CaseStudy

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This R Markdown document includes the codes and figures in Section 4.

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

Summary of Core Parameters

N— size of grid
M— the number of realization
x.sample— initial input data
y.sample— initial output data
g.sample— initial constraint data
d— d-dimension of input variable
lb— lower bound - vector
ub— upper bound - vector
g_constraint— constraint threshold
Sensitivity Analysis— Run Sobol' Analysis Using Saltelli's Scheme

```
lb <- c(125, 150, 600, 7200)
ub <- c(180, 180, 6600, 12000)
eps <- sqrt(.Machine$double.eps)
g_constraint <- 0.96
d <- 4
initial_sample_size <- 50
N <- 500
M <- 10000
```

Load Cure Process Data

```
load("Q22.Rdata")
x.sample <-Q22[,1:4]
y.sample <- Q22[,5]
g.sample <- Q22[,6]
```

Decision Uncertainty Experiment: Optimal Decision Uncertainty & Sensativity Analysis (Section 4)

```
set.seed(123)
result_gp <- gp_opts_constraint(x.sample, y.sample, g.sample, g_constraint, 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 1e-10 1e-10
##   - parameters upper bounds :  1.890909 1.933333 1.953333 1.891667
##   - variance bounds :  0.03166104 5.123977
##   - best initial criterion value(s) :  67.8006
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At X0, 0 variables are exactly at the bounds
## At iterate     0  f=      -67.801  |proj g|=       4.8157
## At iterate     1  f =      -79.666  |proj g|=        1.3889
## At iterate     2  f =      -80.238  |proj g|=        1.3741
## At iterate     3  f =       -81.11  |proj g|=        3.5765
## At iterate     4  f =        -81.4  |proj g|=        1.5847
## At iterate     5  f =      -81.986  |proj g|=        1.5424
## At iterate     6  f =      -82.299  |proj g|=        1.5037
## At iterate     7  f =      -83.257  |proj g|=        4.8287
## At iterate     8  f =      -83.386  |proj g|=        1.4822
## At iterate     9  f =       -83.52  |proj g|=       0.55005
## At iterate    10  f =      -83.522  |proj g|=       0.13967
## At iterate    11  f =      -83.523  |proj g|=       0.17992
## At iterate    12  f =      -83.523  |proj g|=       0.08929
## At iterate    13  f =      -83.523  |proj g|=      0.083954
## At iterate    14  f =      -83.523  |proj g|=      0.015509
## At iterate    15  f =      -83.523  |proj g|=    0.00081121
## At iterate    16  f =      -83.523  |proj g|=    0.00017932
##
## iterations 16
## function evaluations 20
## segments explored during Cauchy searches 20
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 1
## norm of the final projected gradient 0.000179315
## final function value -83.5232
##
## F = -83.5232
## final  value -83.523162
## converged
##
## 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 1e-10 1e-10
##   - parameters upper bounds :  1.890909 1.933333 1.953333 1.891667
##   - variance bounds :  3.054316e-05 0.00587365
##   - best initial criterion value(s) :  209.7215
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At X0, 0 variables are exactly at the bounds
## At iterate     0  f=      -209.72  |proj g|=       1.6862
## At iterate     1  f =       -216.9  |proj g|=        1.6767
## At iterate     2  f =      -219.25  |proj g|=        1.6652
## At iterate     3  f =      -221.61  |proj g|=        1.6609
## At iterate     4  f =      -221.83  |proj g|=        1.6617
## At iterate     5  f =      -221.86  |proj g|=        1.6639
## At iterate     6  f =      -221.91  |proj g|=        1.6698
## At iterate     7  f =      -221.95  |proj g|=        1.6766
## At iterate     8  f =      -221.95  |proj g|=         1.677
## At iterate     9  f =      -221.95  |proj g|=         1.677
## At iterate    10  f =      -221.95  |proj g|=        1.6771
## At iterate    11  f =      -221.96  |proj g|=        1.6771
## At iterate    12  f =      -221.96  |proj g|=         1.677
## At iterate    13  f =      -221.98  |proj g|=        1.6765
## At iterate    14  f =      -222.03  |proj g|=        1.6749
## At iterate    15  f =      -222.14  |proj g|=        1.6706
## At iterate    16  f =       -222.4  |proj g|=        1.6604
## At iterate    17  f =      -222.93  |proj g|=        1.6401
## At iterate    18  f =      -224.11  |proj g|=        1.6056
## At iterate    19  f =      -225.33  |proj g|=        1.5847
## At iterate    20  f =      -225.65  |proj g|=         1.543
## At iterate    21  f =      -225.73  |proj g|=        1.5502
## At iterate    22  f =      -225.75  |proj g|=       0.90517
## At iterate    23  f =      -225.84  |proj g|=       0.88894
## At iterate    24  f =      -225.95  |proj g|=       0.87733
## At iterate    25  f =      -225.95  |proj g|=       0.87458
## At iterate    26  f =      -226.01  |proj g|=       0.88388
## At iterate    27  f =      -226.01  |proj g|=       0.88851
## At iterate    28  f =      -226.03  |proj g|=       0.89157
## At iterate    29  f =      -226.04  |proj g|=       0.88973
## At iterate    30  f =      -226.05  |proj g|=       0.88551
## At iterate    31  f =      -226.05  |proj g|=       0.88626
## At iterate    32  f =      -226.06  |proj g|=       0.87971
## At iterate    33  f =      -226.06  |proj g|=       0.88081
## At iterate    34  f =      -226.07  |proj g|=       0.87088
## At iterate    35  f =      -226.23  |proj g|=       0.82594
## At iterate    36  f =       -228.4  |proj g|=        1.6078
## At iterate    37  f =      -228.43  |proj g|=        1.6069
## At iterate    38  f =      -230.22  |proj g|=        1.6277
## At iterate    39  f =      -230.23  |proj g|=        1.6277
## At iterate    40  f =      -230.78  |proj g|=       0.45868
## At iterate    41  f =      -230.98  |proj g|=       0.68333
## At iterate    42  f =      -230.98  |proj g|=       0.45757
## At iterate    43  f =      -230.98  |proj g|=       0.45756
## At iterate    44  f =      -230.98  |proj g|=       0.45756
## At iterate    45  f =      -230.98  |proj g|=       0.45756
##
## iterations 45
## function evaluations 62
## segments explored during Cauchy searches 50
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 2
## norm of the final projected gradient 0.457563
## final function value -230.978
##
## F = -230.978
## final  value -230.977767
## converged
```

```
x_gp <- result_gp$gp.xhat
y_gp <- result_gp$gp.yhat
g_gp <- result_gp$gp.ghat
surrogate_y <- function(X){result_gp$gpm_y(X)$mean}
surrogate_g <- function(X){result_gp$gpm_g(X)$mean}

opt_mean <- gp_opt_mean_constraint(x.sample, y.sample, g.sample, g_constraint, lb, ub)
```

```
##
## 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 1e-10 1e-10
##   - parameters upper bounds :  1.890909 1.933333 1.953333 1.891667
##   - variance bounds :  0.03166104 5.123977
##   - best initial criterion value(s) :  76.92061
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At X0, 0 variables are exactly at the bounds
## At iterate     0  f=      -76.921  |proj g|=       4.8639
## At iterate     1  f =      -77.459  |proj g|=        1.4192
## At iterate     2  f =      -78.207  |proj g|=         1.395
## At iterate     3  f =      -79.496  |proj g|=         4.726
## At iterate     4  f =      -80.088  |proj g|=        4.6934
## At iterate     5  f =      -82.406  |proj g|=        1.3621
## At iterate     6  f =      -83.158  |proj g|=        1.4797
## At iterate     7  f =       -83.33  |proj g|=         1.457
## At iterate     8  f =      -83.424  |proj g|=        1.2689
## At iterate     9  f =      -83.452  |proj g|=        1.3648
## At iterate    10  f =       -83.49  |proj g|=        1.3436
## At iterate    11  f =      -83.523  |proj g|=        0.3711
## At iterate    12  f =      -83.523  |proj g|=       0.11971
## At iterate    13  f =      -83.523  |proj g|=      0.019497
## At iterate    14  f =      -83.523  |proj g|=      0.018109
##
## iterations 14
## function evaluations 18
## segments explored during Cauchy searches 18
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 1
## norm of the final projected gradient 0.0181093
## final function value -83.5232
##
## F = -83.5232
## final  value -83.523161
## converged
##
## 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 1e-10 1e-10
##   - parameters upper bounds :  1.890909 1.933333 1.953333 1.891667
##   - variance bounds :  3.054316e-05 0.00587365
##   - best initial criterion value(s) :  216.0585
##
## N = 5, M = 5 machine precision = 2.22045e-16
## At X0, 0 variables are exactly at the bounds
## At iterate     0  f=      -216.06  |proj g|=       1.7357
## At iterate     1  f =      -224.11  |proj g|=         1.446
## At iterate     2  f =      -225.51  |proj g|=        0.8018
## At iterate     3  f =      -225.64  |proj g|=       0.81554
## At iterate     4  f =      -225.69  |proj g|=       0.83361
## At iterate     5  f =      -225.69  |proj g|=        1.1663
## At iterate     6  f =       -225.7  |proj g|=       0.82966
## At iterate     7  f =       -225.7  |proj g|=       0.83073
## At iterate     8  f =       -225.7  |proj g|=       0.83056
## At iterate     9  f =      -225.71  |proj g|=       0.82893
## At iterate    10  f =      -225.72  |proj g|=       0.82452
## At iterate    11  f =      -225.74  |proj g|=        1.4608
## At iterate    12  f =       -225.8  |proj g|=        1.4623
## At iterate    13  f =      -227.07  |proj g|=        1.4825
## At iterate    14  f =      -227.27  |proj g|=        1.5297
## At iterate    15  f =      -229.67  |proj g|=        1.4881
## At iterate    16  f =      -230.05  |proj g|=       0.62612
## At iterate    17  f =      -230.05  |proj g|=       0.87658
## At iterate    18  f =      -230.06  |proj g|=        1.3249
## At iterate    19  f =      -230.09  |proj g|=        1.4858
## At iterate    20  f =      -230.16  |proj g|=        1.4808
## At iterate    21  f =      -230.26  |proj g|=         1.472
## At iterate    22  f =      -230.38  |proj g|=        1.5808
## At iterate    23  f =      -230.44  |proj g|=        0.8629
## At iterate    24  f =      -230.44  |proj g|=        1.2415
## At iterate    25  f =      -230.44  |proj g|=        1.1408
## At iterate    26  f =      -230.44  |proj g|=        1.1367
##
## iterations 26
## function evaluations 35
## segments explored during Cauchy searches 32
## BFGS updates skipped 0
## active bounds at final generalized Cauchy point 1
## norm of the final projected gradient 1.13672
## final function value -230.441
##
## F = -230.441
## final  value -230.440696
## converged
```

```
opt_true_A <- c(opt_mean[3]/60,opt_mean[1])
opt_true_B <- c(opt_mean[4]/60,opt_mean[2])
```

Plot Optimal Decision Uncertainty (Figure 4 in Section 4)

```
aa=rbind(cbind(x_gp[ ,2], x_gp[ ,4]/60), cbind(x_gp[,1], x_gp[,3]/60))
df_plot <- data.frame(Time=aa[,2], Temperature=aa[,1])

custom_breaks <- c(0, 0.00005, 0.0001, 0.00015, 0.0002, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1)
ggplot(df_plot, aes(x = Time, y = Temperature)) +
  geom_density_2d_filled(aes(fill = ..level..), breaks = custom_breaks) +
  scale_fill_brewer(palette = "PuBu", name = "Density Level") +
  geom_point(aes(x = opt_true_A[1], y = opt_true_A[2]), color = "red", size = 2.5) +
  geom_point(aes(x = opt_true_B[1], y = opt_true_B[2]), color = "red", size = 2.5) +
  geom_segment(aes(x = 7.5, y = 140, xend = opt_true_A[1], yend = opt_true_A[2]), color = "red") +
  geom_segment(aes(x = opt_true_A[1], y = opt_true_A[2], xend = opt_true_B[1], yend = opt_true_B[2]), color = "re
d") +
  geom_segment(aes(x = opt_true_B[1], y = opt_true_B[2], xend = 200.385, yend = 140), color = "red") +
  ylim(140, 185) +
  xlim(0, 205) +
  theme_minimal() +
  theme(
    axis.title.x = element_text(size = 14),
    axis.title.y = element_text(size = 14),
    axis.text.x = element_text(size = 12),
    axis.text.y = element_text(size = 12),
    plot.margin = unit(c(0.5, 3, 0.5, 3), "cm")
  ) +
  labs(x = "Time", y = "Temperature")
```

Compute Sensitivity Scores

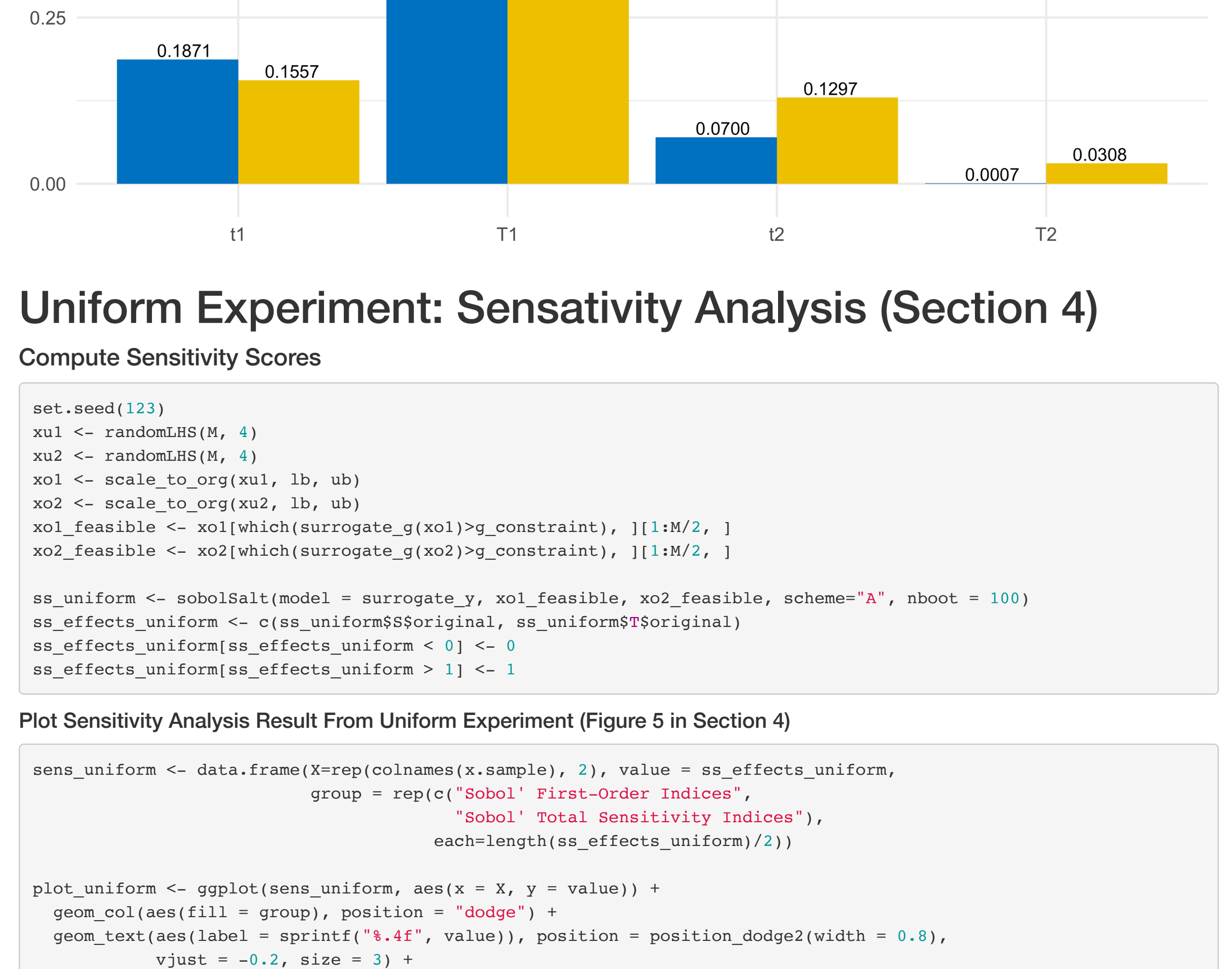
```
X1 <- x_gp[1:(M/2), ]
X2 <- x_gp[(M/2+1):M, ]
sobol_result <- sobolSalt(model = surrogate_y, X1, X2, scheme="A", nboot = 100)

ss_effects_gp <- c(sobol_result$S$original, sobol_result$T$original)
ss_effects_gp[ss_effects_gp < 0] <- 0
ss_effects_gp[ss_effects_gp > 1] <- 1
```

Plot Sensitivity Analysis Result From Decision Uncertainty Experiment (Figure 5 in Section 4)

```
sens_gp <- data.frame(X=rep(colnames(x.sample), 2), value = ss_effects_gp,
                      group = rep(c("Sobol' First-Order Indices",
                                    "Sobol' Total Sensitivity Indices"),
                                  each=length(ss_effects_gp)/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)
```



Uniform Experiment: Sensativity Analysis (Section 4)

Compute Sensitivity Scores

```
set.seed(123)
xu1 <- randomLHS(M, 4)
xu2 <- randomLHS(M, 4)
xo1 <- scale_to_org(xu1, lb, ub)
xo2 <- scale_to_org(xu2, lb, ub)
xo1_feasible <- xo1[which(surrogate_g(xo1)>g_constraint), ][1:M/2, ]
xo2_feasible <- xo2[which(surrogate_g(xo2)>g_constraint), ][1:M/2, ]

ss_uniform <- sobolSalt(model = surrogate_y, xo1_feasible, xo2_feasible, scheme="A", nboot = 100)
ss_effects_uniform <- c(ss_uniform$S$original, ss_uniform$T$original)
ss_effects_uniform[ss_effects_uniform < 0] <- 0
ss_effects_uniform[ss_effects_uniform > 1] <- 1
```

Plot Sensitivity Analysis Result From Uniform Experiment (Figure 5 in Section 4)

```
sens_uniform <- data.frame(X=rep(colnames(x.sample), 2), value = ss_effects_uniform,
                           group = rep(c("Sobol' First-Order Indices",
                                         "Sobol' Total Sensitivity Indices"),
                                       each=length(ss_effects_uniform)/2))

plot_uniform <- ggplot(sens_uniform, 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_uniform, group == "First"),
             position = position_dodge(width = 0.8), size = 4) +
  geom_point(data = subset(sens_uniform, 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(plot_uniform)
```

Combined Plot (Figure 5 in Section 4)

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