A sensitivity analysis of the PAWN sensitivity index

Arnald Puy, Samuele Lo Piano, Andrea Saltelli

Contents

1 Preliminary functions

```
# PRELIMINARY FUNCTIONS ----------------------------------------------------

# Install the development version of the pawnr package
devtools::install_github("arnaldpuy/pawnr", build_vignettes = TRUE)

# Function to read in all required packages in one go:
loadPackages <- function(x) {
  for(i in x) {
    if(!require(i, character.only = TRUE)) {
      install.packages(i, dependencies = TRUE)
      library(i, character.only = TRUE)
    }
  }
}

# Load the packages
loadPackages(c("tidyverse", "data.table", "randtoolbox", "sensitivity",
               "boot", "parallel", "doParallel", "scales", "cowplot",
               "overlapping", "pawnr", "sensobol", "sensitivity", "wesanderson"))

# Set checkpoint

dir.create(".checkpoint")
library("checkpoint")

checkpoint("2019-09-22",
           R.version ="3.6.1",
           checkpointLocation = getwd())
```

2 Check convergence of Sobol' indices and PAWN

```
# DEFINE SETTINGS ----------------------------------------------------------

N <- seq(500, 10000, 250) # Sample sizes
n <- 15 # Number of conditioning intervals
k <- c(2, 3, 8, 20) # Vector with number of model inputs
R <- 100 # Bootstrap replicas
n_cores <- floor(detectCores() * 0.75) # Use 75% of the cores available
type <- "norm" # Define the confidence interval method
conf <- 0.95 # Define the ci
models <- c("Liu", "Ishigami", "Sobol' G", "Morris")
params <- lapply(k, function(x) paste("X", 1:x, sep = ""))
names(params) <- models
```

```r
# Function to compute the Liu et al. function
liu <- function(X1, X2) {
  X1 / X2
}

liu_Mapply <- function(X) {
  X[, 1] <- qchisq(X[, 1], df = 10)
  X[, 2] <- qchisq(X[, 2], df = 13.978)
  return(mapply(liu, X[, 1], X[, 2]))
}
```

2.1 Sample matrix

```r
# CONSTRUCT SAMPLE MATRICES ------------------------------------------------

A <- list()
for(i in k) {
  A[[i]] <-mclapply(N, function(N) sobol_matrices(n = N, k = i), mc.cores = n_cores)
}

A <- A[!sapply(A, is.null)]
names(A) <- models

for(i in names(A)) {
  names(A[[i]]) <- N
}
```

2.2 Model output

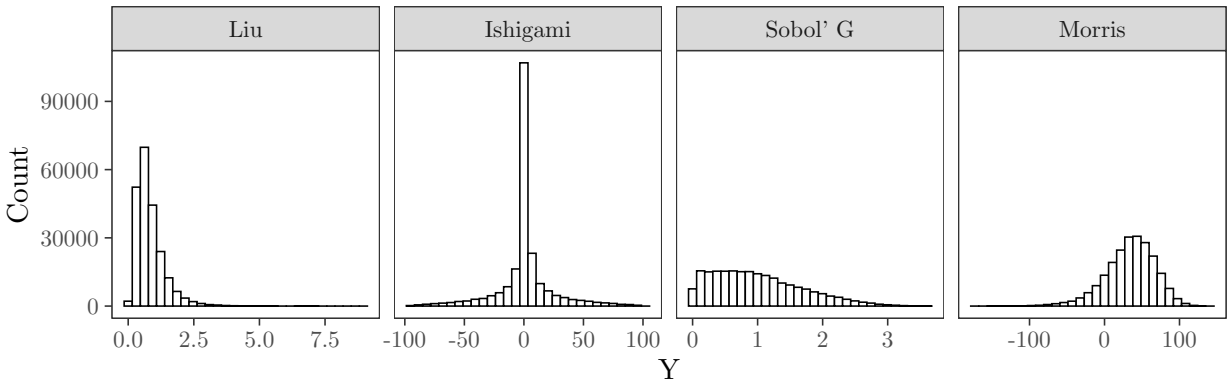
```r
# COMPUTE MODEL OUTPUT -----------------------------------------------------

Y <- list()
for(i in names(A)) {
  if(i == "Liu") {
    Y[[i]] <- lapply(A[[i]], function(x) liu_Mapply(x))
  } else if(i == "Ishigami") {
    Y[[i]] <- lapply(A[[i]], function(x) sensobol::ishigami_Mapply(x))
  } else if(i == "Sobol' G") {
    Y[[i]] <- lapply(A[[i]], function(x) sensobol::sobol_Fun(x))
  } else {
    Y[[i]] <- lapply(A[[i]], function(x) sensitivity::morris.fun(x))
  }
}

names(Y) <- models
for(i in names(Y)) {
  names(Y[[i]]) <- N
```

```
}
```

```
# PLOT MODEL UNCERTAINTY ----------------------------------------------------

lapply(models, function(models) Y[[models]]$`10000`) %>%
  do.call(cbind, .) %>%
  data.table() %>%
  setnames(., 1:4, models) %>%
  melt(., measure.vars = 1:4) %>%
  .[, variable:= factor(variable, levels = models)] %>%
  ggplot(., aes(value)) +
  geom_histogram(color = "black",
                 fill = "white") +
  labs(x = "Y",
       y = "Count") +
  facet_wrap(~ variable,
             scales = "free_x",
             ncol = 4) +
  theme_bw() +
  theme(aspect.ratio = 1,
        panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                         color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA))
```

```
## Warning in (function (..., deparse.level = 1) : number of rows of result is
## not a multiple of vector length (arg 1)
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



2.3 Sobol' indices

```
# COMPUTE SOBOL' INDICES AND THEIR CONFIDENCE INTERVALS ----------------------

out <- out.ci <- list()
```

```
for(i in names(A)) {
  for(j in names(A[[i]])) {
    out[[i]][[j]] <- sobol_indices(Y[[i]][[j]],
                                   params = params[[i]],
                                   n = as.numeric(j),
                                   type = "saltelli",
                                   R = R,
                                   parallel = "multicore",
                                   ncpus = n_cores)
    out.ci[[i]][[j]] <- sobol_ci(out[[i]][[j]],
                                 params = params[[i]],
                                 type = type,
                                 conf = conf)
  }
}
```

```
# SOBOL INDICES AND CONFIDENCE INTERVALS OF DUMMY PARAMETER ------------------

sobol.dummy <- sobol.dummy.ci <- list()
for(i in names(A)) {
  for(j in names(A[[i]])) {
    sobol.dummy[[i]][[j]] <- sobol_dummy(Y[[i]][[j]],
                                         params = params[[i]],
                                         R = R,
                                         n = as.numeric(j),
                                         parallel = "multicore",
                                         ncpus = n_cores)
    sobol.dummy.ci[[i]][[j]] <- sobol_ci_dummy(sobol.dummy[[i]][[j]],
                                               type = type,
                                               conf = conf)
  }
}

sobol.dummy.final <- lapply(sobol.dummy.ci, function(x) rbindlist(x, idcol = "N")) %>%
  rbindlist(., idcol = "model") %>%
  .[, model:= factor(model, levels = c("Liu", "Ishigami",
                                       "Sobol' G", "Morris"))]
```

```
# SOBOL' CONVERGENCE ---------------------------------------------------------

sobol.convergence <- lapply(out.ci, function(x) rbindlist(x, idcol = "N")) %>%
  rbindlist(., idcol = "model") %>%
  .[, N:= as.numeric(N)] %>%
  .[, diff:= high.ci - low.ci] %>%
  .[, model:= factor(model, levels = c("Liu", "Ishigami",
                                       "Sobol' G", "Morris"))] %>%
  .[, parameters:= factor(parameters,
                          levels = paste("X", 1:20, sep = ""))] %>%
```

```
  .[, method:= "Sobol' $S_{Ti}$"] %>%
  .[, .(model, N, parameters, original, low.ci, high.ci, diff, method, sensitivity)]
```

2.4 PAWN

```
# COMPUTE PAWN INDICES AND THEIR CONFIDENCE INTERVALS -------------------------

# Subset to take only the A matrix and the model output of the A matrix
Y.pawn <- A.pawn <- list()
for(i in names(Y)) {
  for(j in names(Y[[i]])) {
    Y.pawn[[i]][[j]] <- Y[[i]][[j]][1:j]
    A.pawn[[i]][[j]] <- A[[i]][[j]][1:j, ]
  }
}

# Compute PAWN indices and their confidence intervals
pawn.indices <- pawn.ci <- list()
for(i in names(A.pawn)) {
  for(j in names(A.pawn[[i]]) ) {
    pawn.indices[[i]][[j]] <- pawn_generic(data = A.pawn[[i]][[j]],
                                           Y = Y.pawn[[i]][[j]],
                                           n = n,
                                           test = median,
                                           R = R)
    pawn.ci[[i]][[j]] <- pawn_ci(pawn.indices[[i]][[j]])
  }
}
```

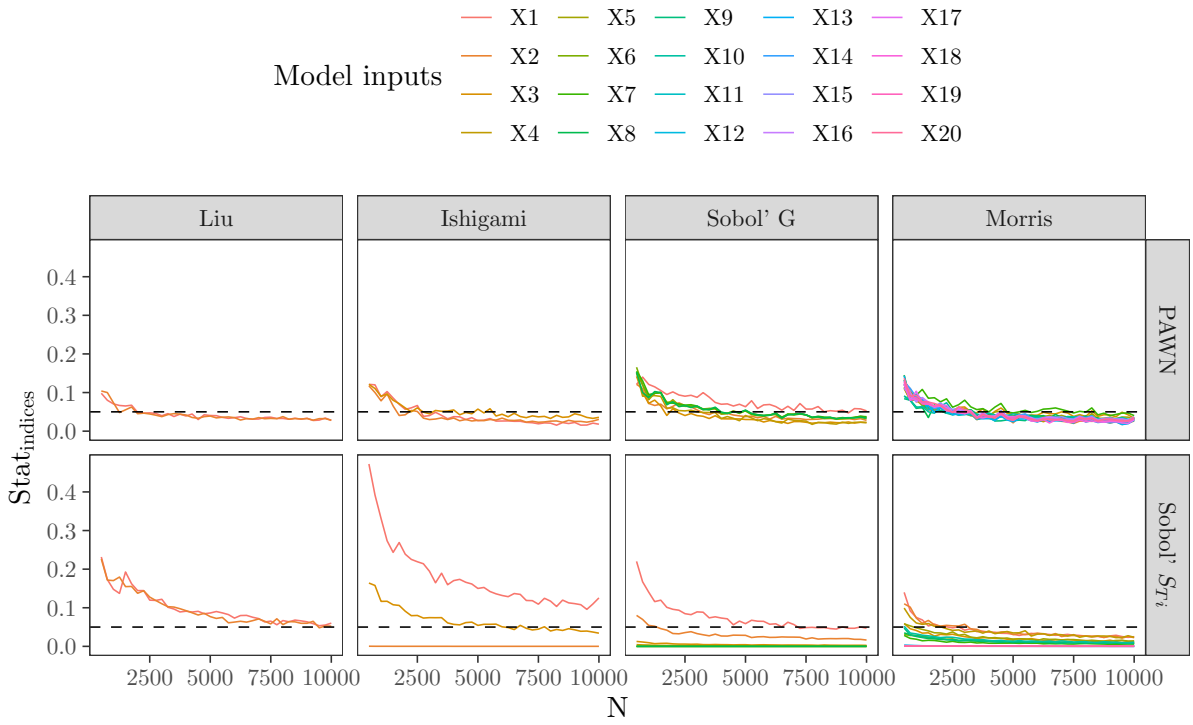
```
# PAWN AND CONFIDENCE INTERVALS OF DUMMY PARAMETER ----------------------------

pawn.index.dummy <- list()
for(i in names(Y)) {
  for(j in names(Y[[i]]) ) {
    pawn.index.dummy[[i]][[j]] <- pawn_dummy(Y = Y[[i]][[j]],
                                             n = n,
                                             R = R)
  }
}

pawn.index.dummy <- lapply(pawn.index.dummy, function(x) rbindlist(x, idcol = "N")) %>%
  rbindlist(., idcol = "model") %>%
  .[, model:= factor(model, levels = c(c("Liu", "Ishigami",
                                         "Sobol' G", "Morris")))]
```

```
# PAWN CONVERGENCE ------------------------------------------------------------

pawn.convergence <- lapply(pawn.ci, function(x) rbindlist(x, idcol = "N")) %>%
```

```
  rbindlist(., idcol = "model") %>%
  .[, N:= as.numeric(N)] %>%
  .[, diff:= high.ci - low.ci] %>%
  .[, model:= factor(model, levels = c("Liu", "Ishigami",
                                       "Sobol' G", "Morris"))] %>%
  .[, parameters:= gsub("V", "X", parameters)] %>%
  .[, parameters:= factor(parameters,
                          levels = paste("X", 1:20, sep = ""))] %>%
  .[, method:= "PAWN"]
```

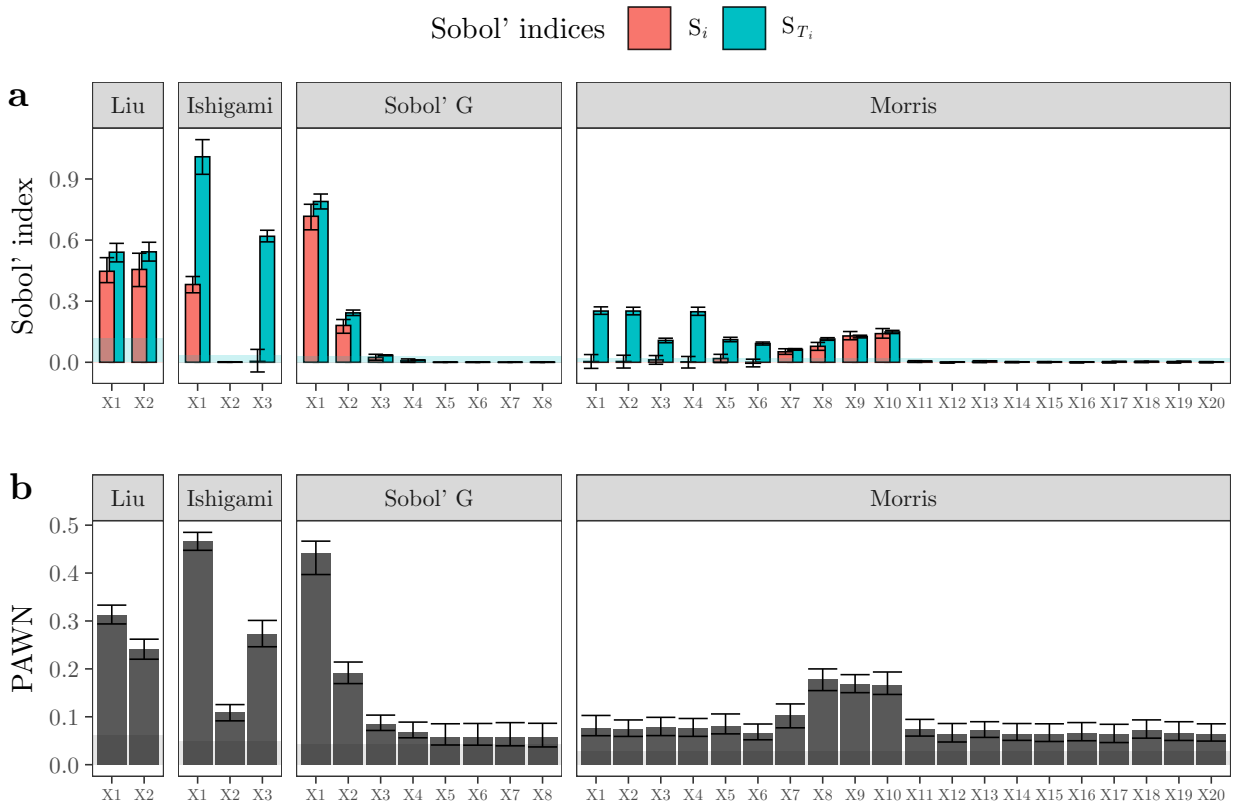
2.5 Plot convergence

```
# PLOT CONVERGENCE ------------------------------------------------------------

sobol.convergence[sensitivity == "STi"] %>%
  .[, sensitivity:= NULL] %>%
  rbind(., pawn.convergence) %>%
  ggplot(., aes(N, diff,
                group = parameters,
                color = parameters)) +
  geom_line() +
  geom_hline(yintercept = 0.05,
             lty = 2) +
  scale_color_discrete(name = "Model inputs") +
  labs(y = expression(Stat[indices]),
       x = "N") +
  facet_grid(method~model) +
  theme_bw() +
  theme(legend.position = "top",
        panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                         color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA))
```

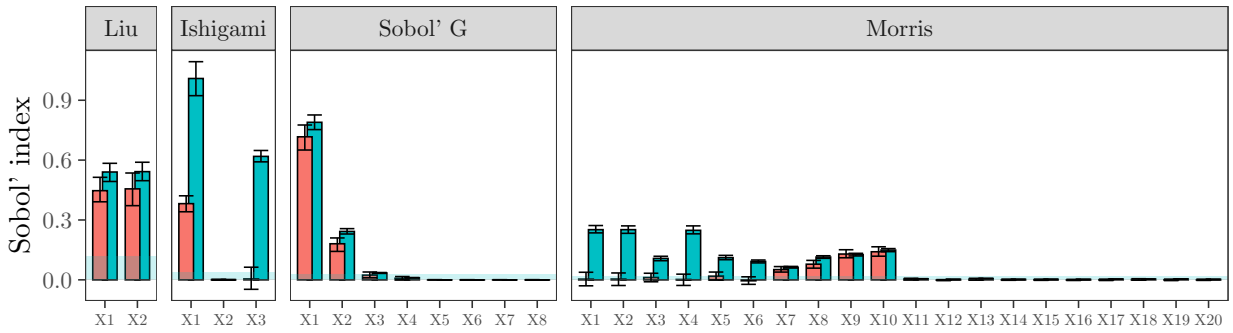



```
# PLOT SOBOL' AND PAWN INDICES ------------------------------------------------

# Sobol' indices
a <- plot_sobol(sobol.convergence[N==4000],
                dummy = sobol.dummy.final[N==4000]) +
  facet_grid(~model,
             scales = "free_x",
             space = "free_x") +
  labs(x = "",
       y = "Sobol' index") +
  theme(axis.text.x = element_text(size = 6),
        legend.position = "none")

# Get legend
legend <- get_legend(a + theme(legend.position = "top"))


# PAWN indices
b <- pawn.convergence[N==4000] %>%
  plot_pawn(.) +
  geom_rect(data = pawn.index.dummy[N==4000],
            aes(ymin = 0,
                ymax = high.ci,
                xmin = -Inf,
                xmax = Inf),
            fill = "black",
            alpha = 0.1,
```

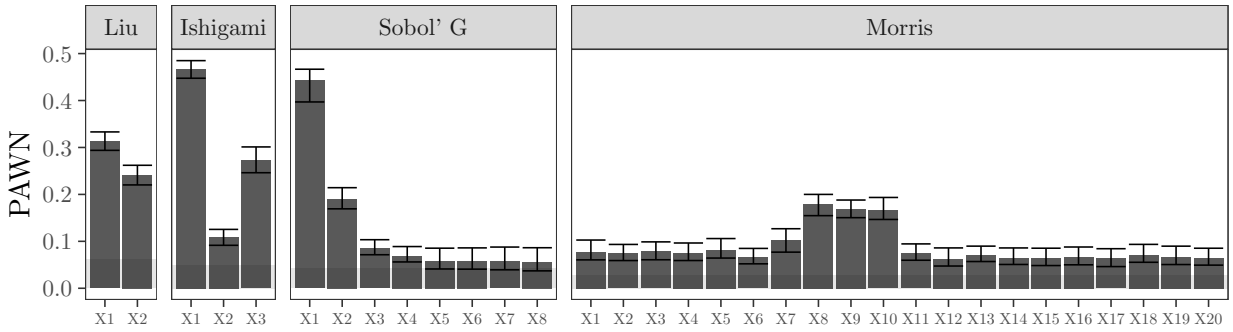
```
            inherit.aes = FALSE) +
  labs(x = "",
       y = "PAWN") +
  facet_grid(~ model,
             scales = "free_x",
             space = "free_x") +
  theme(axis.text.x = element_text(size = 6))

# Merge
bottom <- plot_grid(a, b,
                    ncol = 1,
                    labels = "auto",
                    align = "h")

plot_grid(legend, bottom,
          labels = c("", ""),
          ncol = 1,
          align = "",
          rel_heights = c(0.1, 1))
```




```
# PLOT SOBOL' AND PAWN INDICES (INDIVIDUAL PLOTS) ----------------------------

a
```



b



3 Sensitivity of PAWN to its design parameters

3.1 The model

```
# THE MODEL ------------------------------------------------------------------

# Function to divide a vector into chunks
chunks <- function(x,n) split(x, cut(seq_along(x), n, labels = FALSE))

# The model
model_pawn <- function(Model, N, n, epsilon, theta) {
  # Check which model to apply to set the number of
  # parameters
  if(Model == 1) {
    k <- 2
  } else if(Model == 2) {
    k <- 3
  } else if(Model == 3) {
    k <- 8
  } else {
    k <- 20
  }
  # Create the Sobol' matrix
  data <- randtoolbox::sobol(n = N, dim = k)
  # Transform distribution:
  if(Model == 1) {
```

```
    ModelRun <- liu_Mapply
  } else if(Model == 2) {
    ModelRun <- sensobol::ishigami_Mapply
  } else if(Model == 3) {
    ModelRun <- sensobol::sobol_Fun
  } else {
    ModelRun <- sensitivity::morris.fun
  }
  # Run the model
  Y <- ModelRun(data)
  # Set seed to fix the random number generator
  # for the sample function below
  set.seed(epsilon)
  # Sample the unconditional model output
  index <- sample(1:nrow(data),
                  size = floor(nrow(data) / n),
                  # Without replacement
                  replace = FALSE)
  # Bind model inputs and model output
  dt <- data.table::data.table(cbind(data, Y))
  # Subset and obtain the unconditional model output
  Y_unc <- dt[index, Y]
  # Create the intervals
  melted <- data.table::melt(dt,
                             measure.vars = 1:(ncol(dt) - 1),
                             variable.name = "parameters")
  # Compute PAWN indices
  out <- melted[order(parameters, value)][
    , .(chunks(Y, n)), parameters][
    , Y_unc:= .(rep(.(Y_unc), times = n * ncol(data)))][
    , ID:= .I][
    , results:= .(.(mapply(stats::ks.test, Y_unc, V1))), ID][
    , statistic:= sapply(results, function(x) x[, 1]$statistic)]
  if(theta == 1) {
    final <-  out[, mean(statistic), parameters][, V1]
  } else if(theta == 2) {
    final <-  out[, median(statistic), parameters][, V1]
  } else {
    final <-  out[, max(statistic), parameters][, V1]
  }
  return(final)
}
```

3.2 Settings

```
# DEFINE SETTINGS ----------------------------------------------------------
```

```r
# Set sample size
n <- 2 ^ 13

# Define N.min and N.max
N.min <- 200
N.max <- 2000

# Set parameters
parameters <- c("N", "n", "epsilon", "theta")

# Vector with name of functions
models <- c("Liu", "Ishigami", "Sobol' G", "Morris")
```

3.3 Sample matrix

```r
# CREATION OF THE MATRICES ------------------------------------------------

# Create the A, B and AB matrices, also for the
# computation of second and third-order indices
tmp <- lapply(1:4, function(x)
  sobol_matrices(n = n,
                 k = length(parameters),
                 second = TRUE,
                 third = TRUE) %>%
    data.table())

# Name the slots
names(tmp) <- 1:4

# Rename columns
tmp <- lapply(tmp, setnames, parameters) %>%
  rbindlist(., idcol = "Model")

# Create two copies of the sample matrix and list the
# original and the copies. One would be to run the
# calculations in the max in theta setting; the
# other one for the max not in theta setting,
# and the other in the optimum setting
max <- copy(tmp)
A <- list(tmp, max, copy(tmp))

# Name the slots
names(A) <- c("max", "no.max", "optimum")

# Transform all distributions
for(i in names(A)) {
  if(i == "max") {
```

```
    # where 1=mean, 2=median, 3=max in the model
    A[[i]][, N:= floor(qunif(N, N.min, N.max))]
    A[[i]][, n:= floor(qunif(n, 5, 20))]
    A[[i]][, theta:= floor(theta * (3 - 1 + 1)) + 1]
  } else if(i == "no.max") {
    A[[i]][, N:= floor(qunif(N, N.min, N.max))]
    A[[i]][, n:= floor(qunif(n, 5, 20))]
    A[[i]][, theta:= floor(theta * (2 - 1 + 1)) + 1]
  } else {
    A[[i]][, N:= floor(qunif(N, N.max, 4000))]
    A[[i]][, n:= floor(qunif(n, 15, 20))]
    A[[i]][, theta:= floor(theta * (2 - 1 + 1)) + 1]
  }
}

# Transform all the other distributions
A.pawn <- rbindlist(A, idcol = "setting")[
  , epsilon:= floor(qunif(epsilon, 1, 1000))][
  , Model:= as.numeric(Model)]

print(A.pawn)
```

```
##          setting Model    N  n epsilon theta
##       1:     max     1 1100 12     500     2
##       2:     max     1 1550  8     750     1
##       3:     max     1  650 16     250     3
##       4:     max     1  875 10     625     1
##       5:     max     1 1775 18     125     2
##      ---
## 1572860: optimum     4 2500 18     508     2
## 1572861: optimum     4 3500 16       9     1
## 1572862: optimum     4 3000 19     258     2
## 1572863: optimum     4 2000 17     758     1
## 1572864: optimum     4 2000 19     889     2
```

3.4 Run the model

```
# RUN MODEL ------------------------------------------------------------------

# Define parallel computing
cl <- makeCluster(n_cores)
registerDoParallel(cl)

# Compute
Y.pawn <- foreach(i=1:nrow(A.pawn),
                  .packages = "data.table") %dopar%
  {
```

```
    model_pawn(epsilon = A.pawn[[i, "epsilon"]],
               N = A.pawn[[i, "N"]],
               n = A.pawn[[i, "n"]],
               theta = A.pawn[[i, "theta"]],
               Model = A.pawn[[i, "Model"]])
  }

# Stop parallel cluster
stopCluster(cl)
```

```
# EXTRACT DATA ------------------------------------------------------------

rowNumber <- lapply(1:4, function(x) A.pawn[, .I[Model == x]])
names(rowNumber) <- models

out <- list()
for(i in models) {
  out[[i]] <- Y.pawn[rowNumber[[i]]]
}

dt.models <- list()
for(i in seq_along(1:4)) {
  dt.models[[i]] <- cbind(A.pawn[Model == i], data.table(do.call(rbind, out[[i]])))
}
```

3.5 Uncertainty analysis

```
# DATASET FOR UNCERTAINTY ANALYSIS ----------------------------------------

AB.pawn <- lapply(dt.models, function(x)  {
  x[, .SD[1: (2 * (2 ^ 13))], setting] %>%
    melt(., measure.vars = patterns("V"),
         variable.name = "parameter")
  }) %>%
  rbindlist() %>%
  .[, Model:= ifelse(Model == 1, models[1],
                     ifelse(Model == 2, models[2],
                            ifelse(Model == 3, models[3], models[4])))] %>%
  .[, parameter:= gsub("V", "X", parameter)] %>%
  .[, parameter:= factor(parameter,
                         levels = paste("X", 1:20, sep = ""))] %>%
  .[, Model:= factor(Model,
                     levels = c("Liu", "Ishigami", "Sobol' G", "Morris"))] %>%
  .[, setting:= ifelse(setting == "max", "$max \\in \\theta$",
                       ifelse(setting == "no.max", "$max \\notin \\theta$", "Optimum"))]
```

```r
# CHECK OVERLAP ------------------------------------------------------------

overlap.dt <- split(AB.pawn, AB.pawn$setting)

overlap.results <- mclapply(overlap.dt, function(x) {
  split(x, x$Model, drop = TRUE) %>%
    lapply(., function(x) split(x, x$parameter, drop = TRUE)) %>%
    lapply(., function(x) lapply(x, function(y) y[, value])) %>%
    lapply(., function(x) overlap(x))},
  mc.cores = n_cores)

tmp <- lapply(overlap.results, function(x) lapply(x, function(y) {
  cbind(y$OV) %>%
    data.frame() %>%
    setDT(., keep.rownames = TRUE)
  }))

pawn.overlap.results <- lapply(tmp, function(x)
  rbindlist(x, idcol = "Model")) %>%
  rbindlist(., idcol = "setting") %>%
  setnames(., ".", "overlap")

par.overlap <- paste("X", 1:6, sep = "")

final.overlap <- lapply(models, function(x) pawn.overlap.results[Model==x, .SD, setting]) %>%
  lapply(., function(x) x[, "overlap":= round(.SD, 3), .SDcols = "overlap"])

final.overlap
```

```
## [[1]]
##                   setting Model    rn overlap
## 1:    $max \\in \\theta$   Liu X1-X2   0.253
## 2: $max \\notin \\theta$   Liu X1-X2   0.127
## 3:                Optimum   Liu X1-X2   0.013
##
## [[2]]
##                   setting    Model    rn overlap
## 1:    $max \\in \\theta$ Ishigami X1-X2   0.009
## 2:    $max \\in \\theta$ Ishigami X1-X3   0.051
## 3:    $max \\in \\theta$ Ishigami X2-X3   0.095
## 4: $max \\notin \\theta$ Ishigami X1-X2   0.001
## 5: $max \\notin \\theta$ Ishigami X1-X3   0.016
## 6: $max \\notin \\theta$ Ishigami X2-X3   0.038
## 7:                Optimum Ishigami X1-X2   0.000
## 8:                Optimum Ishigami X1-X3   0.000
## 9:                Optimum Ishigami X2-X3   0.000
##
```

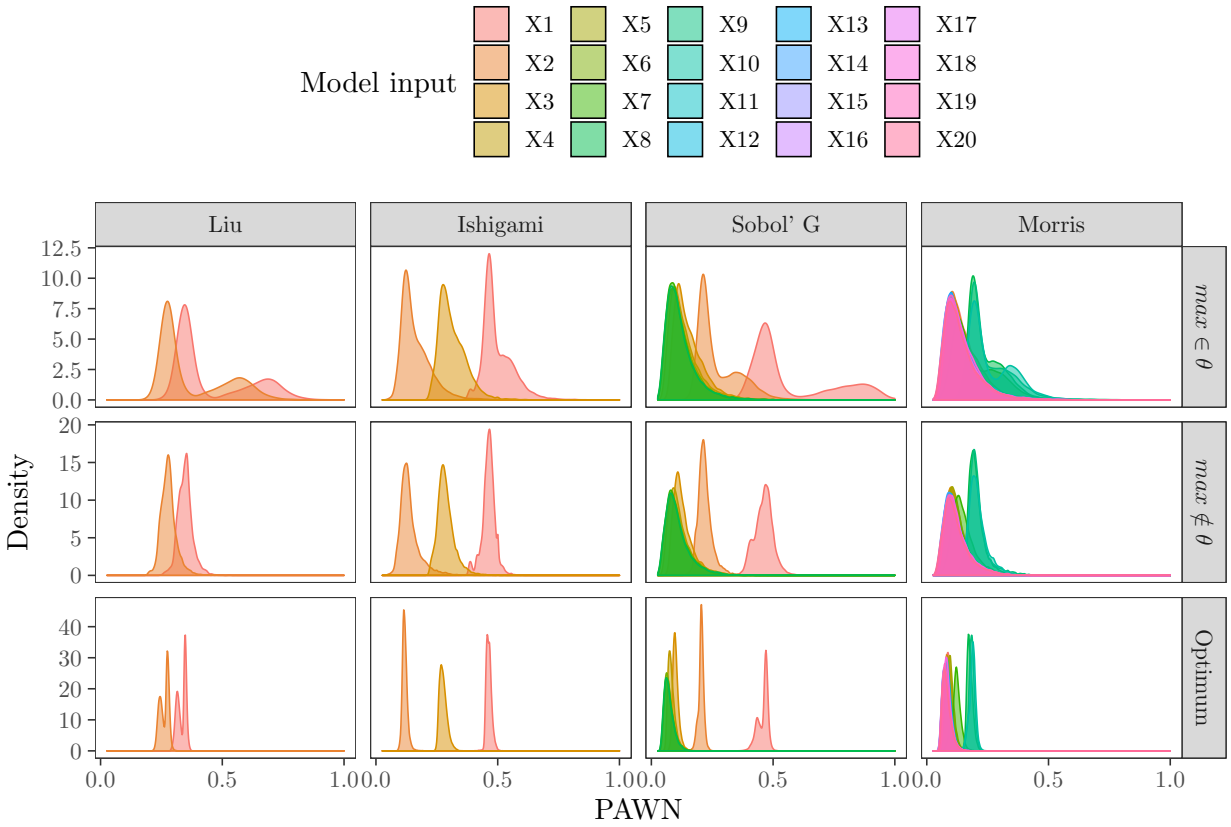
```
## [[3]]
##                    setting    Model    rn overlap
##  1:    $max \\in \\theta$ Sobol' G X1-X2   0.101
##  2:    $max \\in \\theta$ Sobol' G X1-X3   0.010
##  3:    $max \\in \\theta$ Sobol' G X1-X4   0.011
##  4:    $max \\in \\theta$ Sobol' G X1-X5   0.006
##  5:    $max \\in \\theta$ Sobol' G X1-X6   0.006
##  6:    $max \\in \\theta$ Sobol' G X1-X7   0.006
##  7:    $max \\in \\theta$ Sobol' G X1-X8   0.009
##  8:    $max \\in \\theta$ Sobol' G X2-X3   0.192
##  9:    $max \\in \\theta$ Sobol' G X2-X4   0.138
## 10:    $max \\in \\theta$ Sobol' G X2-X5   0.108
## 11:    $max \\in \\theta$ Sobol' G X2-X6   0.107
## 12:    $max \\in \\theta$ Sobol' G X2-X7   0.100
## 13:    $max \\in \\theta$ Sobol' G X2-X8   0.103
## 14:    $max \\in \\theta$ Sobol' G X3-X4   0.702
## 15:    $max \\in \\theta$ Sobol' G X3-X5   0.592
## 16:    $max \\in \\theta$ Sobol' G X3-X6   0.568
## 17:    $max \\in \\theta$ Sobol' G X3-X7   0.544
## 18:    $max \\in \\theta$ Sobol' G X3-X8   0.544
## 19:    $max \\in \\theta$ Sobol' G X4-X5   0.839
## 20:    $max \\in \\theta$ Sobol' G X4-X6   0.808
## 21:    $max \\in \\theta$ Sobol' G X4-X7   0.779
## 22:    $max \\in \\theta$ Sobol' G X4-X8   0.777
## 23:    $max \\in \\theta$ Sobol' G X5-X6   0.952
## 24:    $max \\in \\theta$ Sobol' G X5-X7   0.920
## 25:    $max \\in \\theta$ Sobol' G X5-X8   0.913
## 26:    $max \\in \\theta$ Sobol' G X6-X7   0.951
## 27:    $max \\in \\theta$ Sobol' G X6-X8   0.950
## 28:    $max \\in \\theta$ Sobol' G X7-X8   0.961
## 29: $max \\notin \\theta$ Sobol' G X1-X2   0.003
## 30: $max \\notin \\theta$ Sobol' G X1-X3   0.001
## 31: $max \\notin \\theta$ Sobol' G X1-X4   0.002
## 32: $max \\notin \\theta$ Sobol' G X1-X5   0.001
## 33: $max \\notin \\theta$ Sobol' G X1-X6   0.001
## 34: $max \\notin \\theta$ Sobol' G X1-X7   0.001
## 35: $max \\notin \\theta$ Sobol' G X1-X8   0.002
## 36: $max \\notin \\theta$ Sobol' G X2-X3   0.095
## 37: $max \\notin \\theta$ Sobol' G X2-X4   0.089
## 38: $max \\notin \\theta$ Sobol' G X2-X5   0.076
## 39: $max \\notin \\theta$ Sobol' G X2-X6   0.078
## 40: $max \\notin \\theta$ Sobol' G X2-X7   0.075
## 41: $max \\notin \\theta$ Sobol' G X2-X8   0.076
## 42: $max \\notin \\theta$ Sobol' G X3-X4   0.648
## 43: $max \\notin \\theta$ Sobol' G X3-X5   0.569
## 44: $max \\notin \\theta$ Sobol' G X3-X6   0.548
## 45: $max \\notin \\theta$ Sobol' G X3-X7   0.527
## 46: $max \\notin \\theta$ Sobol' G X3-X8   0.525
```

```
## 47: $max \\notin \\theta$ Sobol' G X4-X5   0.852
## 48: $max \\notin \\theta$ Sobol' G X4-X6   0.821
## 49: $max \\notin \\theta$ Sobol' G X4-X7   0.797
## 50: $max \\notin \\theta$ Sobol' G X4-X8   0.793
## 51: $max \\notin \\theta$ Sobol' G X5-X6   0.952
## 52: $max \\notin \\theta$ Sobol' G X5-X7   0.927
## 53: $max \\notin \\theta$ Sobol' G X5-X8   0.919
## 54: $max \\notin \\theta$ Sobol' G X6-X7   0.956
## 55: $max \\notin \\theta$ Sobol' G X6-X8   0.953
## 56: $max \\notin \\theta$ Sobol' G X7-X8   0.958
## 57:               Optimum Sobol' G X1-X2   0.000
## 58:               Optimum Sobol' G X1-X3   0.000
## 59:               Optimum Sobol' G X1-X4   0.000
## 60:               Optimum Sobol' G X1-X5   0.000
## 61:               Optimum Sobol' G X1-X6   0.000
## 62:               Optimum Sobol' G X1-X7   0.000
## 63:               Optimum Sobol' G X1-X8   0.000
## 64:               Optimum Sobol' G X2-X3   0.002
## 65:               Optimum Sobol' G X2-X4   0.001
## 66:               Optimum Sobol' G X2-X5   0.001
## 67:               Optimum Sobol' G X2-X6   0.001
## 68:               Optimum Sobol' G X2-X7   0.001
## 69:               Optimum Sobol' G X2-X8   0.001
## 70:               Optimum Sobol' G X3-X4   0.276
## 71:               Optimum Sobol' G X3-X5   0.191
## 72:               Optimum Sobol' G X3-X6   0.183
## 73:               Optimum Sobol' G X3-X7   0.184
## 74:               Optimum Sobol' G X3-X8   0.174
## 75:               Optimum Sobol' G X4-X5   0.542
## 76:               Optimum Sobol' G X4-X6   0.523
## 77:               Optimum Sobol' G X4-X7   0.516
## 78:               Optimum Sobol' G X4-X8   0.490
## 79:               Optimum Sobol' G X5-X6   0.957
## 80:               Optimum Sobol' G X5-X7   0.947
## 81:               Optimum Sobol' G X5-X8   0.907
## 82:               Optimum Sobol' G X6-X7   0.953
## 83:               Optimum Sobol' G X6-X8   0.919
## 84:               Optimum Sobol' G X7-X8   0.954
##                   setting    Model    rn overlap
##
## [[4]]
##                 setting  Model      rn overlap
##   1: $max \\in \\theta$ Morris   X1-X2   0.907
##   2: $max \\in \\theta$ Morris   X1-X3   0.940
##   3: $max \\in \\theta$ Morris   X1-X4   0.890
##   4: $max \\in \\theta$ Morris   X1-X5   0.887
##   5: $max \\in \\theta$ Morris   X1-X6   0.814
##  ---
```

```
## 566:            Optimum Morris X17-X19   0.884
## 567:            Optimum Morris X17-X20   0.971
## 568:            Optimum Morris X18-X19   0.756
## 569:            Optimum Morris X18-X20   0.680
## 570:            Optimum Morris X19-X20   0.890
```

```r
# Export results
rbindlist(final.overlap) %>%
  fwrite(., "pawn.overlap.csv")
```

```r
# PLOT UNCERTAINTY ------------------------------------------------------------

plot.uncertainty.pawn <- ggplot(AB.pawn, aes(value,
                                             fill = parameter,
                                             color = parameter)) +
  geom_density(alpha = 0.5,
               position = "identity") +
  facet_grid(setting~Model,
             scales = "free_y") +
  scale_fill_discrete(name = "Model input") +
  scale_color_discrete(guide = FALSE) +
  labs(x = "PAWN",
       y = "Density") +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  theme_bw() +
  theme(legend.position = "top",
        legend.box = "horizontal",
        panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                         color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA))

plot.uncertainty.pawn
```




```
# EXPORT AB MATRIX FOR PAWN ------------------------------------------------

fwrite(AB.pawn, "AB.pawn.csv")
```

3.6 Sensitivity analysis

```
# DATASET FOR SENSITIVITY ANALYSIS -----------------------------------------

dt.pawn.sens <- lapply(dt.models, function(x)
  melt(x, measure.vars = patterns("V"), variable.name = "model.input")) %>%
  rbindlist() %>%
  .[, Model:= ifelse(Model == 1, models[1],
                     ifelse(Model == 2, models[2],
                            ifelse(Model == 3, models[3], models[4])))] %>%
  .[, model.input:= gsub("V", "X", model.input)] %>%
  .[, model.input:= factor(model.input,
                           levels = paste("X", 1:20, sep = ""))] %>%
  .[, Model:= factor(Model,
                     levels = c("Liu", "Ishigami", "Sobol' G", "Morris"))] %>%
  setnames(., "value", "Y")

# EXPORT AB MATRIX FOR SENSITIVITY -----------------------------------------

fwrite(dt.pawn.sens, "dt.pawn.sens.csv")
```

```r
# SENSITIVITY ANALYSIS -----------------------------------------------------

pawn.sensitivity <- dt.pawn.sens[, sobol_indices(Y,
                                                 params = parameters,
                                                 R = R,
                                                 n = 2 ^ 13,
                                                 parallel = "multicore",
                                                 second = TRUE,
                                                 third = TRUE,
                                                 ncpus = n_cores),
                                 .(setting, Model, model.input)]
```

```r
# CONFIDENCE INTERVALS -----------------------------------------------------

# Arrange data
tmp3 <- split(pawn.sensitivity, pawn.sensitivity$setting) %>%
  lapply(., function(x) split(x, x$Model)) %>%
  lapply(., function(x) lapply(x, function(y) split(y, y$model.input, drop = TRUE)))

# Compute confidence intervals
pawn.ci <- list()
for(i in names(tmp3)) {
  for(j in names(tmp3[[i]])) {
    for(k in names(tmp3[[i]][[j]])) {
      pawn.ci[[i]][[j]][[k]] <- sobol_ci(tmp3[[i]][[j]][[k]],
                                         params = parameters,
                                         type = type,
                                         conf = conf,
                                         second = TRUE,
                                         third = TRUE)
    }
  }
}

# Rearrange data
final.pawn.ci <- lapply(pawn.ci, function(x)
  lapply(x, function(y) rbindlist(y, idcol = "model.input"))) %>%
  lapply(., function(x) rbindlist(x, idcol = "model")) %>%
  rbindlist(., idcol = "setting") %>%
  .[, model:= factor(model, levels = c("Liu", "Ishigami",
                                       "Sobol' G", "Morris"))] %>%
  .[, model.input:= factor(model.input, levels = paste("X", 1:20, sep = ""))] %>%
  .[, parameters:= gsub("epsilon", "$\\\\varepsilon$", parameters)] %>%
  .[, parameters:= gsub("theta", "$\\\\theta$", parameters)] %>%
  .[, setting:= ifelse(setting == "max", "$max \\in \\theta$",
                       ifelse(setting == "no.max", "$max \\notin \\theta$", "Optimum"))]
```

```r
# EXPORT DATA ------------------------------------------------------------------

fwrite(final.pawn.ci, "final.pawn.ci.csv")
```

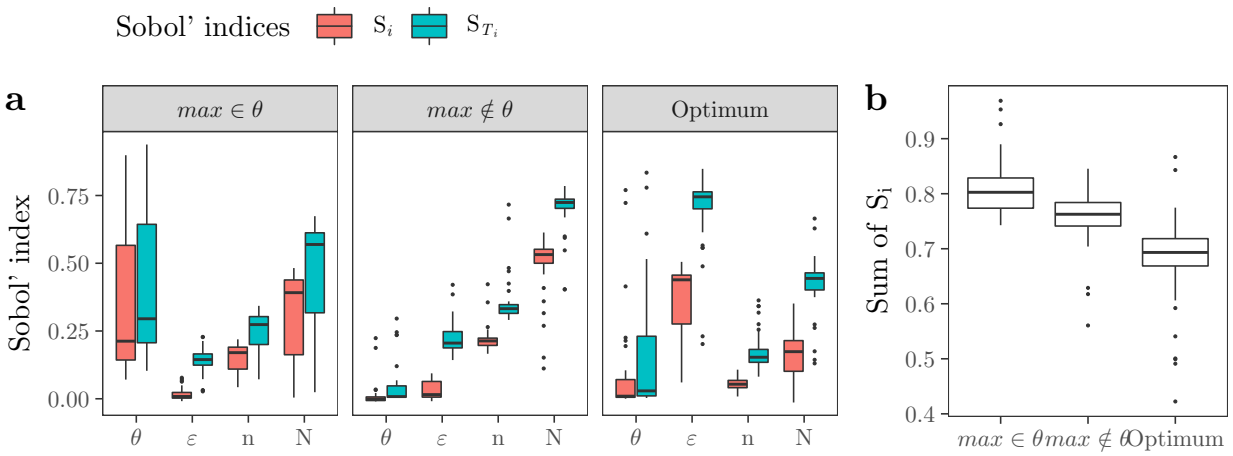
```r
# PLOT AGGREGATED SOBOL' INDICES -----------------------------------------------

a <- final.pawn.ci[sensitivity == "Si" | sensitivity == "STi"] %>%
  ggplot(., aes(parameters, original,
                fill = sensitivity)) +
  geom_boxplot(outlier.size = 0.2) +
  labs(x = "",
       y = "Sobol' index") +
  scale_fill_discrete(name = "Sobol' indices",
                      labels = c(expression(S[italic(i)]),
                                 expression(S[italic(T[i])]))) +
  theme_bw() +
  facet_wrap(~ setting) +
  theme(panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                         color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA),
        legend.position = "none")

legend <- get_legend(a + theme(legend.position = "top"))

# PLOT SUM OF SOBOL' SI --------------------------------------------------------

b <- final.pawn.ci[sensitivity == "Si"][
  , sum(original), .(setting, model, model.input)] %>%
  ggplot(., aes(setting, V1)) +
  geom_boxplot(outlier.size = 0.2) +
  labs(x = "",
       y = expression(paste("Sum of"~S[i]))) +
  theme_bw() +
  theme(panel.grid.major = element_blank(),
        panel.grid.minor = element_blank())

# MERGE AGGREGATED SOBOL' AND SUM OF SOBOL' ------------------------------------

up <- plot_grid(legend, NULL,
                ncol = 2)

bottom <- plot_grid(a, b,
                    ncol = 2,
                    align = "hv",
```

```
                    labels = "auto",
                    rel_widths = c(2.2, 1))
```

```
## Warning: Graphs cannot be vertically aligned unless the axis parameter is
## set. Placing graphs unaligned.
```

```
## Warning: Graphs cannot be horizontally aligned unless the axis parameter is
## set. Placing graphs unaligned.
```

```
plot_grid(up, bottom,
          ncol = 1,
          align = "hv",
          rel_heights = c(0.21, 1))
```



4 Sensitivity of Sobol' indices to its design parameters

4.1 The model

```
# THE MODEL ------------------------------------------------------------------

# Functions to create A and AB matrices to compute Ti
scrambled_sobol <- function(A, B) {
  X <- rbind(A, B)
  for(i in 1:ncol(A)) {
    AB <- A
    AB[, i] <- B[, i]
    X <- rbind(X, AB)
  }
  AB <- rbind(A, X[((2*nrow(A)) + 1):nrow(X), ])
  return(AB)
}

sobol_matrix <- function(n, k) {
  df <- randtoolbox::sobol(n = n, dim = k * 2)
  A <- df[, 1:k]
```

```
  B <- df[, (k + 1) : (k * 2)]
  out <- scrambled_sobol(A = A, B = B)
  return(out)
}

# Functions to estimate Ti
sobol_all <- function(Y_A, Y_AB, type) {
  n <- length(Y_A[!is.na(Y_A)])
  f0 <- (1 / n) * sum(Y_A)
  VY <- 1 / n * sum((Y_A - f0) ^ 2)
  if(type == "jansen") {
    STi <- ((1 / (2 * n)) * sum((Y_A - Y_AB) ^ 2)) / VY
  } else if(type == "homma") {
    STi <- (VY - (1 / n) * sum(Y_A * Y_AB) + f0 ^ 2) / VY
  } else if(type == "sobol") {
    STi <- ((1 / n) * sum(Y_A * (Y_A - Y_AB))) / VY
  } else {
    stop("type should  be either jansen, sobol or homma")
  }
  return(STi)
}

sobol_Ti_Mapply <- function(d, type) {
  return(mapply(sobol_all,
                MoreArgs = list(type = type),
                d[, "Y_A"],
                d[, "Y_AB"]))
}

sobol_Ti <- function(Y, params, type) {
  k <- length(params)
  p <- length(1:(length(Y) / (k + 1)))
  Y_A <- Y[1:p]
  Y_AB <- Y[(p + 1):length(Y)]
  parameters <- rep(params, each = length(Y_A))
  vec <- cbind(Y_A, Y_AB)
  out <- data.table(vec, parameters)
  output <- out[, sobol_Ti_Mapply(.SD, type = type), parameters][, V1]
  return(output)
}

# The model
model_sobol <- function(Model, N, k, Theta) {
  data <- sobol_matrix(n = N, k = k)
  if(Model == 1) {
    Y <- liu_Mapply(data)
  } else if(Model == 2) {
```

```
    Y <- sensobol::ishigami_Mapply(data)
  } else if(Model == 3) {
    Y <- sensobol::sobol_Fun(data)
  } else {
    Y <- sensitivity::morris.fun(data)
  }
  out <- sobol_Ti(Y, params = paste("X", 1:k, sep = ""), type = Theta)
  return(out)
}
```

4.2 Settings

```
# DEFINE SETTINGS ---------------------------------------------------------

# Set parameters
parameters.sobol <- c("N", "Theta")
```

4.3 Sample matrix

```
# CREATION OF THE MATRICES ------------------------------------------------

# Create the A and AB matrices, also for the
# computation of second and third-order indices
tmp <- lapply(models, function(x)
  sobol_matrices(n = n, k = length(parameters.sobol)) %>%
    data.table())

# Rename columns and transform distributions
A <- lapply(tmp, setnames, parameters.sobol) %>%
  rbindlist(., idcol = "Model")

# Create two copies of the sample matrix and list the
# original and the copies. One would be to run the
# calculations with uncertainty in N and Theta,
# the other with uncertainty in N only.
N.only <- copy(A)
A.DT <- list(A, N.only)
names(A.DT) <- c("N.Theta", "N")

A <- rbindlist(A.DT, idcol = "setting")

A.sobol <- A[, k:= ifelse(Model == 1, 2, ifelse(Model == 2, 3, ifelse(Model == 3, 8, 20)))][
    , N:= floor(qunif(N, N.min, N.max))][
    , Model:= as.numeric(Model)][
    , Theta:= floor(Theta * (3 - 1 + 1)) + 1][
    , Theta:= ifelse(Theta == 1, "jansen", ifelse(Theta == 2, "homma", "sobol"))][
    , Theta:= ifelse(setting == "N", "jansen", Theta)]
```

```r
print(A.sobol)
```

```
##         setting Model    N  Theta  k
##      1: N.Theta     1 1100  homma  2
##      2: N.Theta     1 1550 jansen  2
##      3: N.Theta     1  650  sobol  2
##      4: N.Theta     1  875  homma  2
##      5: N.Theta     1 1775  sobol  2
##     ---
## 262140:       N     4  650 jansen 20
## 262141:       N     4 1550 jansen 20
## 262142:       N     4 1100 jansen 20
## 262143:       N     4  200 jansen 20
## 262144:       N     4  200 jansen 20
```

```r
print(n)
```

```
## [1] 8192
```

4.4 Run the model

```r
# RUN MODEL ------------------------------------------------------------------

# Define parallel computing
cl <- makeCluster(n_cores)
registerDoParallel(cl)

# Compute
Y.sobol <- foreach(i=1:nrow(A.sobol),
                   .packages = "data.table") %dopar%
  {
    model_sobol(N = A.sobol[[i, "N"]],
                Theta = A.sobol[[i, "Theta"]],
                Model = A.sobol[[i, "Model"]],
                k = A.sobol[[i, "k"]])
  }

# Stop parallel cluster
stopCluster(cl)
```

```r
# EXTRACT MODEL OUTPUT -------------------------------------------------------

rowNumber <- lapply(1:4, function(x) A.sobol[, .I[Model == x]])
names(rowNumber) <- models

out <- list()
for(i in models) {
  out[[i]] <- Y.sobol[rowNumber[[i]]]
```

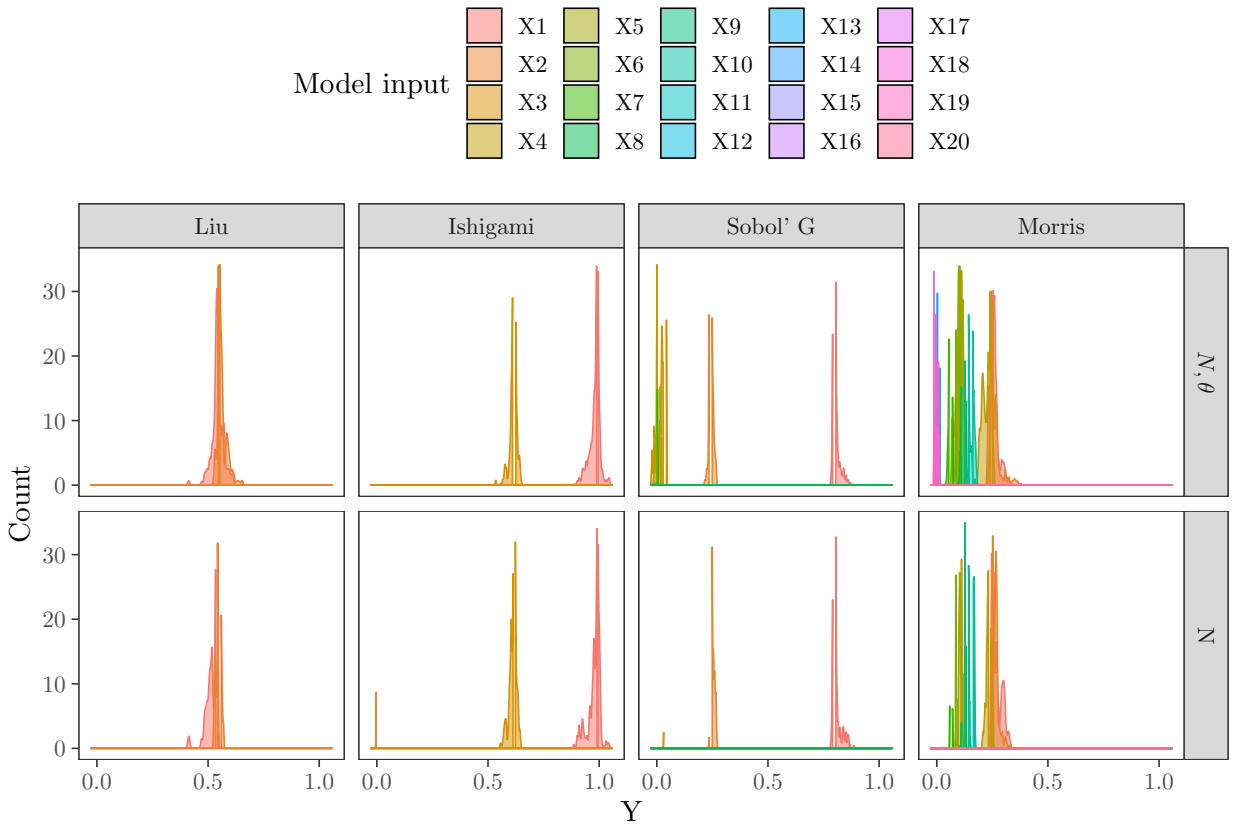
```
}

dt.models <- list()
for(i in seq_along(1:4)) {
  dt.models[[i]] <- cbind(A[Model == i], data.table(do.call(rbind, out[[i]])))
}
```

4.5 Uncertainty analysis

```
# DATASET FOR UNCERTAINTY ANALYSIS ----------------------------------------

AB.sobol <- lapply(dt.models, function(x) {
  x[, .SD[1: (2 * (2 ^ 13))], setting] %>%
  melt(., measure.vars = patterns("V"),
       variable.name = "parameter")}) %>%
  rbindlist(.) %>%
  .[, Model:= ifelse(Model == 1, models[1],
                     ifelse(Model == 2, models[2],
                            ifelse(Model == 3, models[3], models[4])))] %>%
  .[, k:= NULL] %>%
  .[, parameter:= gsub("V", "X", parameter)] %>%
  .[, parameter:= factor(parameter,
                         levels = paste("X", 1:20, sep = ""))] %>%
  .[, Model:= factor(Model,
                     levels = c("Liu", "Ishigami", "Sobol' G", "Morris"))] %>%
  .[, setting:= ifelse(setting == "N.Theta", "$N,\\theta$", setting)]

# EXPORT AB MATRIX FOR SOBOL' ---------------------------------------------

fwrite(AB.sobol, "AB.sobol.csv")
```

```
# PLOT UNCERTAINTY --------------------------------------------------------

AB.sobol %>%
  ggplot(., aes(value,
                fill = parameter,
                color = parameter)) +
  geom_density(alpha = 0.5,
               position = "identity") +
  facet_grid(setting~Model) +
  scale_fill_discrete(name = "Model input") +
  scale_color_discrete(guide = FALSE) +
  labs(x = "Y",
       y = "Count") +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  scale_y_continuous(limits = c(0, 35)) +
  theme_bw() +
```

```
  theme(legend.position = "top",
        legend.box = "horizontal",
        panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                         color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA))
```




```
# CHECK OVERLAP ------------------------------------------------------------

overlap.dt <- split(AB.sobol, AB.sobol$setting)

overlap.results <- mclapply(overlap.dt, function(x) {
  split(x, x$Model, drop = TRUE) %>%
    lapply(., function(x) split(x, x$parameter, drop = TRUE)) %>%
    lapply(., function(x) lapply(x, function(y) y[, value])) %>%
    lapply(., function(x) overlap(x))},
  mc.cores = n_cores)

tmp <- lapply(overlap.results, function(x) lapply(x, function(y) {
  cbind(y$OV) %>%
    data.frame() %>%
    setDT(., keep.rownames = TRUE)
```

```
}))

sobol.overlap.results <- lapply(tmp, function(x)
  rbindlist(x, idcol = "Model")) %>%
  rbindlist(., idcol = "setting") %>%
  setnames(., ".", "overlap")

par.overlap <- paste("X", 1:6, sep = "")

final.overlap <- lapply(models, function(x) sobol.overlap.results[Model==x, .SD, setting]) %>%
  lapply(., function(x) x[, "overlap":= round(.SD, 3), .SDcols = "overlap"])

final.overlap
```

```
## [[1]]
##        setting Model    rn overlap
## 1: $N,\\theta$   Liu X1-X2   0.340
## 2:           N   Liu X1-X2   0.185
##
## [[2]]
##        setting    Model    rn overlap
## 1: $N,\\theta$ Ishigami X1-X2       0
## 2: $N,\\theta$ Ishigami X1-X3       0
## 3: $N,\\theta$ Ishigami X2-X3       0
## 4:           N Ishigami X1-X2       0
## 5:           N Ishigami X1-X3       0
## 6:           N Ishigami X2-X3       0
##
## [[3]]
##         setting    Model    rn overlap
##  1: $N,\\theta$ Sobol' G X1-X2   0.000
##  2: $N,\\theta$ Sobol' G X1-X3   0.000
##  3: $N,\\theta$ Sobol' G X1-X4   0.000
##  4: $N,\\theta$ Sobol' G X1-X5   0.000
##  5: $N,\\theta$ Sobol' G X1-X6   0.000
##  6: $N,\\theta$ Sobol' G X1-X7   0.000
##  7: $N,\\theta$ Sobol' G X1-X8   0.000
##  8: $N,\\theta$ Sobol' G X2-X3   0.000
##  9: $N,\\theta$ Sobol' G X2-X4   0.000
## 10: $N,\\theta$ Sobol' G X2-X5   0.000
## 11: $N,\\theta$ Sobol' G X2-X6   0.000
## 12: $N,\\theta$ Sobol' G X2-X7   0.000
## 13: $N,\\theta$ Sobol' G X2-X8   0.000
## 14: $N,\\theta$ Sobol' G X3-X4   0.033
## 15: $N,\\theta$ Sobol' G X3-X5   0.001
## 16: $N,\\theta$ Sobol' G X3-X6   0.001
## 17: $N,\\theta$ Sobol' G X3-X7   0.001
```

```
## 18: $N,\\theta$ Sobol' G X3-X8   0.001
## 19: $N,\\theta$ Sobol' G X4-X5   0.025
## 20: $N,\\theta$ Sobol' G X4-X6   0.036
## 21: $N,\\theta$ Sobol' G X4-X7   0.026
## 22: $N,\\theta$ Sobol' G X4-X8   0.026
## 23: $N,\\theta$ Sobol' G X5-X6   0.779
## 24: $N,\\theta$ Sobol' G X5-X7   0.209
## 25: $N,\\theta$ Sobol' G X5-X8   0.666
## 26: $N,\\theta$ Sobol' G X6-X7   0.258
## 27: $N,\\theta$ Sobol' G X6-X8   0.588
## 28: $N,\\theta$ Sobol' G X7-X8   0.224
## 29:           N Sobol' G X1-X2   0.000
## 30:           N Sobol' G X1-X3   0.000
## 31:           N Sobol' G X1-X4   0.000
## 32:           N Sobol' G X1-X5   0.000
## 33:           N Sobol' G X1-X6   0.000
## 34:           N Sobol' G X1-X7   0.000
## 35:           N Sobol' G X1-X8   0.000
## 36:           N Sobol' G X2-X3   0.000
## 37:           N Sobol' G X2-X4   0.000
## 38:           N Sobol' G X2-X5   0.000
## 39:           N Sobol' G X2-X6   0.000
## 40:           N Sobol' G X2-X7   0.000
## 41:           N Sobol' G X2-X8   0.000
## 42:           N Sobol' G X3-X4   0.000
## 43:           N Sobol' G X3-X5   0.000
## 44:           N Sobol' G X3-X6   0.000
## 45:           N Sobol' G X3-X7   0.000
## 46:           N Sobol' G X3-X8   0.000
## 47:           N Sobol' G X4-X5   0.000
## 48:           N Sobol' G X4-X6   0.000
## 49:           N Sobol' G X4-X7   0.000
## 50:           N Sobol' G X4-X8   0.000
## 51:           N Sobol' G X5-X6   0.372
## 52:           N Sobol' G X5-X7   0.603
## 53:           N Sobol' G X5-X8   0.678
## 54:           N Sobol' G X6-X7   0.269
## 55:           N Sobol' G X6-X8   0.264
## 56:           N Sobol' G X7-X8   0.684
##         setting    Model    rn overlap
##
## [[4]]
##          setting  Model      rn overlap
##   1: $N,\\theta$ Morris   X1-X2   0.447
##   2: $N,\\theta$ Morris   X1-X3   0.000
##   3: $N,\\theta$ Morris   X1-X4   0.291
##   4: $N,\\theta$ Morris   X1-X5   0.000
##   5: $N,\\theta$ Morris   X1-X6   0.000
```

```
##  ---
## 376:           N Morris X17-X19   0.060
## 377:           N Morris X17-X20   0.000
## 378:           N Morris X18-X19   0.026
## 379:           N Morris X18-X20   0.000
## 380:           N Morris X19-X20   0.000
```

```
# Export results
rbindlist(final.overlap) %>%
  fwrite(., "sobol.overlap.csv")
```

4.6 Sensitivity analysis

```
# DATASET FOR SENSITIVITY ANALYSIS ----------------------------------------

full.dataset.sobol <- lapply(dt.models, function(x)
  melt(x, measure.vars = patterns("V"),
       variable.name = "parameter")) %>%
  rbindlist(.) %>%
  .[, Model:= ifelse(Model == 1, models[1],
                     ifelse(Model == 2, models[2],
                            ifelse(Model == 3, models[3], models[4])))] %>%
  .[, k:= NULL] %>%
  .[, parameter:= gsub("V", "X", parameter)] %>%
  .[, parameter:= factor(parameter,
                         levels = paste("X", 1:20, sep = ""))] %>%
  .[, Model:= factor(Model,
                     levels = c("Liu", "Ishigami", "Sobol' G", "Morris"))] %>%
  .[, setting:= ifelse(setting == "N.Theta", "$N,\\theta$", setting)]

# EXPORT SENSITIVITY MATRIX -----------------------------------------------

fwrite(full.dataset.sobol, "full.dataset.sobol.csv")
```

```
# SENSITIVITY ANALYSIS ----------------------------------------------------

sobol.sensitivity <- full.dataset.sobol[, sobol_indices(value,
                                                        type = "jansen",
                                                        params = parameters.sobol,
                                                        n = 2 ^ 13,
                                                        R = R,
                                                        parallel = "multicore",
                                                        ncpus = n_cores),
                                        .(Model, parameter, setting)]
```

```
# CONFIDENCE INTERVALS ----------------------------------------------------

# Arrange data
```

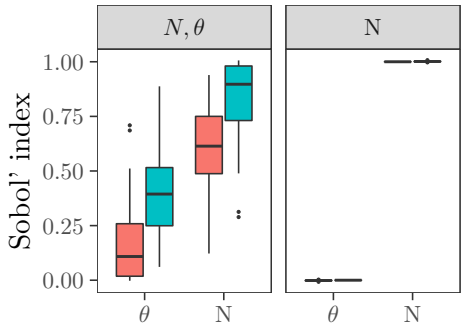
```r
tmp3 <- split(sobol.sensitivity, sobol.sensitivity$setting) %>%
  lapply(., function(x) split(x, x$Model)) %>%
  lapply(., function(x) lapply(x, function(y) split(y, y$parameter, drop = TRUE)))

# Compute confidence intervals
out <- list()
for(i in names(tmp3)) {
  for(j in names(tmp3[[i]])) {
    for(k in names(tmp3[[i]][[j]])) {
      out[[i]][[j]][[k]] <- sobol_ci(tmp3[[i]][[j]][[k]],
                                     params = parameters.sobol,
                                     type = type,
                                     conf = conf)
    }
  }
}
```

```
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
```

```
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to  1 \n Cannot calculate confidence intervals"
```

```
# ARRANGE DATA ------------------------------------------------------------

final.sobol <- lapply(out, function(x)
  lapply(x, function(y) rbindlist(y, idcol = "model.input"))) %>%
  lapply(., function(x) rbindlist(x, idcol = "Model")) %>%
  rbindlist(., idcol = "setting") %>%
  .[, Model:= factor(Model, levels = c("Liu", "Ishigami", "Sobol' G", "Morris"))] %>%
  .[, model.input:= factor(model.input, levels = paste("X", 1:20, sep = ""))] %>%
  .[, parameters:= gsub("Theta", "$\\\\theta$", parameters)]

# EXPORT DATA -------------------------------------------------------------

fwrite(final.sobol, "final.sobol.csv")
```

```
# PLOT SOBOL INDICES ------------------------------------------------------

ggplot(final.sobol, aes(parameters, original,
                        fill = sensitivity)) +
  geom_boxplot(outlier.size = 0.2) +
  labs(x = "",
       y = "Sobol' index") +
  scale_fill_discrete(name = "Sobol' indices",
                      labels = c(expression(S[italic(i)]),
                                 expression(S[italic(T[i])]))) +
  theme_bw() +
  facet_wrap(~setting) +
  theme(panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                         color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA),
        legend.position = "none")
```

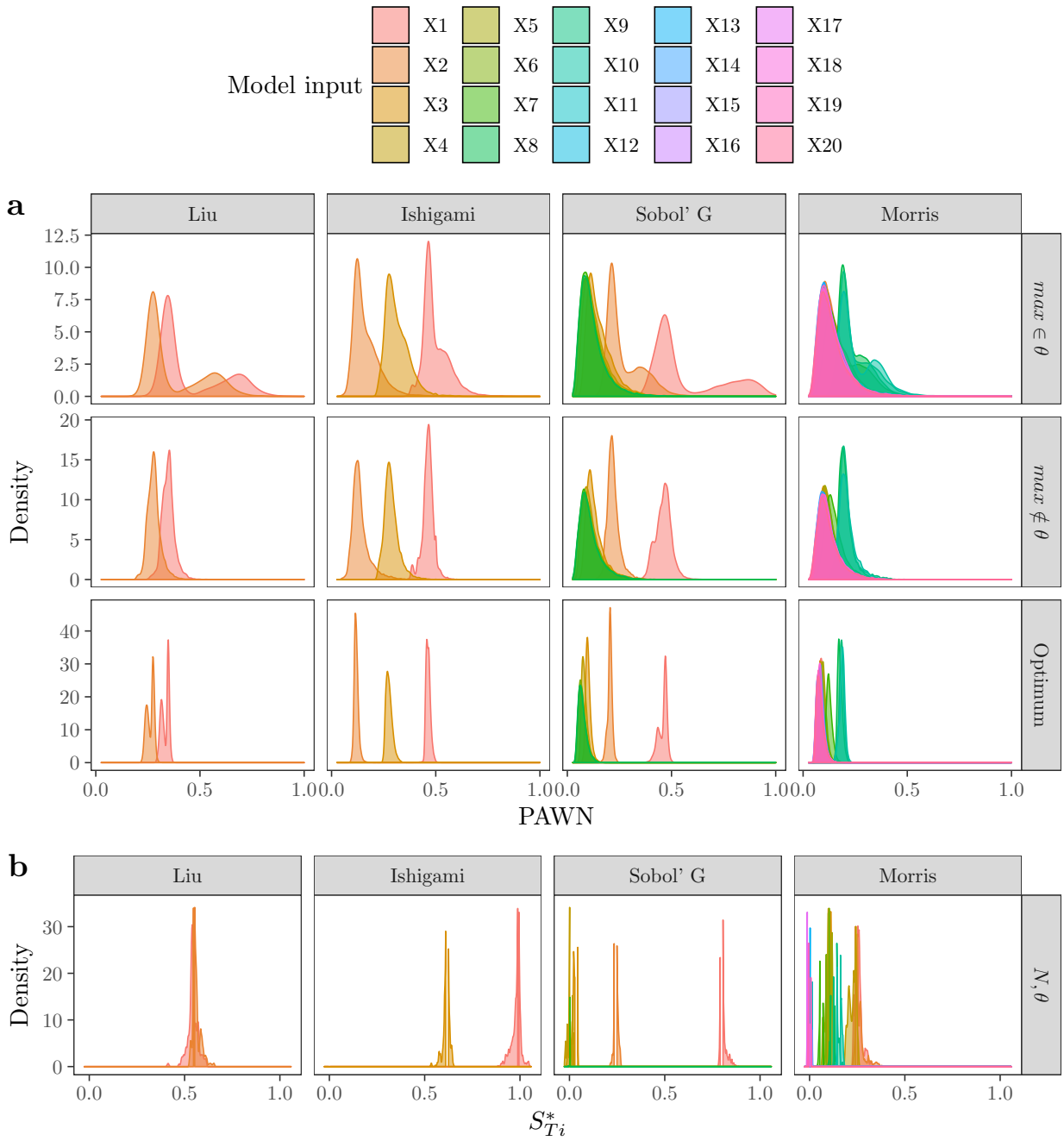


5 Extra plots

```
# MERGE UNCERTAINTY IN PAWN AND SOBOL'----------------------------------------

a <- plot.uncertainty.pawn +
  theme(legend.position = "none")

b <- AB.sobol[!setting == "N"] %>%
  ggplot(., aes(value,
                fill = parameter,
                color = parameter)) +
  geom_density(alpha = 0.5,
               position = "identity") +
  facet_grid(setting~Model) +
  scale_fill_discrete(name = "Model input") +
  scale_color_discrete(guide = FALSE) +
  labs(x = "$S_{Ti}^*$",
       y = "Density") +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  scale_y_continuous(limits = c(0, 35)) +
  theme_bw() +
  theme(legend.position = "none",
        legend.box = "horizontal",
        panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                         color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA))

# Get legend
legend <- get_legend(a + theme(legend.position = "top"))

# Merge
bottom <- plot_grid(a, b,
                    ncol = 1,
                    labels = "auto",
                    align = "h",
                    rel_heights = c(1, 0.46))
```

```
## Warning: Graphs cannot be horizontally aligned unless the axis parameter is
## set. Placing graphs unaligned.
```

```
plot_grid(legend, bottom,
          labels = c("", ""),
          ncol = 1,
          align = "",
          rel_heights = c(0.2, 1))
```




```
# PLOT AGGREGATED SOBOL' INDICES ------------------------------------------

a <- final.pawn.ci[sensitivity == "Si" | sensitivity == "STi"] %>%
  ggplot(., aes(parameters, original,
                fill = sensitivity)) +
  geom_boxplot(outlier.size = 0.2) +
  labs(x = "",
       y = "Sobol' index") +
  scale_fill_discrete(name = "Sobol' indices",
                      labels = c(expression(S[italic(i)]),
```

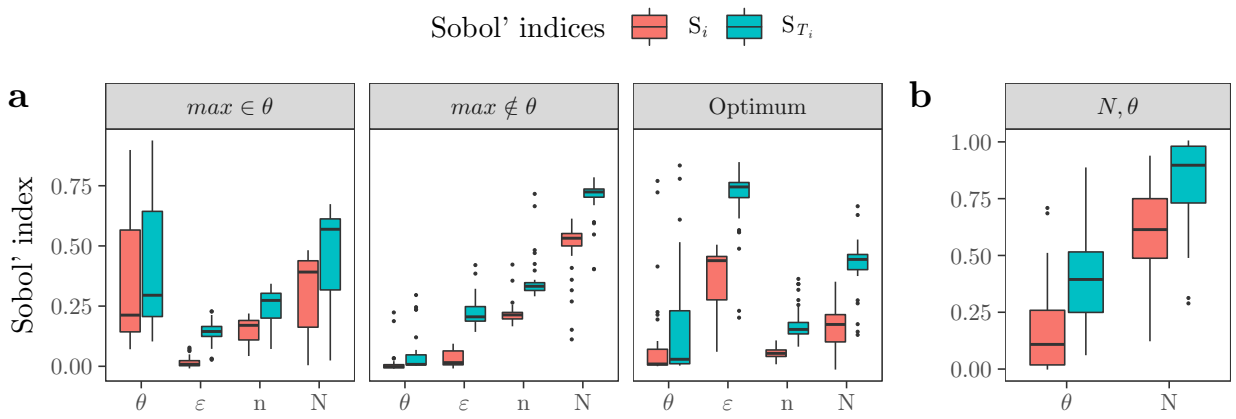
```
                                  expression(S[italic(T[i])]))) +
  theme_bw() +
  facet_wrap(~ setting) +
  theme(panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                         color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA),
        legend.position = "none")

legend <- get_legend(a + theme(legend.position = "top"))


b <- final.sobol[!setting == "N"] %>%
  ggplot(., aes(parameters, original, fill = sensitivity)) +
  geom_boxplot(outlier.size = 0.2) +
  labs(x = "",
       y = "") +
  scale_fill_discrete(name = expression(paste("Sobol'"~T[i])),
                      labels = c(expression(S[italic(i)]),
                                 expression(S[italic(T[i])]))) +
  facet_wrap(~ setting) +
  theme_bw() +
  theme(panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                         color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA),
        legend.position = "none")

bottom <- plot_grid(a, b,
                    ncol = 2,
                    align = "hv",
                    labels = "auto",
                    rel_widths = c(2.58, 1))
```

```
## Warning: Graphs cannot be vertically aligned unless the axis parameter is
## set. Placing graphs unaligned.
```

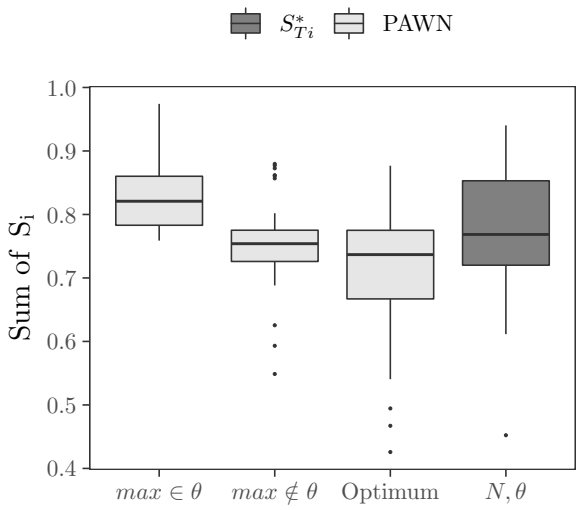
```
plot_grid(legend, bottom,
          ncol = 1,
          align = "hv",
          rel_heights = c(0.21, 1))
```

```
## Warning: Graphs cannot be vertically aligned unless the axis parameter is
## set. Placing graphs unaligned.
```

```
## Warning: Graphs cannot be horizontally aligned unless the axis parameter is
## set. Placing graphs unaligned.
```




```
# PLOT AGGREGATED SUM OF SI ----------------------------------------------------

final.sobol2 <- setnames(final.sobol, "Model", "model")

rbind(final.pawn.ci[sensitivity == "Si"][, type:= "PAWN"],
      final.sobol2[!setting == "N" & sensitivity == "Si"][, type:= "$S_{Ti}^*$"]) %>%
  .[, sum(original), .(setting, model, model.input, type)] %>%
  .[, setting:= factor(setting, levels = c("$max \\in \\theta$",
                                           "$max \\notin \\theta$",
                                           "Optimum",
                                           "$N,\\theta$"))] %>%
  ggplot(., aes(setting, V1, fill = type)) +
  scale_fill_grey(start = 0.5, end = 0.9,
                  name = "") +
  geom_boxplot(outlier.size = 0.2) +
  labs(x = "",
       y = expression(paste("Sum of"~S[i]))) +
  theme_bw() +
  theme(legend.position = "top",
        panel.grid.major = element_blank(),
        panel.grid.minor = element_blank())
```

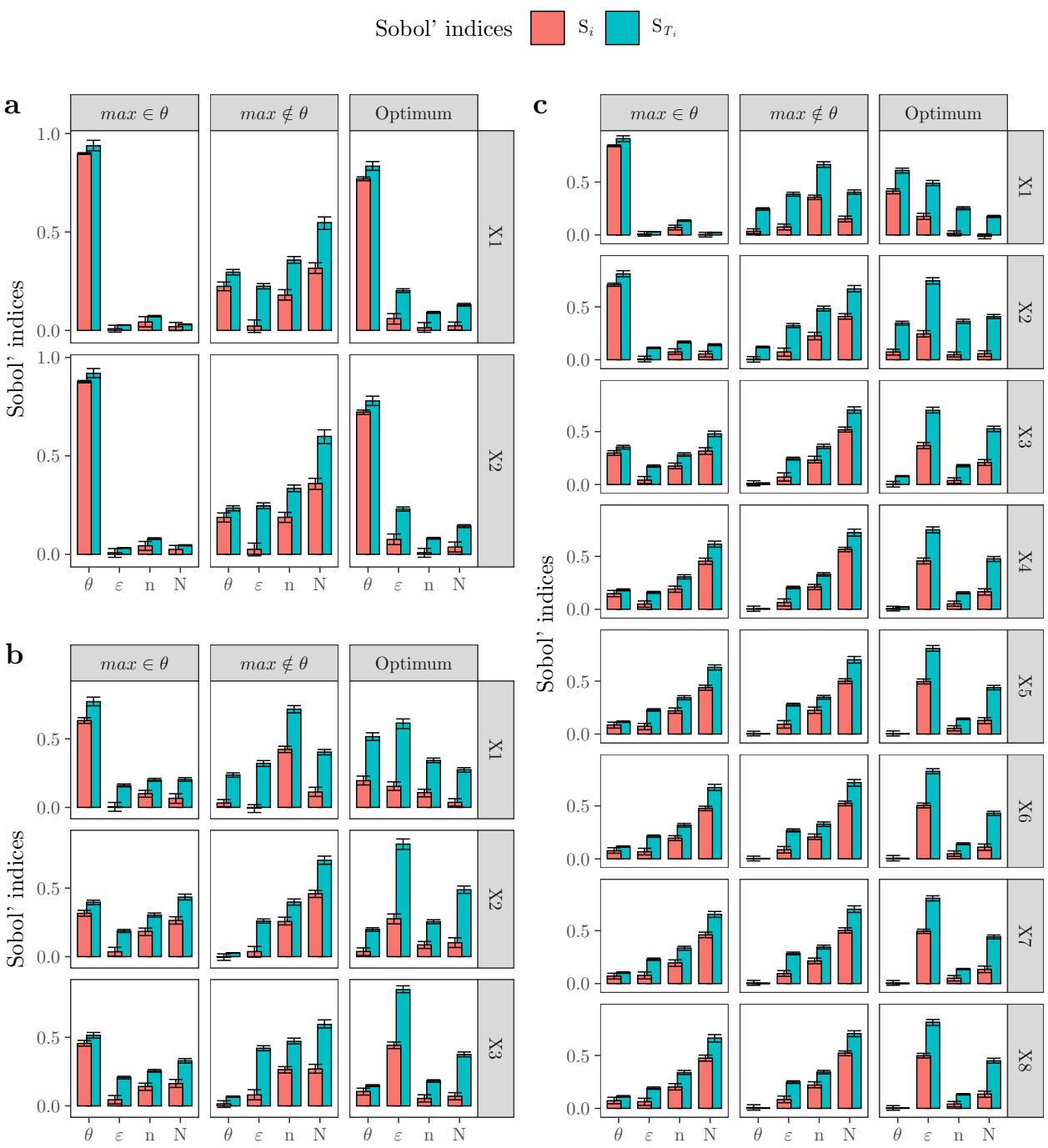



```
# ARRANGE TO PLOT SOBOL' INDICES FOR EACH FUNCTION ---------------------------

tmp <- split(final.pawn.ci, final.pawn.ci$model)
gg <- list()
for(i in names(tmp)) {
  for(j in 1:3) {
    gg[[i]][[j]] <- plot_sobol(tmp[[i]], type = j) +
      scale_y_continuous(breaks = pretty_breaks(n = 3)) +
      facet_grid(model.input ~ setting) +
      labs(x = "",
           y = "Sobol' indices") +
      theme(legend.position = "none")
  }
}
# Extract legend
legend <- get_legend(gg[[1]][[1]] + theme(legend.position = "top"))

# PLOT SOBOL' INDICES FOR LIU, ISHIGAMI AND SOBOL' G --------------------------

all <- lapply(1:3, function(x) {
  left <- plot_grid(gg[[1]][[x]], gg[[2]][[x]],
                    labels = c("a", "b"),
                    align = "h",
                    ncol = 1)
  plot_grid(left, gg[[3]][[x]],
            labels = c("", "c"),
            ncol = 2)
})
```

```
## Warning: Graphs cannot be horizontally aligned unless the axis parameter is
## set. Placing graphs unaligned.

## Warning: Graphs cannot be horizontally aligned unless the axis parameter is
```

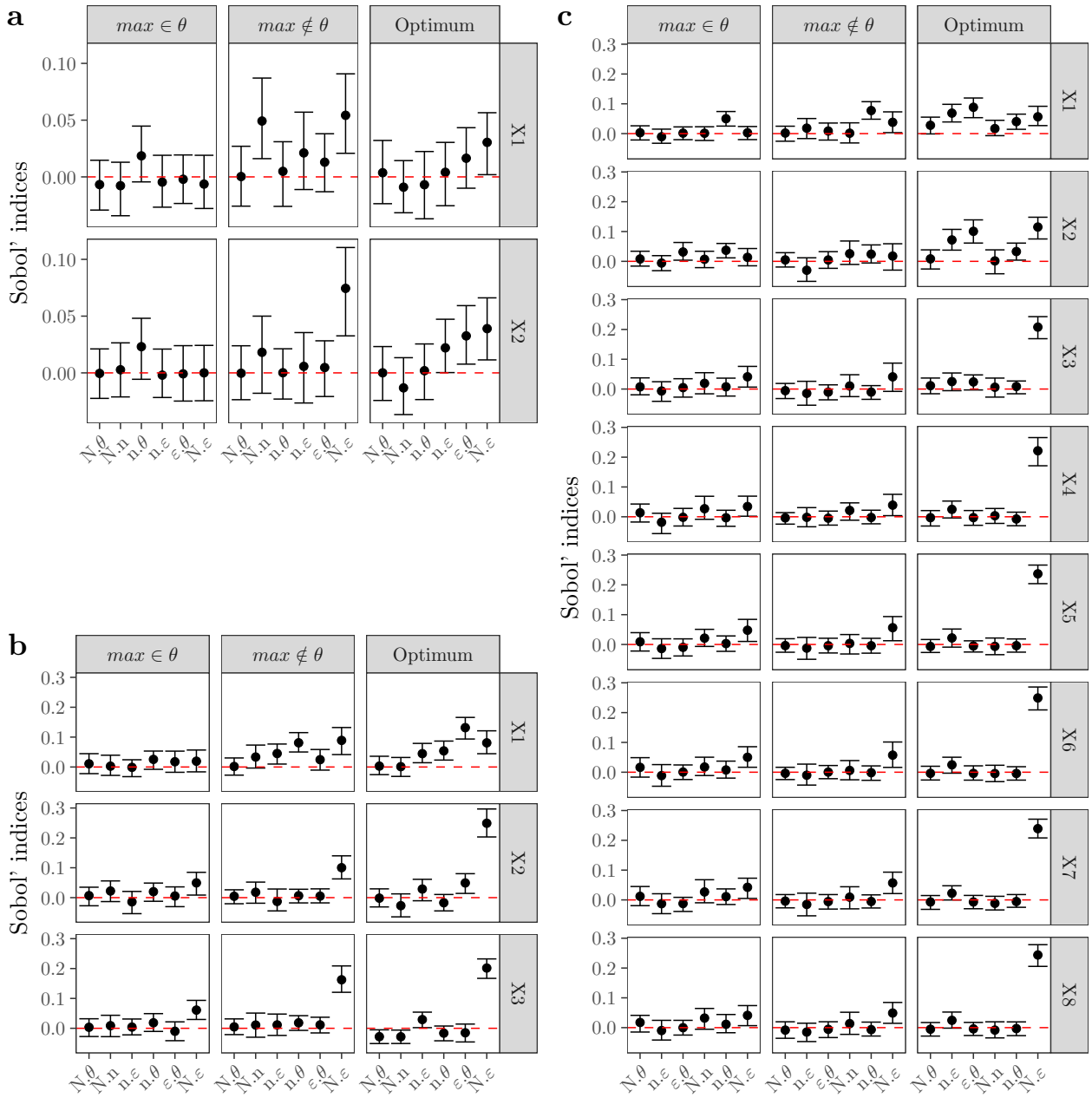
```
## set. Placing graphs unaligned.

## Warning: Graphs cannot be horizontally aligned unless the axis parameter is
## set. Placing graphs unaligned.
```

```
plot_grid(legend, all[[1]],
          ncol = 1,
          rel_heights = c(0.1, 1))
```

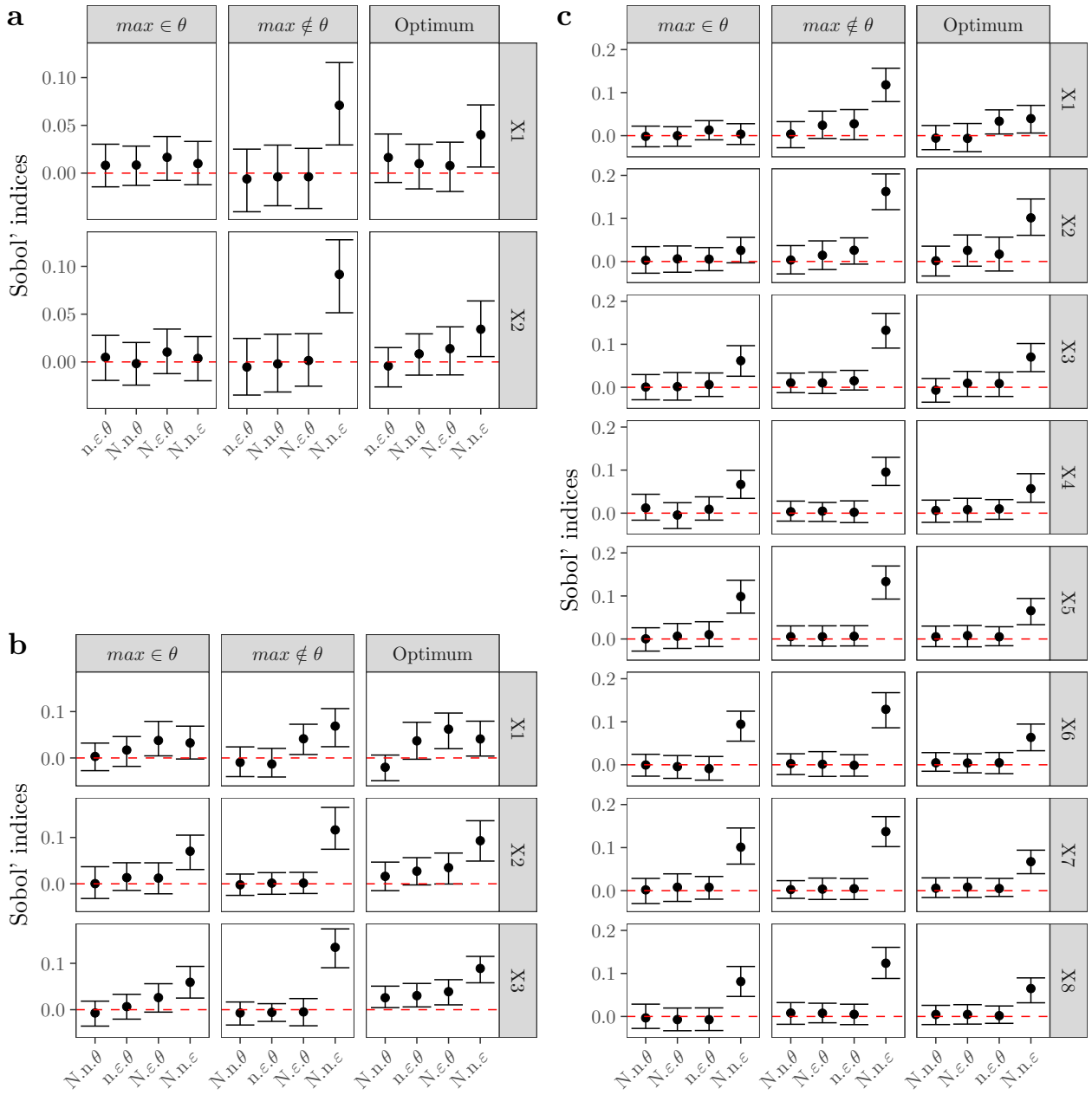


```
lapply(2:3, function(x) all[x])
```

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

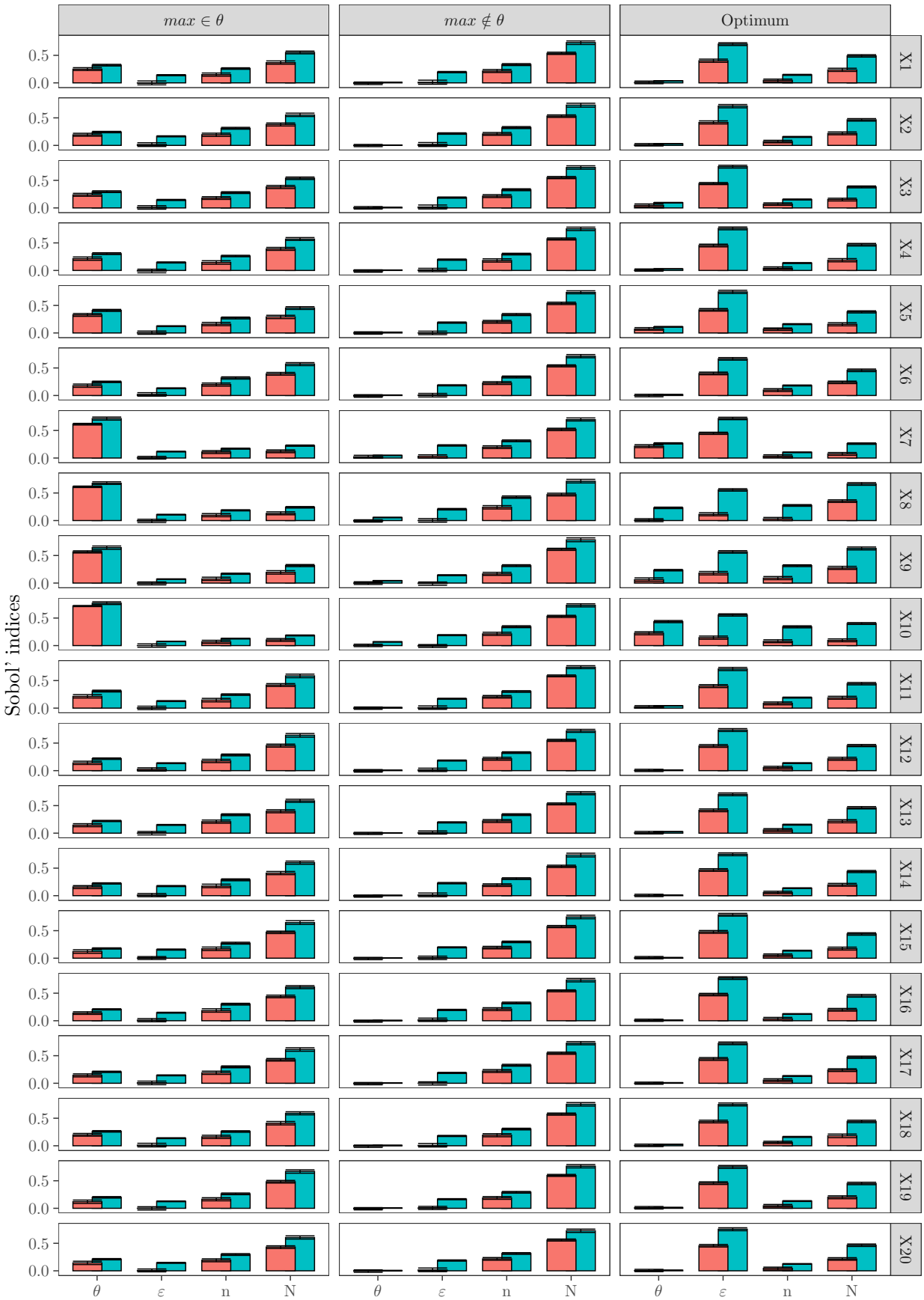



```
##
##
## [[2]]
## [[2]][[1]]
```

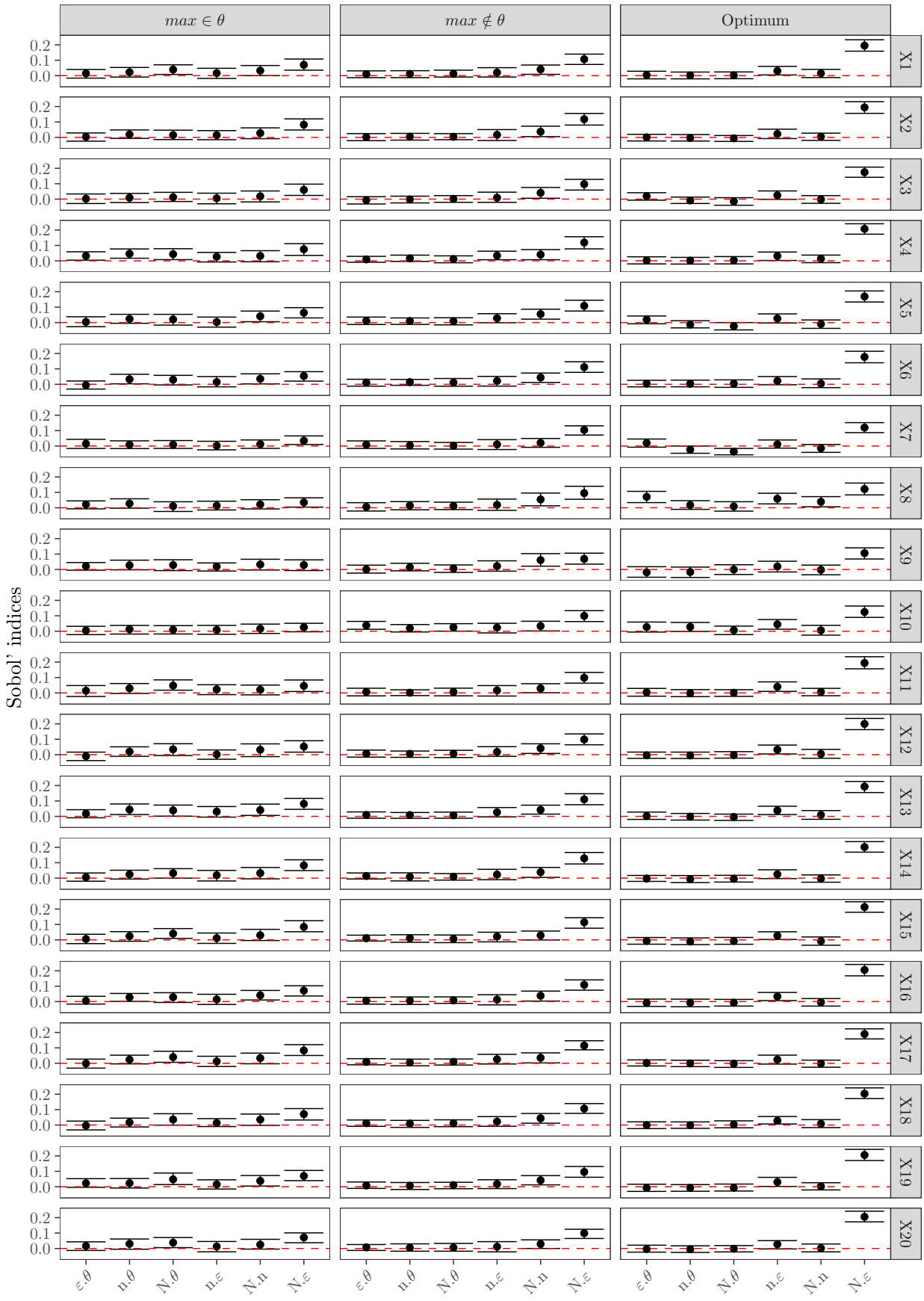



```
# PLOT SOBOL' INDICES FOR THE MORRIS FUNCTION ---------------------------------

lapply(1:3, function(x) gg[[4]][[x]])
```

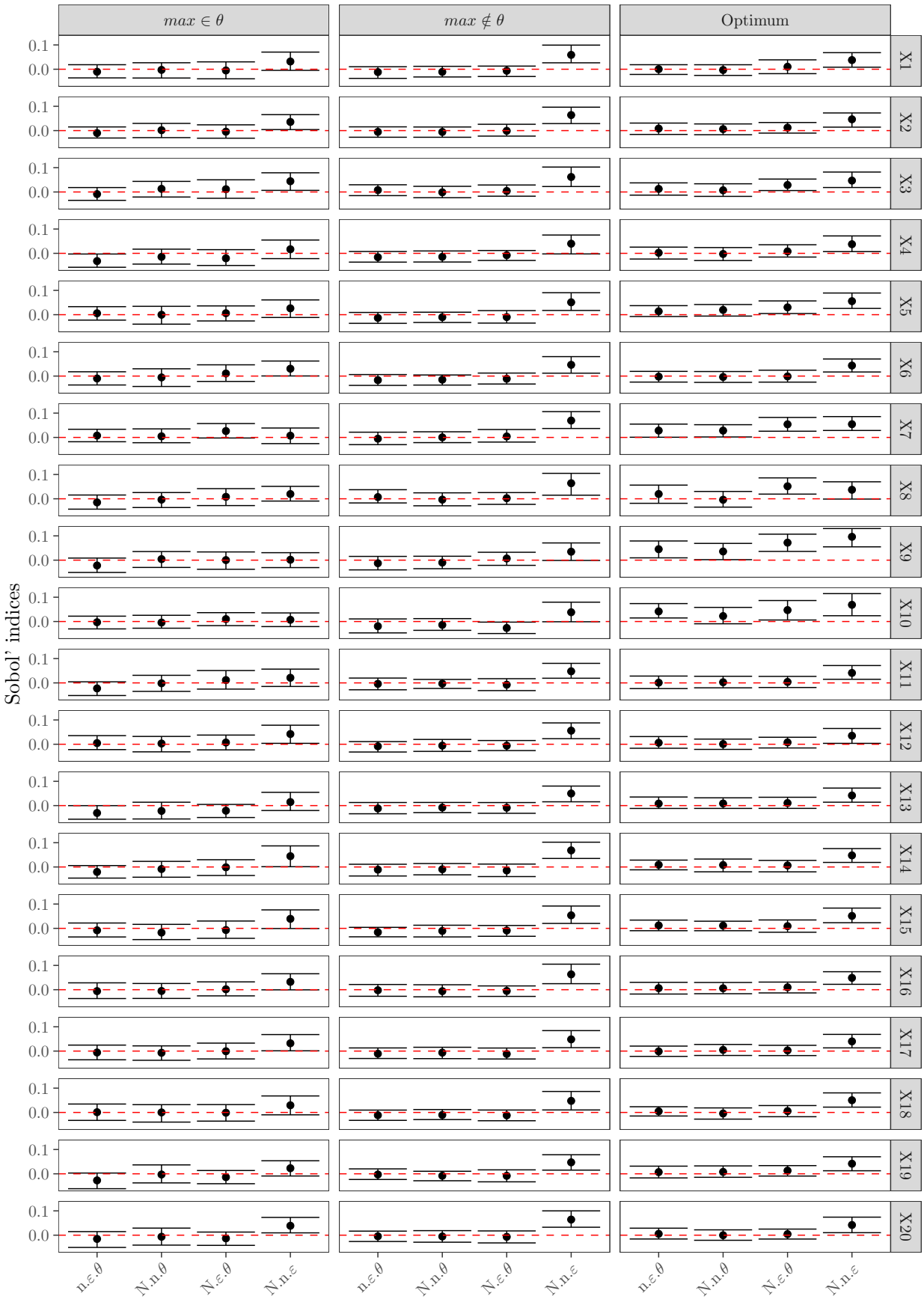
```
## [[1]]
```


$max \in \theta$
$max \notin \theta$
Optimum
X1
X2
X3
X4
X5
X6
X7
X8
X9
X10
X11
X12
X13
X14
X15
X16
X17
X18
X19
X20
Sobol' indices
0.0
0.5
θ
ε
n
N

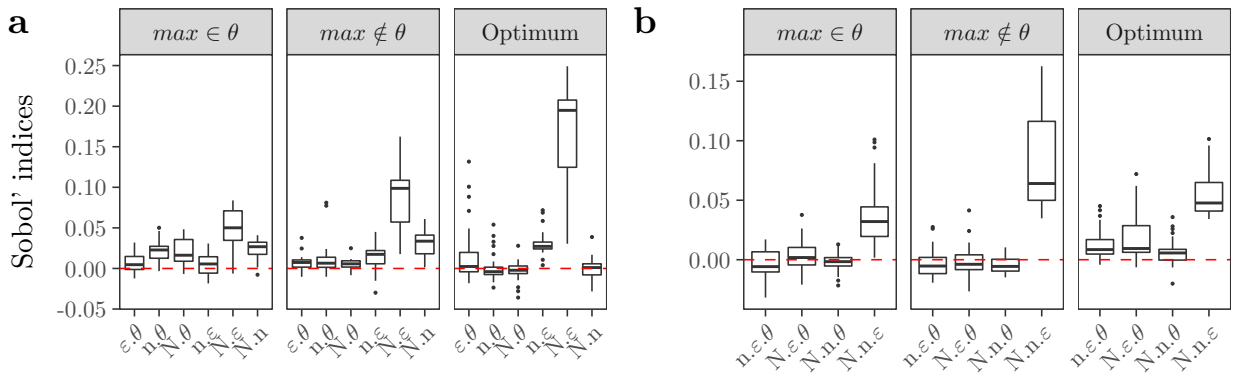
```
##
## [[2]]
```


$max \in \theta$
$max \notin \theta$
Optimum
X1
X2
X3
X4
X5
X6
X7
X8
X9
X10
X11
X12
X13
X14
X15
X16
X17
X18
X19
X20
Sobol' indices
0.0
0.1
0.2
ε.θ
n.θ
N.θ
n.ε
N.n
N.ε

```
##
## [[3]]
```


$max \in \theta$
$max \notin \theta$
Optimum
Sobol' indices
0.1
0.0
X1
X2
X3
X4
X5
X6
X7
X8
X9
X10
X11
X12
X13
X14
X15
X16
X17
X18
X19
X20
n.ε.θ
N.n.θ
N.ε.θ
N.n.ε

```r
# MERGE SECOND AND THIRD-ORDER EFFECTS ----------------------------------------

gg <- list()
second.third <- c("Sij", "Sijk")
for(i in second.third) {
  gg[[i]] <- final.pawn.ci[sensitivity == i] %>%
    ggplot(., aes(parameters, original)) +
    geom_boxplot(outlier.size = 0.2) +
    labs(x = NULL,
         y = "Sobol' indices") +
    scale_fill_discrete(name = "Sobol' indices",
                        labels = c(expression(S[italic(i)]),
                                   expression(S[italic(T[i])]))) +
    theme_bw() +
    geom_hline(yintercept = 0,
               lty = 2,
               color = "red") +
    facet_wrap(~ setting) +
    theme(legend.position = "none",
          panel.grid.major = element_blank(),
          panel.grid.minor = element_blank(),
          axis.text.x = element_text(angle = 45,
                                     hjust = 1))
}

# PLOT SECOND AND THIRD-ORDER EFFECTS ----------------------------------------

plot_grid(gg[[1]],
          gg[[2]] + labs(x = "", y = ""),
          ncol = 2,
          labels = "auto",
          align = "hv")
```




```r
# PLOT AGGREGATED SOBOL' INDICES AFTER WEIGHTING ------------------------------

final.pawn.ci[sensitivity == "Si" |sensitivity == "STi"] %>%
  # For each function, setting and design parameter, compute
```

```
# the median value of Si and STi
.[, .(Median = median(original)),
  by = .(setting, model, sensitivity, parameters)] %>%
# Compute the aggregated median and the percentiles
.[, .(aggregated.median = median(Median),
      low.ci = quantile(Median, probs = 0.025),
      high.ci = quantile(Median, probs = 0.975)),
  by = .(setting, sensitivity, parameters)] %>%
ggplot(., aes(parameters, aggregated.median,
              color = sensitivity)) +
geom_point(position = position_dodge(0.6)) +
geom_errorbar(aes(ymin = low.ci,
                  ymax = high.ci),
              position = position_dodge(0.6)) +
labs(x = "",
     y = "Sobol' indices") +
scale_color_discrete(name = "Sobol' indices",
                     labels = c(expression(S[italic(i)]),
                                expression(S[italic(T[i])]))) +
theme_bw() +
facet_wrap(~ setting) +
theme(panel.grid.major = element_blank(),
      panel.grid.minor = element_blank(),
      legend.background = element_rect(fill = "transparent",
                                       color = NA),
      legend.key = element_rect(fill = "transparent",
                                color = NA),
      legend.position = "top")
```