.sample, y.sample, lb, ub, N, M, d)
```

```
##
## optimisation start
## ------------------
## * estimation method   : MLE
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~1
## * covariance model :
##   - type :  matern5_2
##   - nugget : 1.490116e-08
##   - parameters lower bounds :  1e-10 1e-10
##   - parameters upper bounds :  1.982623 1.979489
##   - variance bounds :  0.04594482 5.930558
##   - best initial criterion value(s) :  167.4151
##
## N = 3, M = 5 machine precision = 2.22045e-16
## At X0, 0 variables are exactly at the bounds
## At iterate     0  f=      -167.42  |proj g|=       5.5957
## At iterate     1  f =      -189.82  |proj g|=        1.7759
## At iterate     2  f =      -196.91  |proj g|=        5.1143
## At iterate     3  f =      -198.31  |proj g|=        5.0535
## At iterate     4  f =       -198.8  |proj g|=        5.0079
## At iterate     5  f =      -200.53  |proj g|=        4.8256
## At iterate     6  f =      -203.04  |proj g|=        4.5687
## At iterate     7  f =      -208.33  |proj g|=        4.0833
## At iterate     8  f =       -215.9  |proj g|=        3.3708
## At iterate     9  f =      -220.53  |proj g|=        2.4913
## At iterate    10  f =      -221.29  |proj g|=        1.6394
## At iterate    11  f =      -223.66  |proj g|=        1.8261
## At iterate    12  f =       -225.7  |proj g|=        1.9481
## At iterate    13  f =      -226.14  |proj g|=        1.8848
## At iterate    14  f =      -226.28  |proj g|=       0.28398
## At iterate    15  f =      -226.28  |proj g|=       0.12597
## At iterate    16  f =      -226.28  |proj g|=      0.072816
## At iterate    17  f =      -226.28  |proj g|=    0.00019726
## At iterate    18  f =      -226.28  |proj g|=    1.9616e-06
##
## iterations 18
## function evaluations 22
## segments explored during Cauchy searches 20
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 1
## norm of the final projected gradient 1.96164e-06
## final function value -226.277
##
## F = -226.277
## final  value -226.276511
## converged
```

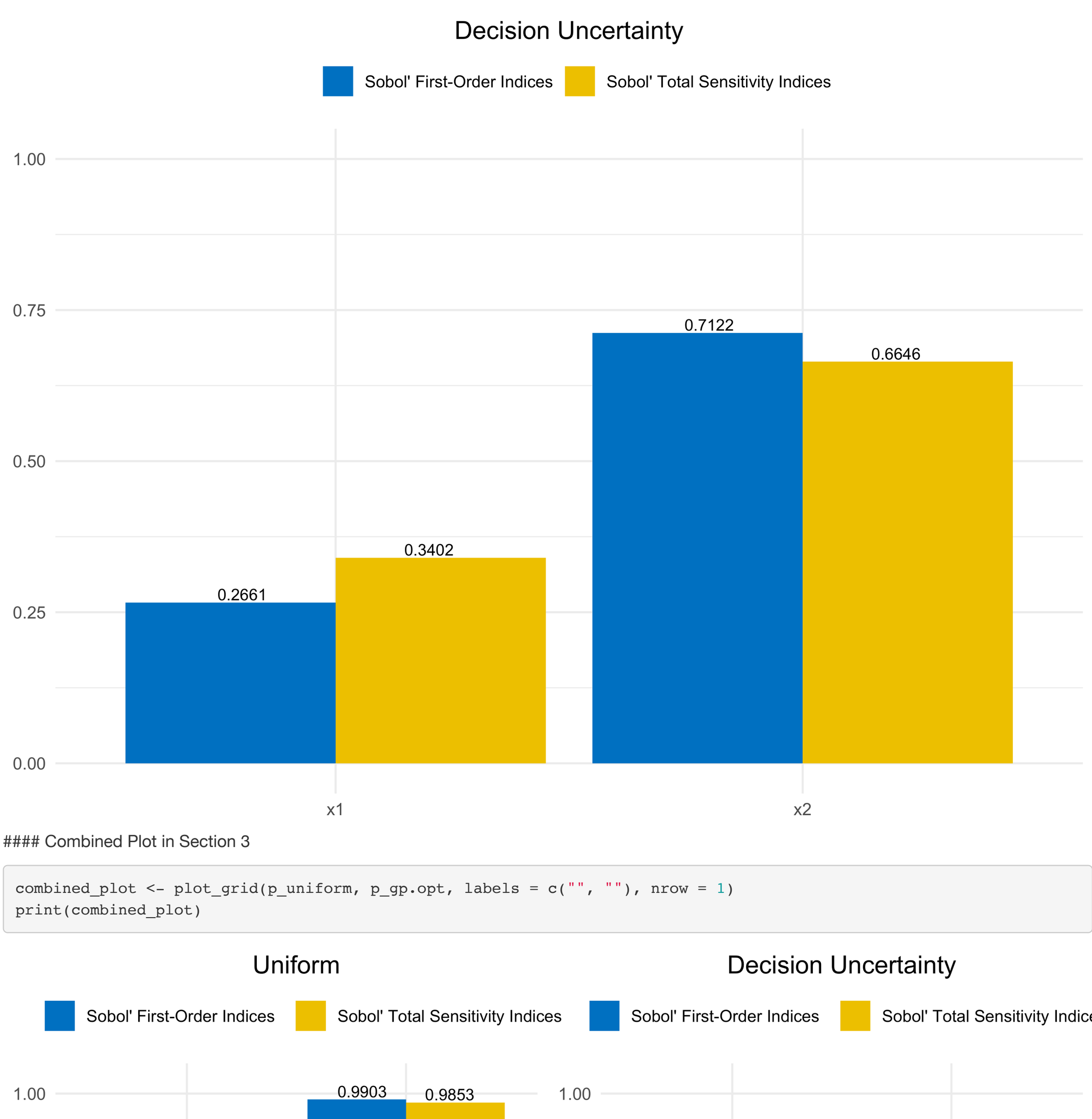
```
x_gp <- result_gp[[2]]
y_gp <- result_gp[[3]]
surrogate_y <- function(X){result_gp$gpm_y(X)$mean}

gp_mean <- gp_opt_mean_unconstraint(x.sample, y.sample, lb, ub, d)
```

```
##
## optimisation start
## ------------------
## * estimation method   : MLE
## * optimisation method : BFGS
## * analytical gradient : used
## * trend model : ~1
## * covariance model :
##   - type :  matern5_2
##   - nugget : 1.490116e-08
##   - parameters lower bounds :  1e-10 1e-10
##   - parameters upper bounds :  1.982623 1.979489
##   - variance bounds :  0.04594482 5.930558
##   - best initial criterion value(s) :  144.8808
##
## N = 3, M = 5 machine precision = 2.22045e-16
## At X0, 0 variables are exactly at the bounds
## At iterate     0  f=      -144.88  |proj g|=       5.2228
## At iterate     1  f =       -183.9  |proj g|=        1.6959
## At iterate     2  f =      -197.85  |proj g|=        1.8862
## At iterate     3  f =      -210.07  |proj g|=        3.1596
## At iterate     4  f =      -213.52  |proj g|=        2.9805
## At iterate     5  f =      -222.38  |proj g|=        1.9313
## At iterate     6  f =       -223.3  |proj g|=        1.8073
## At iterate     7  f =      -224.16  |proj g|=        1.8668
## At iterate     8  f =      -225.64  |proj g|=        1.9425
## At iterate     9  f =      -226.14  |proj g|=        1.8852
## At iterate    10  f =      -226.27  |proj g|=        1.5964
## At iterate    11  f =      -226.28  |proj g|=      0.062273
## At iterate    12  f =      -226.28  |proj g|=    0.00042146
## At iterate    13  f =      -226.28  |proj g|=    5.9556e-06
##
## iterations 13
## function evaluations 15
## segments explored during Cauchy searches 15
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 1
## norm of the final projected gradient 5.95563e-06
## final function value -226.277
##
## F = -226.277
## final  value -226.276511
## converged
```

```
gp_mean_y <- surrogate_y(matrix(gp_mean, nrow = 1))

X1 <- x_gp[1:(M/2), ]
X2 <- x_gp[(M/2+1):M, ]
sobol_result_gp <- sobolSalt(model = surrogate_y, X1, X2, scheme="A", nboot = 100)
```

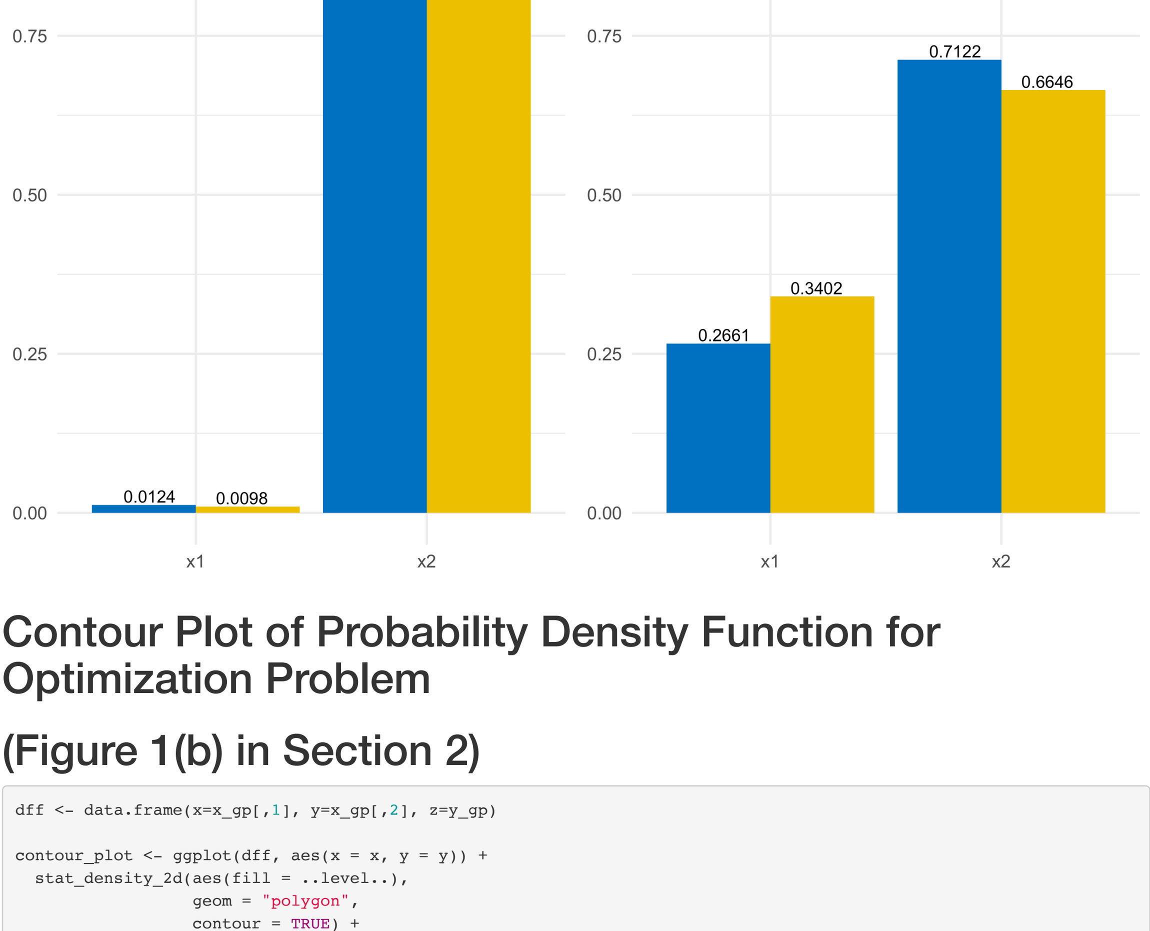
Plot Sensativity Analysis Result for Decision Uncertainty Experiment (Figure 2(b) in Section 3)

```
ss_effects_gp <- c(sobol_result_gp$S$original, sobol_result_gp$T$original)
sens_gp <- data.frame(X=rep(c('x1','x2'), 2), value = ss_effects_gp,
                      group = rep(c("Sobol' First-Order Indices",
                                    "Sobol' Total Sensitivity Indices"), each=2))

p_gp.opt <- ggplot(sens_gp, aes(x = X, y = value)) +
  geom_col(aes(fill = group), position = "dodge") +
  geom_text(aes(label = sprintf("%.4f", value)), position = position_dodge2(width = 0.8),
            vjust = -0.2, size = 3) +
  geom_point(data = subset(sens_gp, group == "First"),
             position = position_dodge(width = 0.8), size = 4) +
  geom_point(data = subset(sens_gp, group == "Total"),
             position = position_dodge(width = 0.8), size = 4) +
  scale_color_manual(values = c("#0073C2FF", "#EFC000FF"), name = " ") +
  scale_fill_manual(values = c("#0073C2FF", "#EFC000FF"), name = " ") +
  scale_y_continuous(limits = c(0, 1)) +
  labs(title = "Decision Uncertainty", x=NULL, y=NULL) +
  theme_minimal() +
  theme(plot.title = element_text(hjust = 0.5),
        legend.position = "top",
        legend.title = element_text(size = 8),
        axis.text = element_text(size = 9))
print(p_gp.opt)
```



Combined Plot in Section 3

```
combined_plot <- plot_grid(p_uniform, p_gp.opt, labels = c("", ""), nrow = 1)
print(combined_plot)
```



Contour Plot of Probability Density Function for Optimization Problem

(Figure 1(b) in Section 2)

```
dff <- data.frame(x=x_gp[,1], y=x_gp[,2], z=y_gp)

contour_plot <- ggplot(dff, aes(x = x, y = y)) +
  stat_density_2d(aes(fill = ..level..),
                  geom = "polygon",
                  contour = TRUE) +
  scale_fill_viridis_c(option = "viridis", direction = -1) +
  theme_minimal() +
  labs(x = "X1", y = "X2")

print(contour_plot)
```