A sensitivity analysis of the PAWN sensitivity index

Arnald Puy, Samuele Lo Piano, Andrea Saltelli

Contents

1 Preliminary functions

```r
# 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

```r
# 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

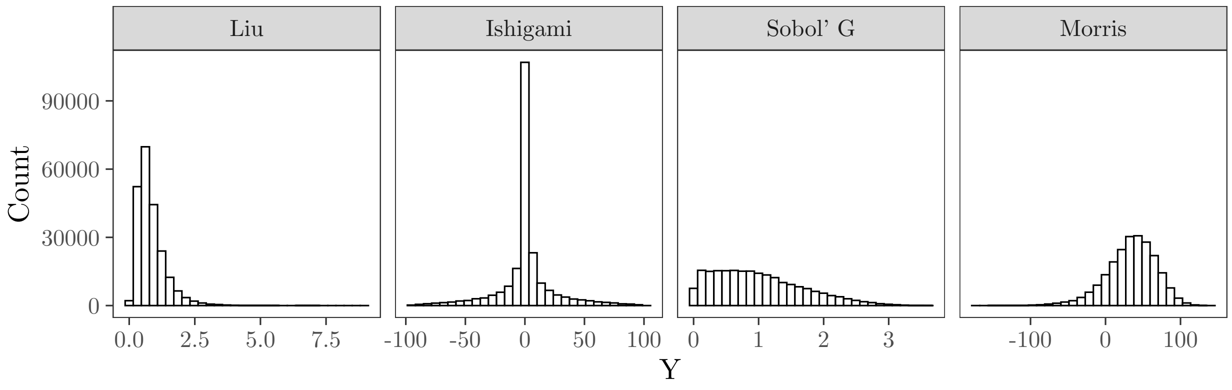
```r
# CONSTRUCT SAMPLE MATRICES -----------------------------------------------------

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
}
```

```r
# 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

```r
# 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]])
  }
}
```

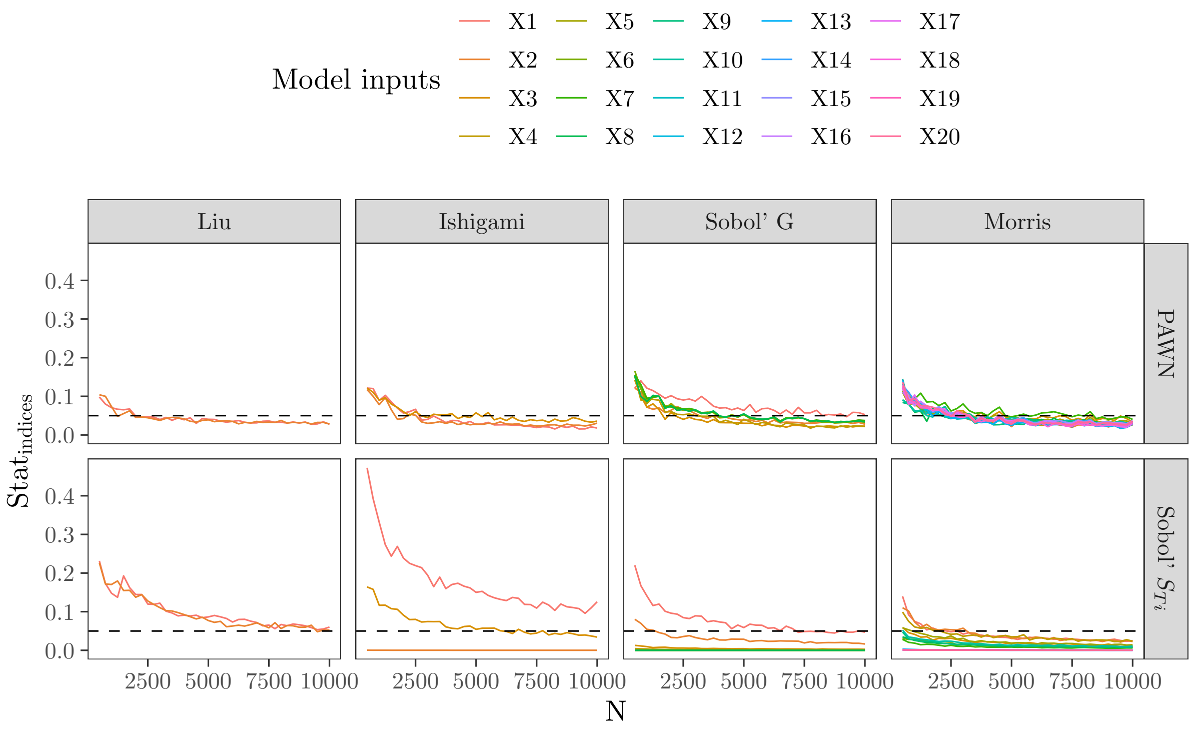
```
# PAWN AND CONFIDENCE INTERVALS OF DUMMY PARAMETER ----------------------------

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")) %>%
```

```r
  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"]
```

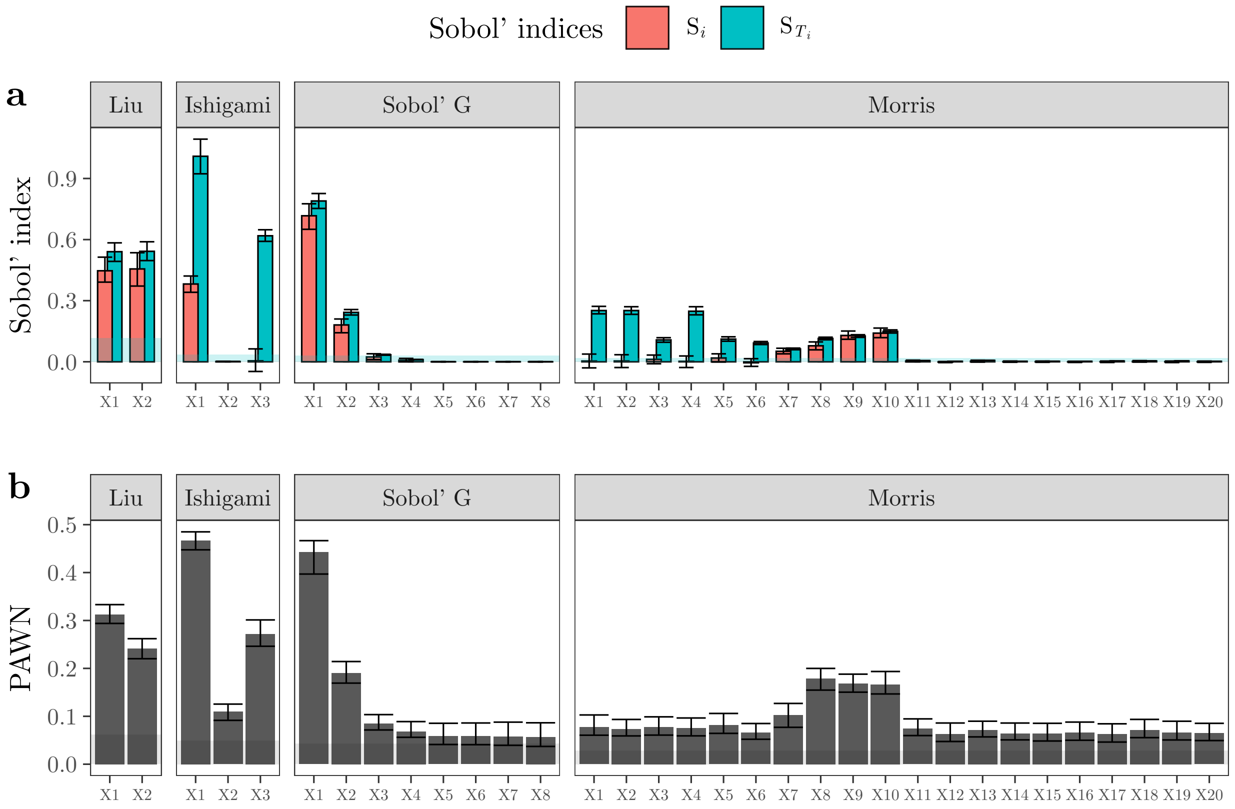
2.5 Plot convergence

```r
# 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))
```

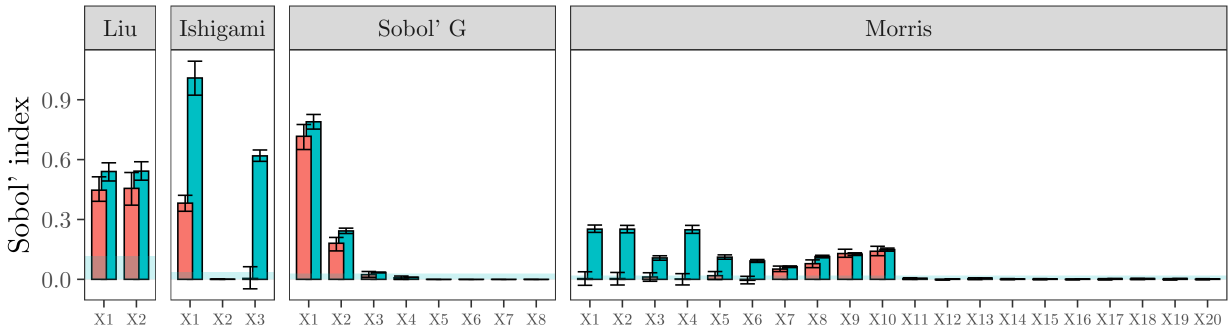


```
# PLOT SOBOL' AND PAWN INDICES -----------------------------------------------

# 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,
```

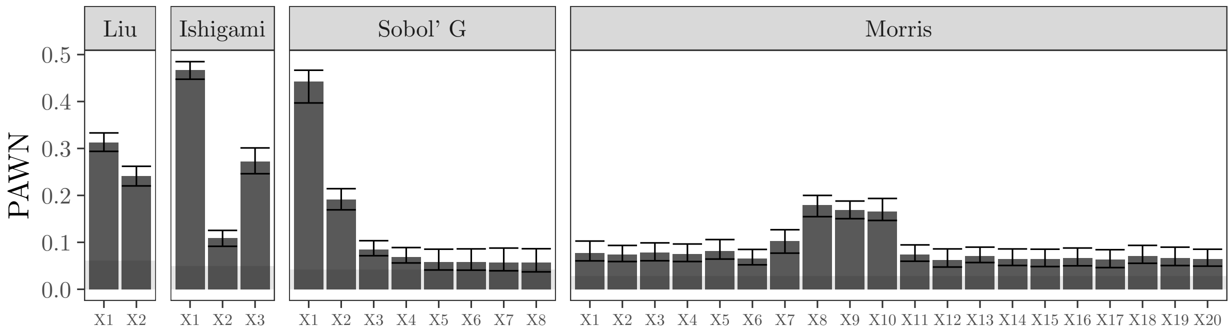
```r
             inherit.aes = FALSE) +
  labs(x = "",
       y = "PAWN") +
  facet_grid(~ model,
             scales = "free_x",
             space = "free_x") +
  theme(axis.text.x = element_text(size = 6))

# 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))
```



```r
# 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"))]
```

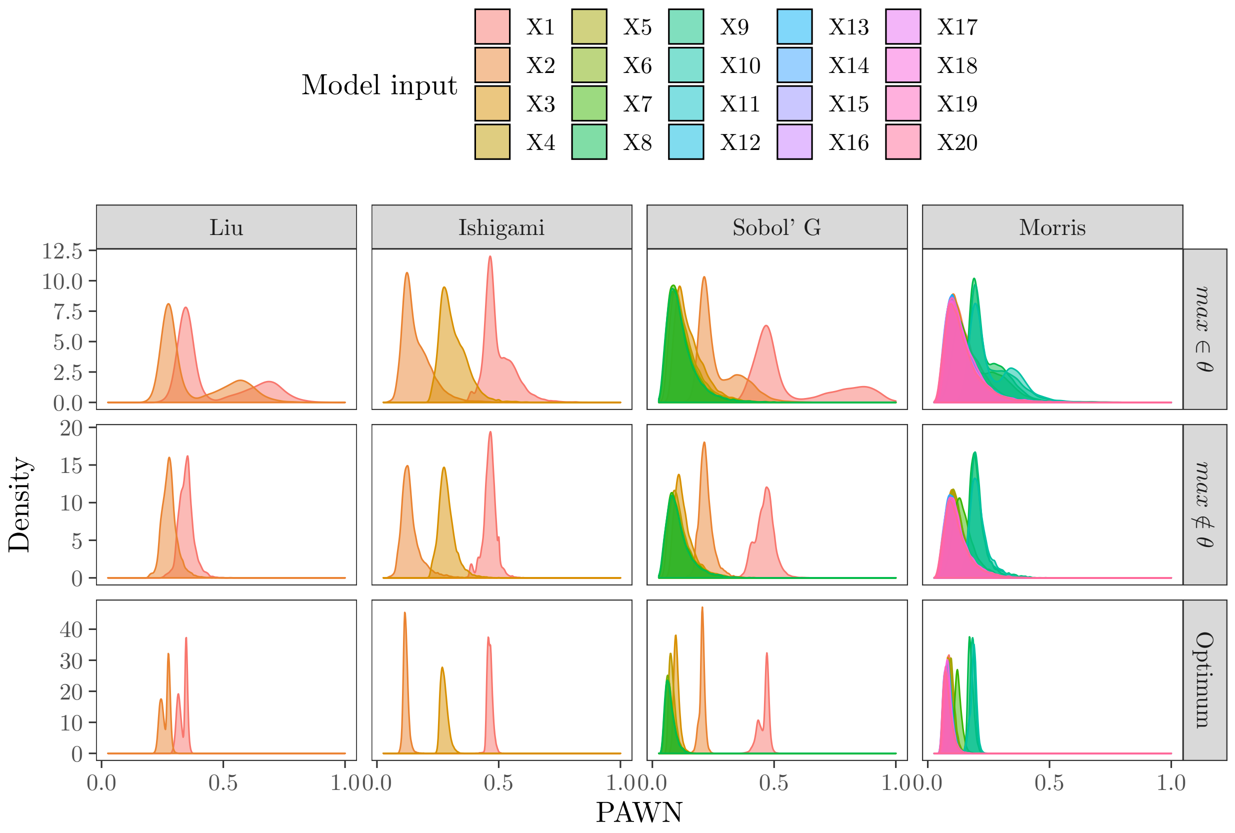
```r
# CHECK OVERLAP ----------------------------------------------------------------

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"))]
```

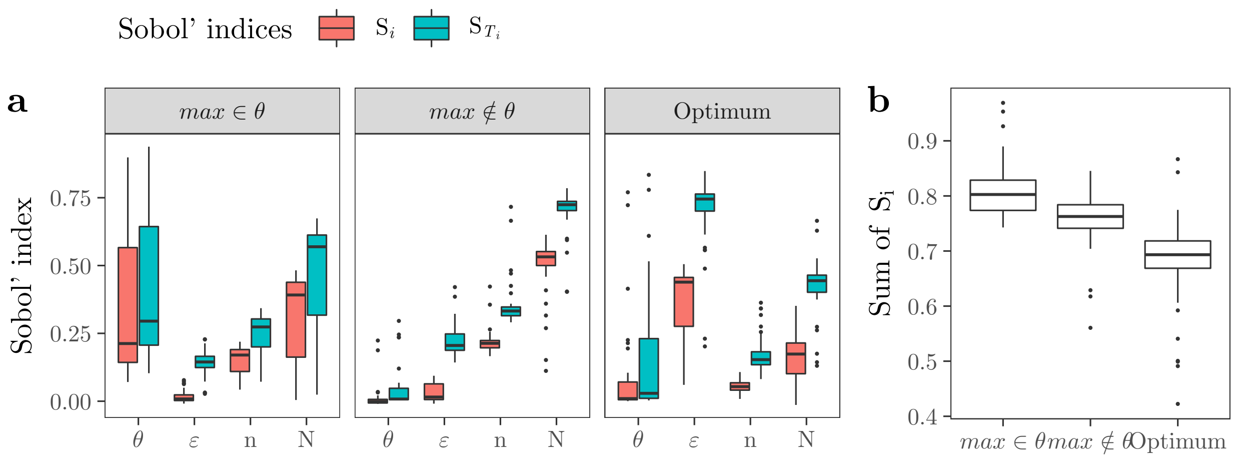
```r
# EXPORT DATA -----------------------------------------------------------------

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.
```

```r
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

```r
# 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

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

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

4.3 Sample matrix

```r
# 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

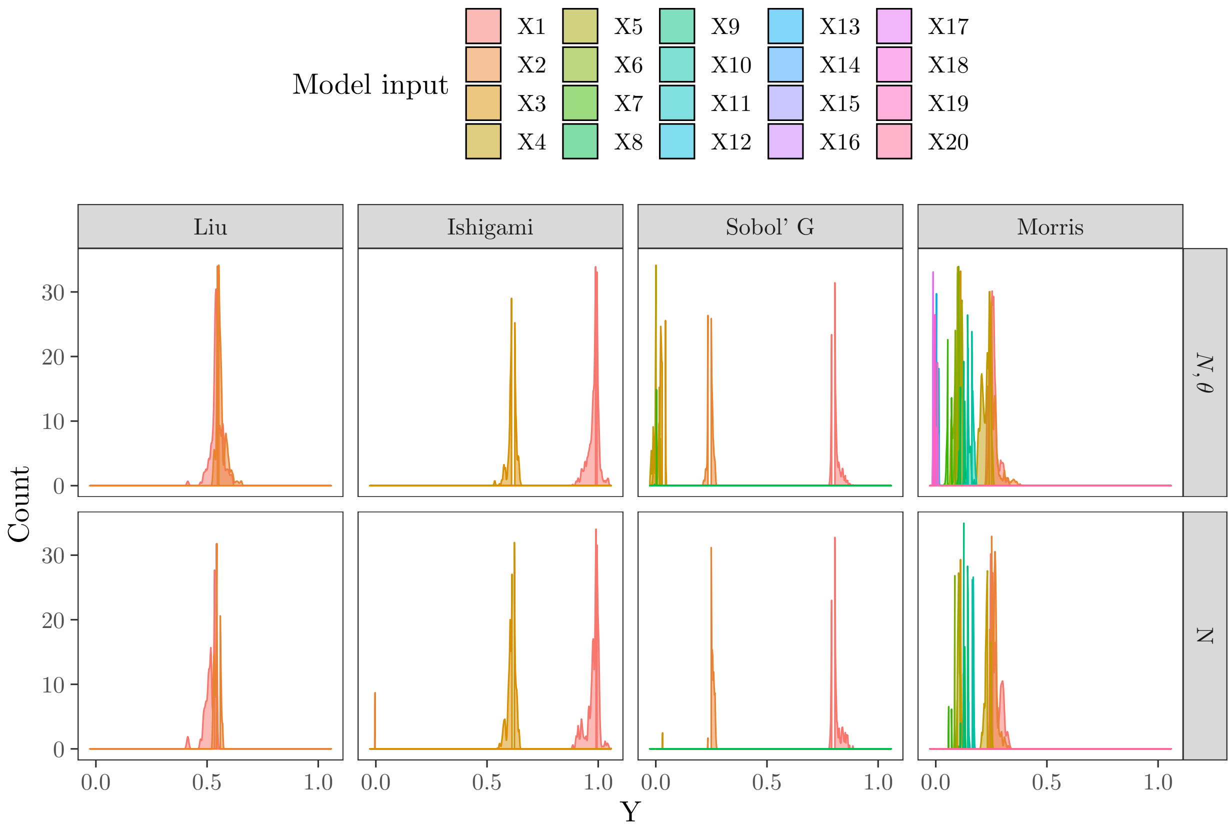
```r
# RUN MODEL -------------------------------------------------------------------

# 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

```r
# 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")
```

```r
# 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))
```



```r
# 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)]
```

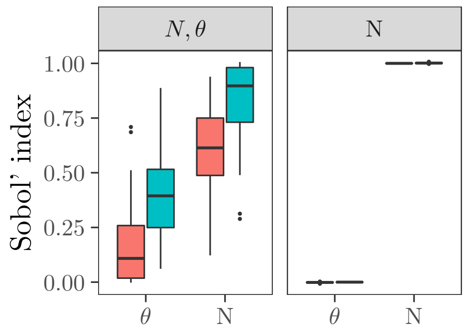
```
# CONFIDENCE INTERVALS -------------------------------------------------------

# 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"
```

```r
# 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")
```

```r
# 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")
```

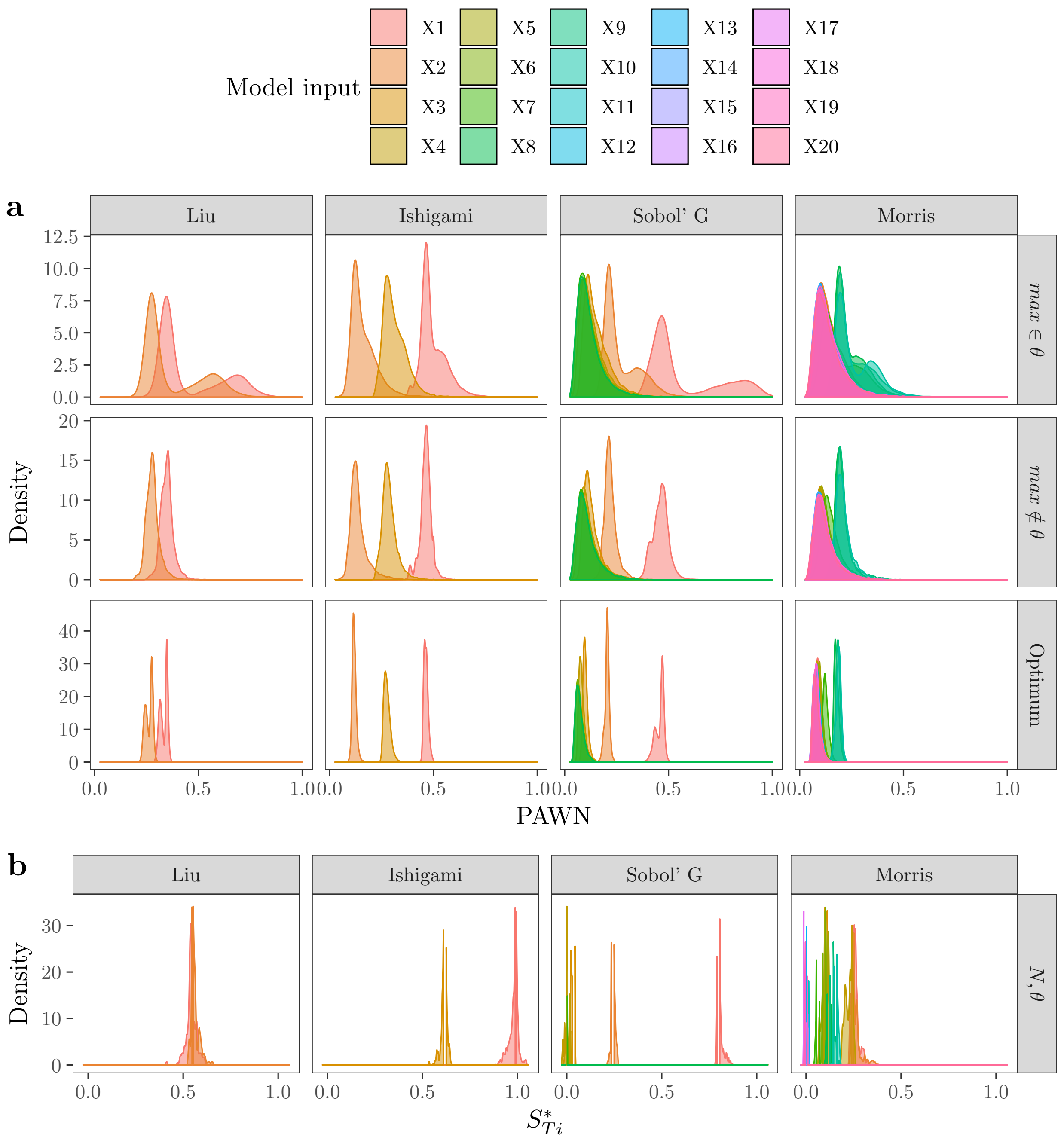


5 Extra plots

```r
# 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.
```

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

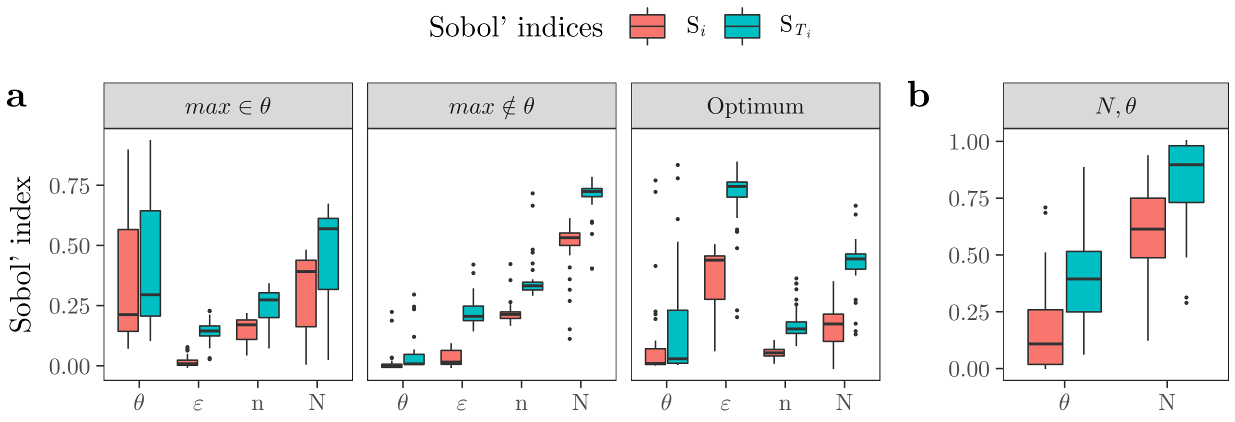


```
# PLOT AGGREGATED SOBOL' INDICES -----------------------------------------------

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))
```

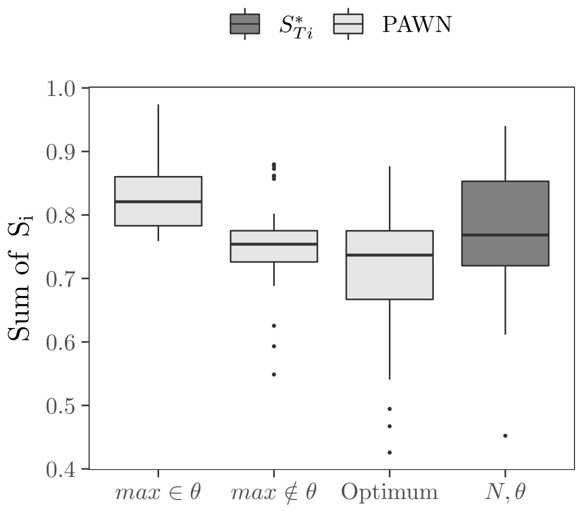
```
## Warning: Graphs cannot be vertically aligned unless the axis parameter is
## set. Placing graphs unaligned.
```

```
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.
```



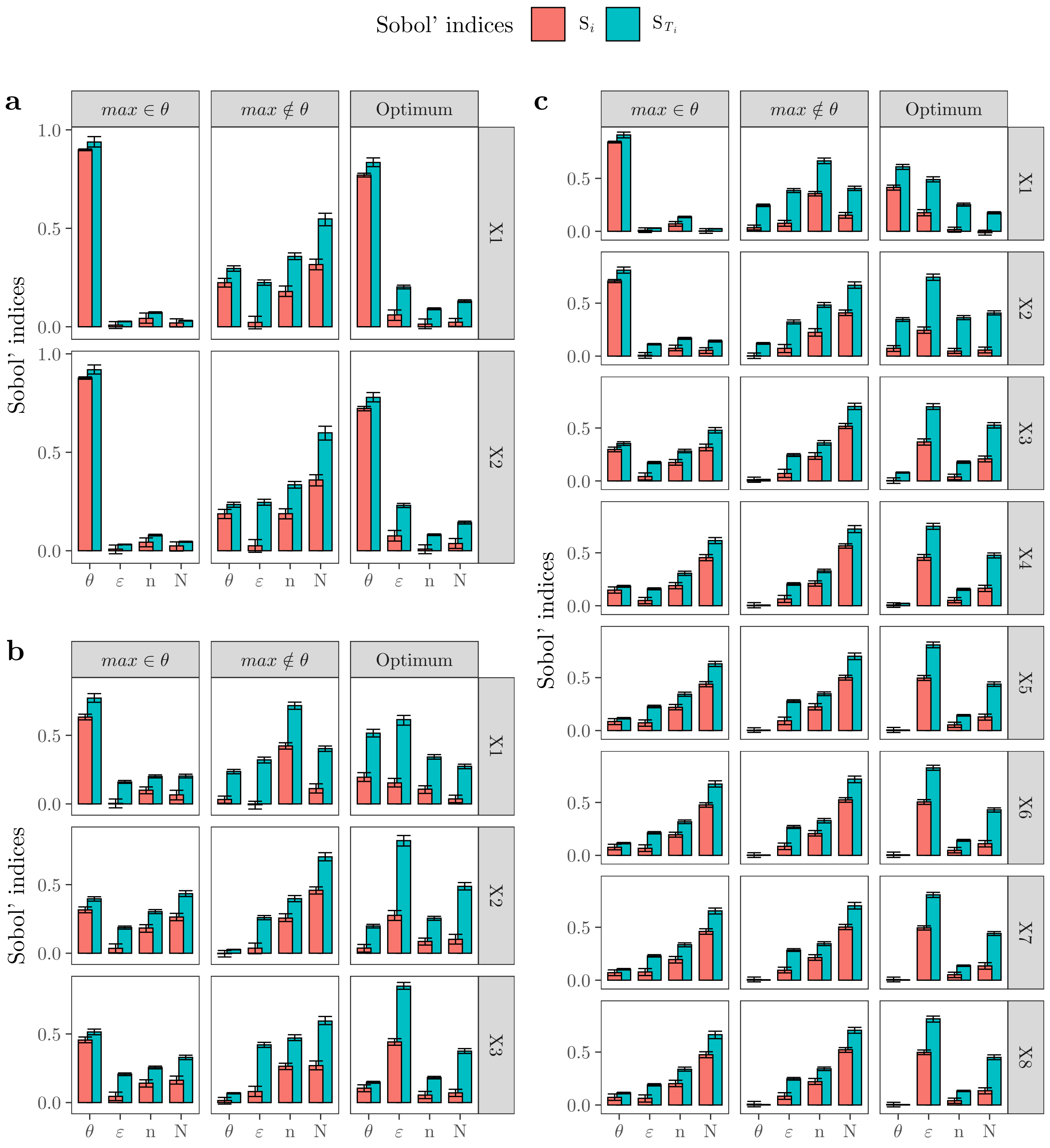
```
# PLOT AGGREGATED SUM OF SI ---------------------------------------------------

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())
```



```r
# 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)
})
```

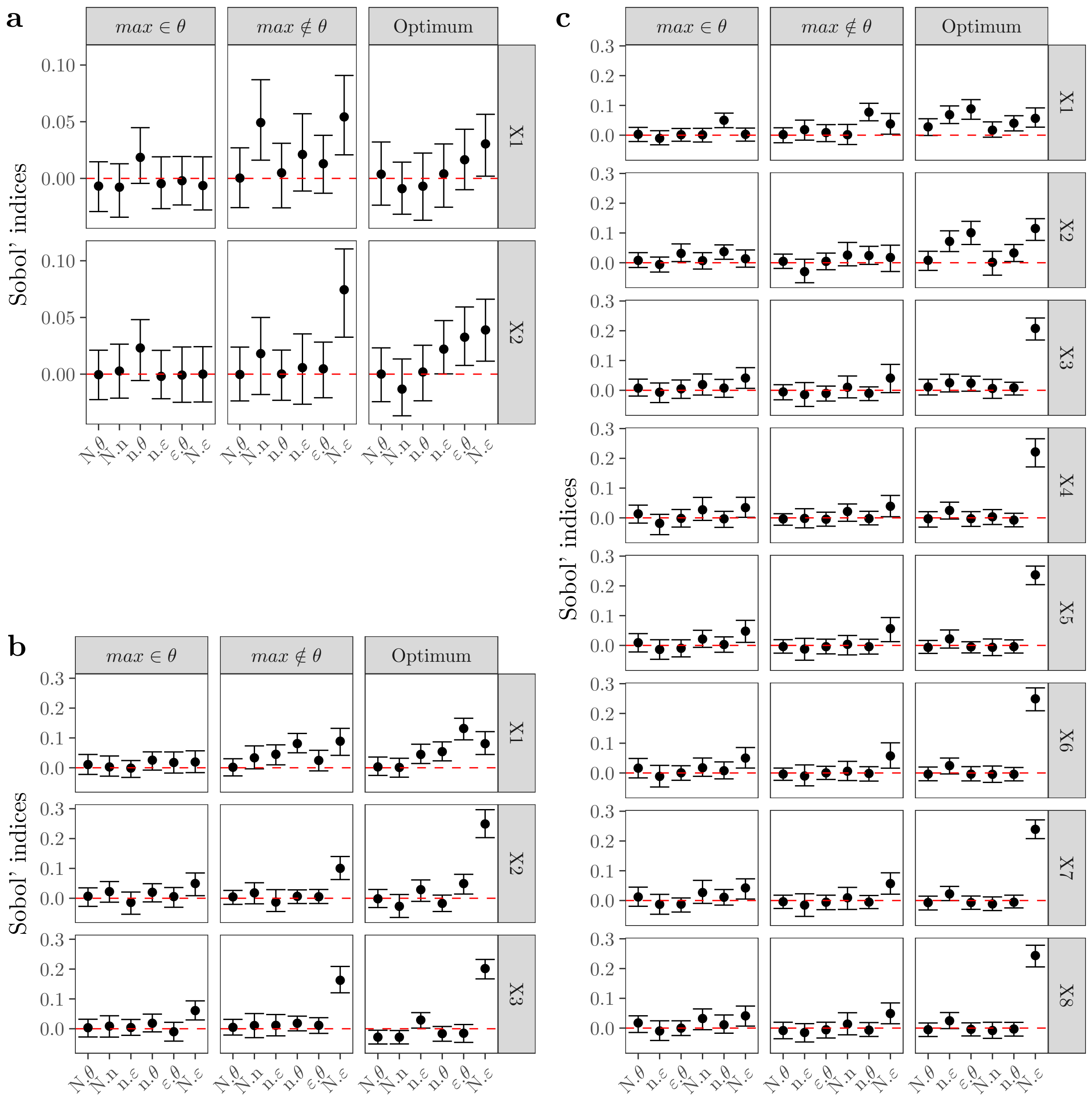
```
## Warning: Graphs cannot be horizontally aligned unless the axis parameter is
## set. Placing graphs unaligned.

## 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))
```

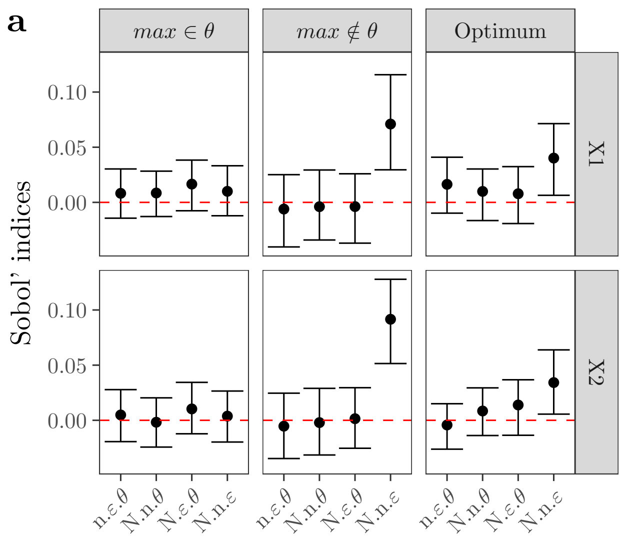


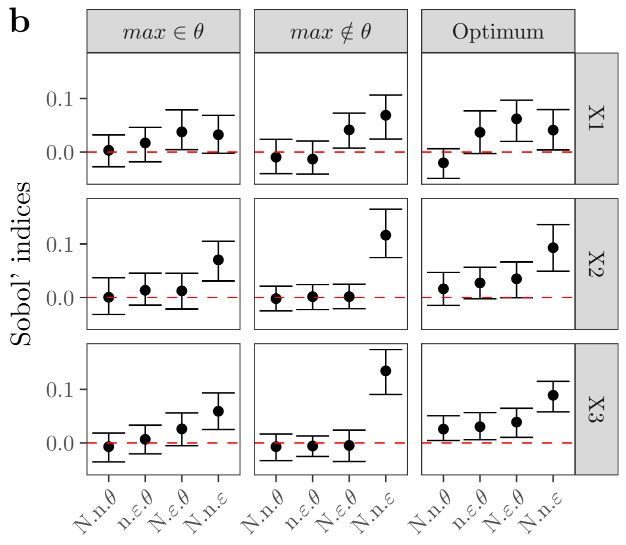
```
lapply(2:3, function(x) all[x])
```

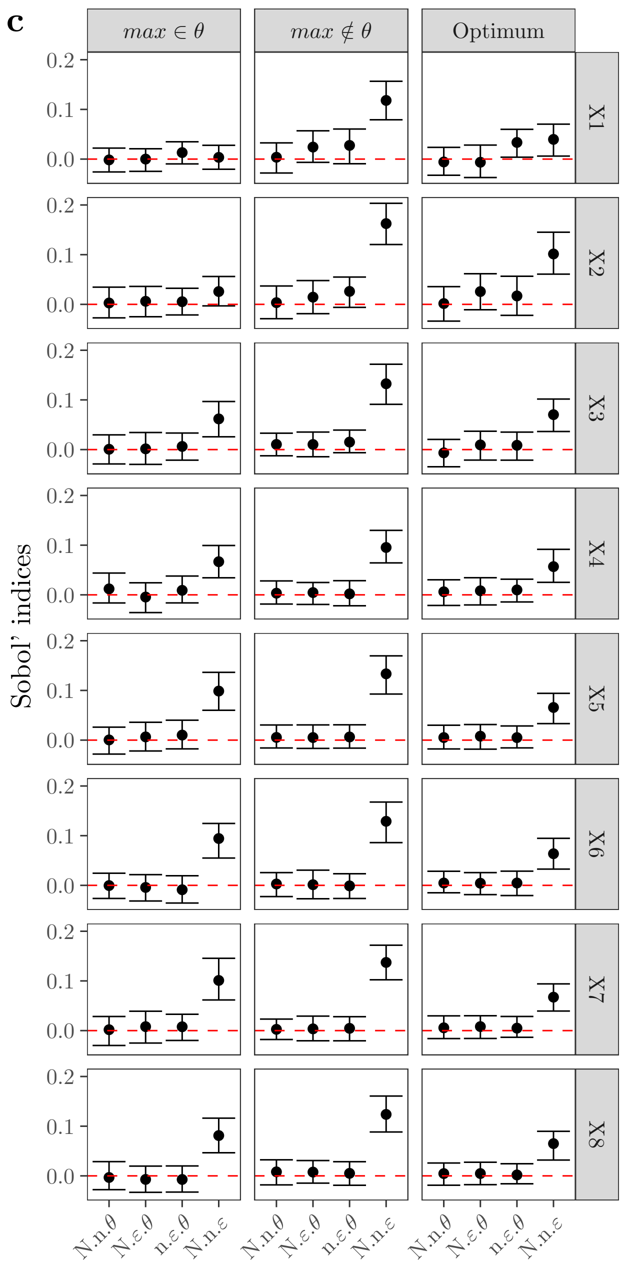
```
## [[1]]
## [[1]][[1]]
```



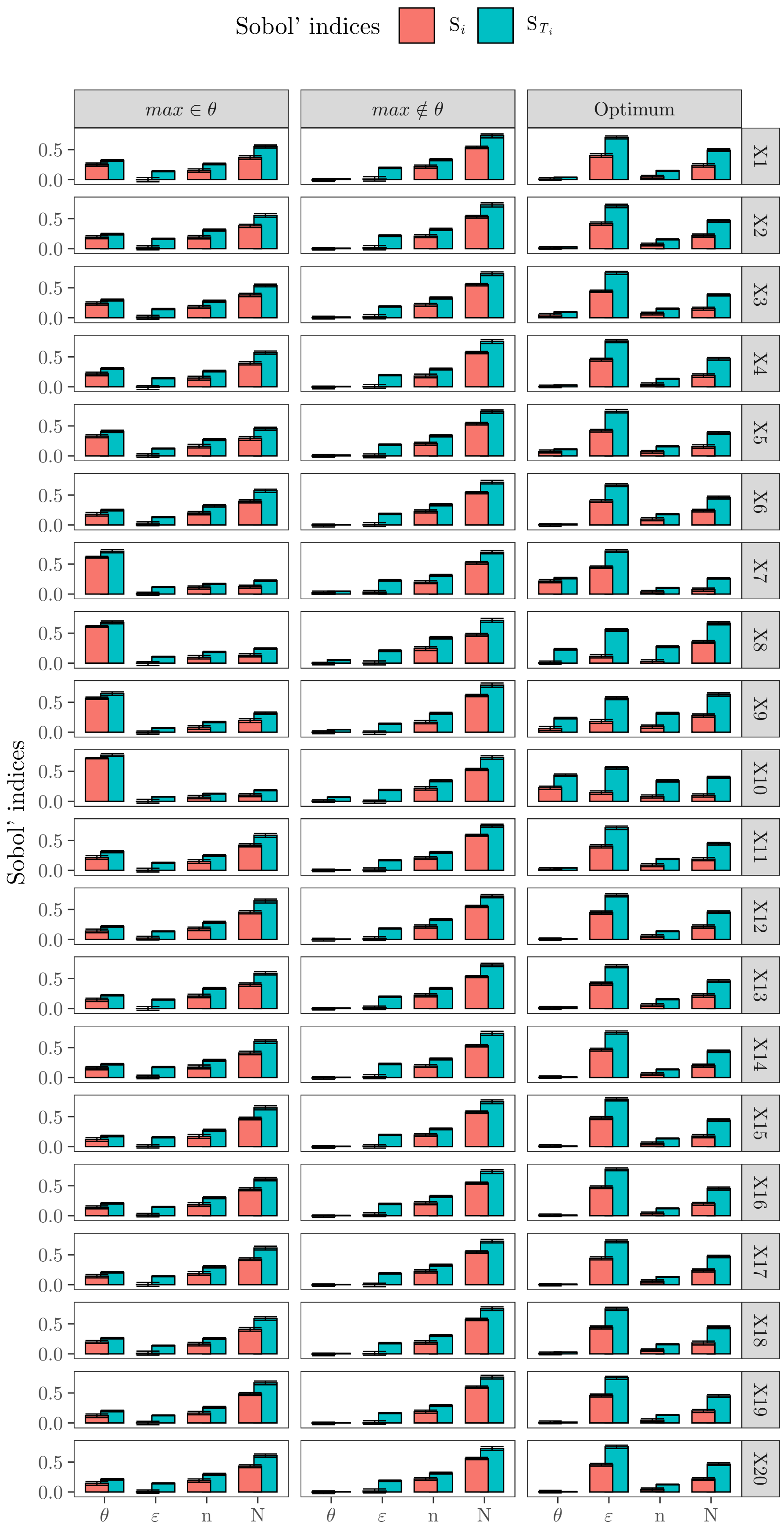
```
##
##
## [[2]]
## [[2]][[1]]
```





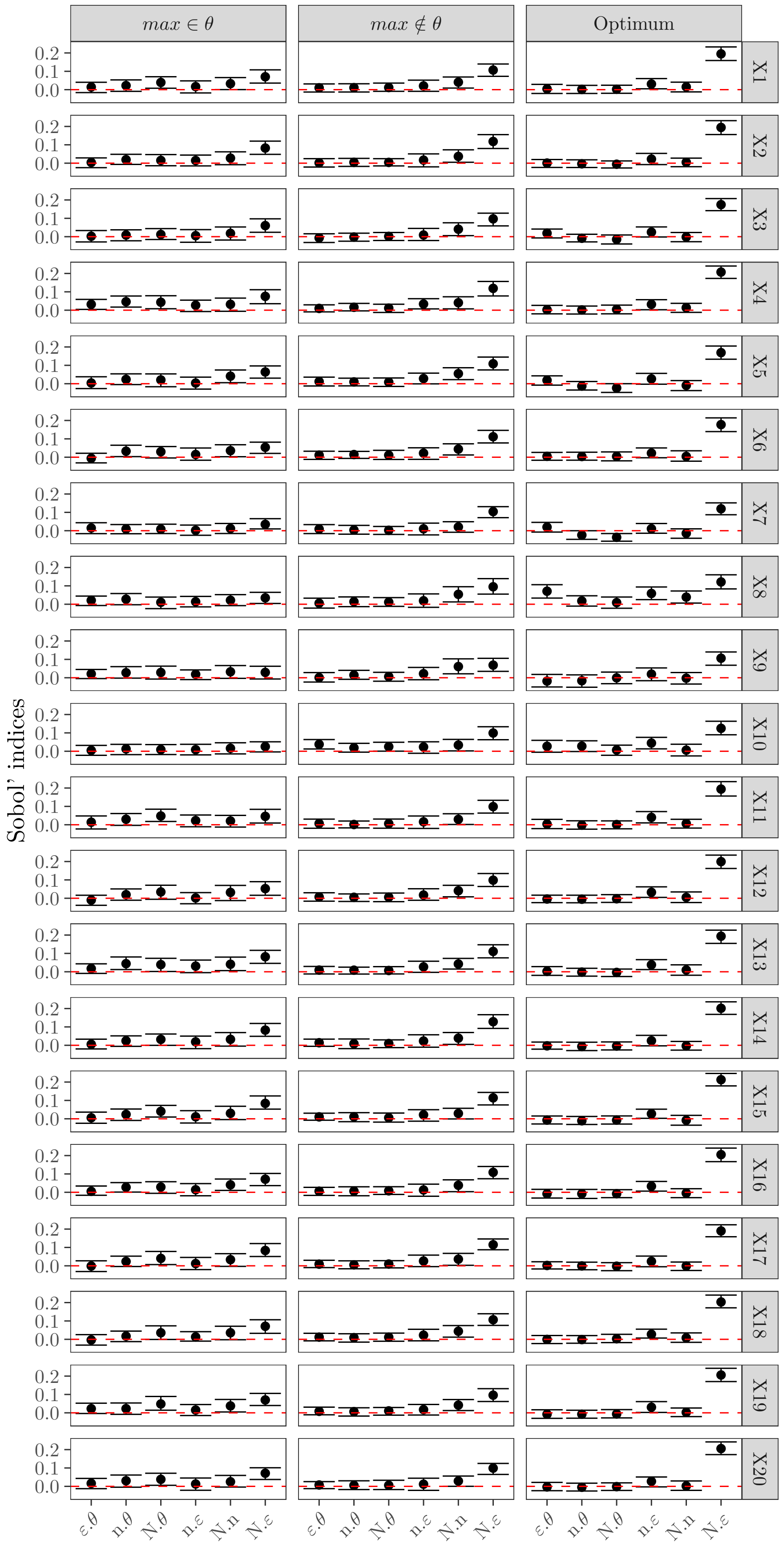


```
# PLOT SOBOL' INDICES FOR THE MORRIS FUNCTION ---------------------------------

plot_grid(legend, gg[[4]][[1]],
          ncol = 1,
          rel_heights = c(0.07, 1))
```


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

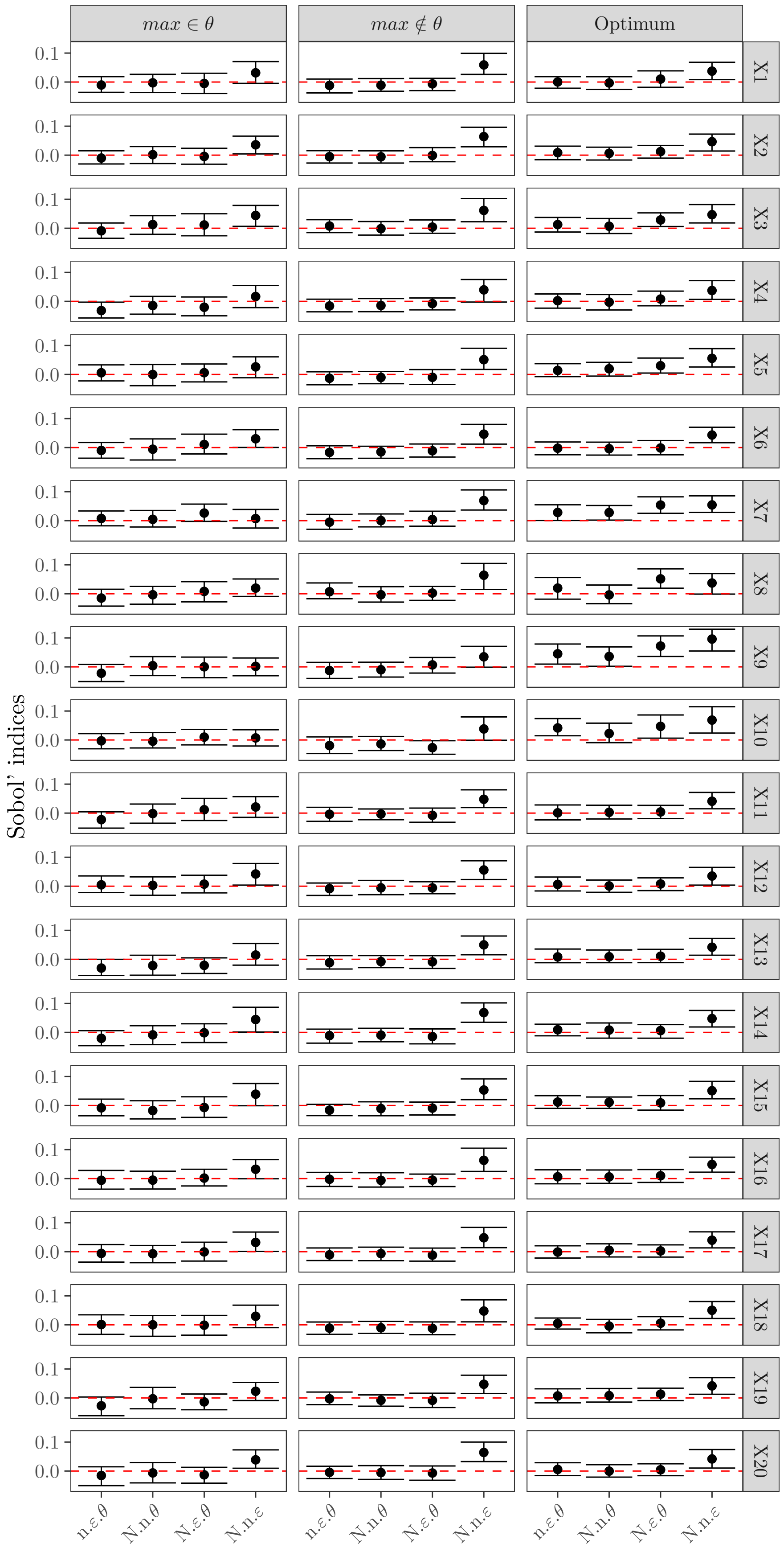
```r
lapply(2:3, function(x) gg[[4]][[x]])
```

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



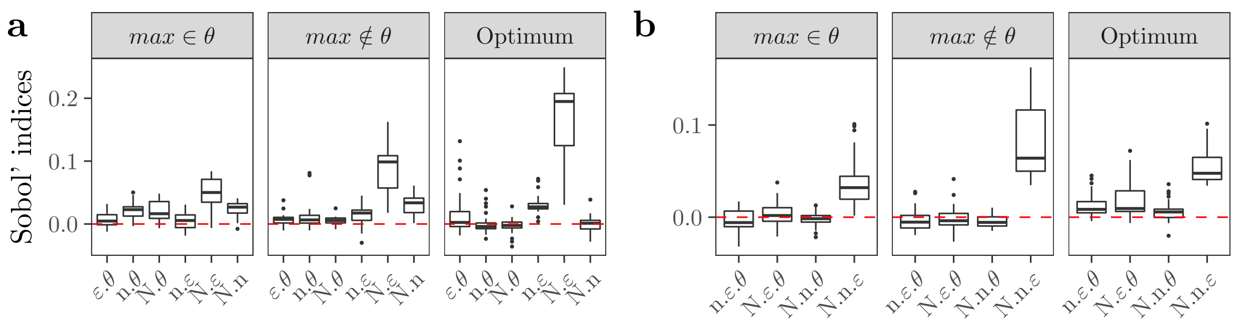
$max \in \theta$
$max \notin \theta$
Optimum
Sobol' indices
0.2
0.1
0.0
X1
X2
X3
X4
X5
X6
X7
X8
X9
X10
X11
X12
X13
X14
X15
X16
X17
X18
X19
X20
$\varepsilon.\theta$
$n.\theta$
$N.\theta$
$n.\varepsilon$
$N.n$
$N.\varepsilon$

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



$max \in \theta$
$max \notin \theta$
Optimum
0.1
0.0
X1
X2
X3
X4
X5
X6
X7
X8
X9
X10
X11
X12
X13
X14
X15
X16
X17
X18
X19
X20
Sobol' indices
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") +
    scale_y_continuous(breaks = pretty_breaks(n = 3)) +
    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")
```



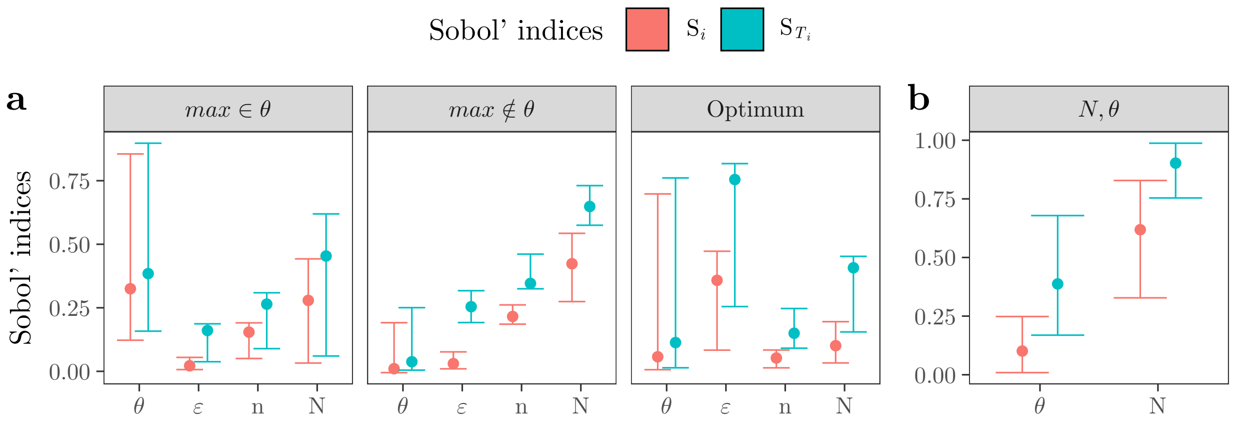
```r
# PLOT AGGREGATED SOBOL' INDICES AFTER WEIGHTING ------------------------------

a <- 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(legend.position = "none",
        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))

b <- final.sobol[!setting == "N"] %>%
  # 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 = NULL) +
```

```r
  scale_color_discrete(name = "Sobol' indices",
                       labels = c(expression(S[italic(i)]),
                                  expression(S[italic(T[i])]))) +
  theme_bw() +
  facet_wrap(~ setting) +
  theme(legend.position = "none",
        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))

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

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

```r
plot_grid(legend, all,
          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.
```

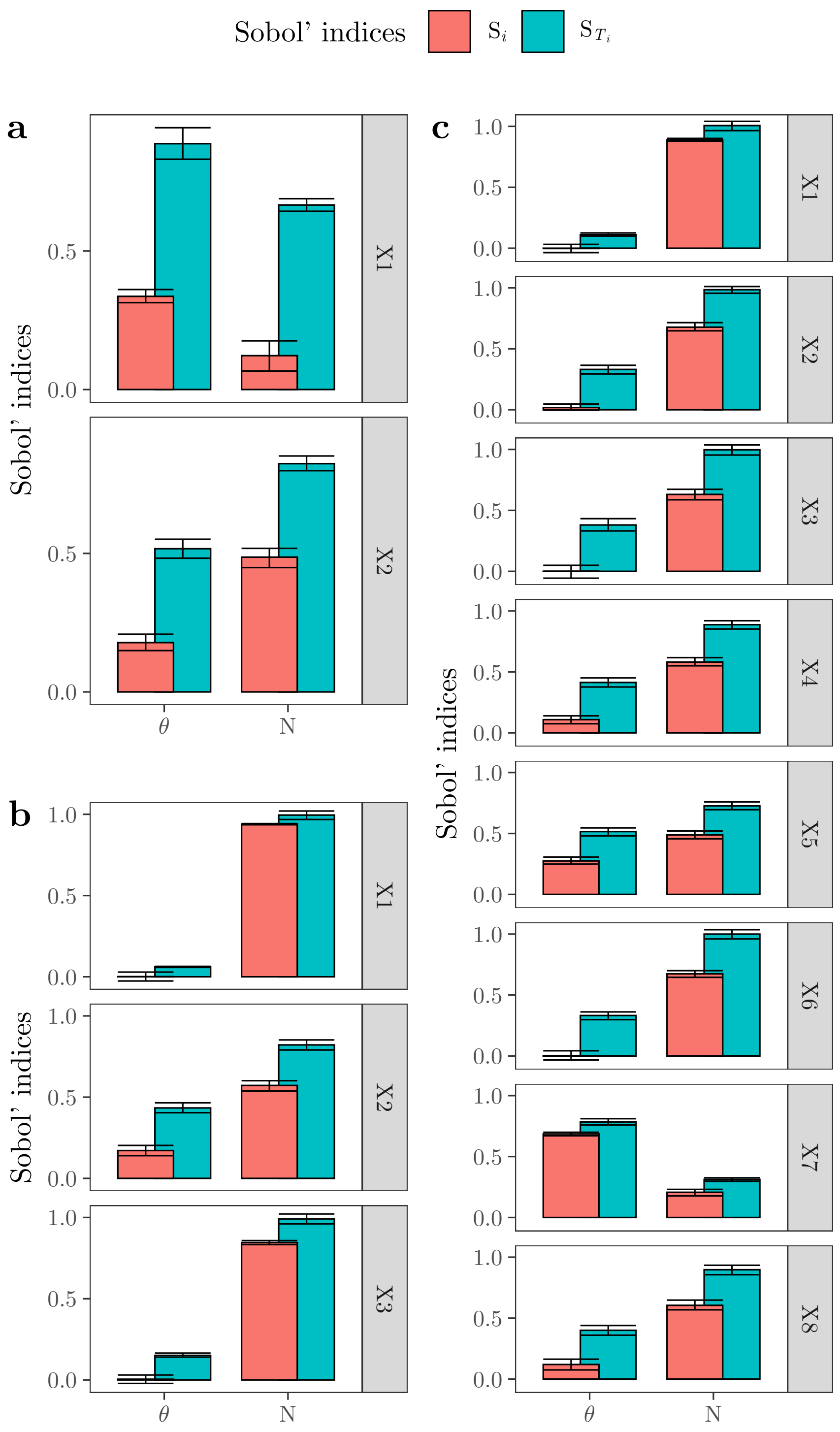


```r
# PLOT DESIGN PARAMETERS FOR SOBOL: ALL FUNCTIONS -----------------------------

tmp <- final.sobol[!setting == "N"] %>%
  split(., .$Model)
```

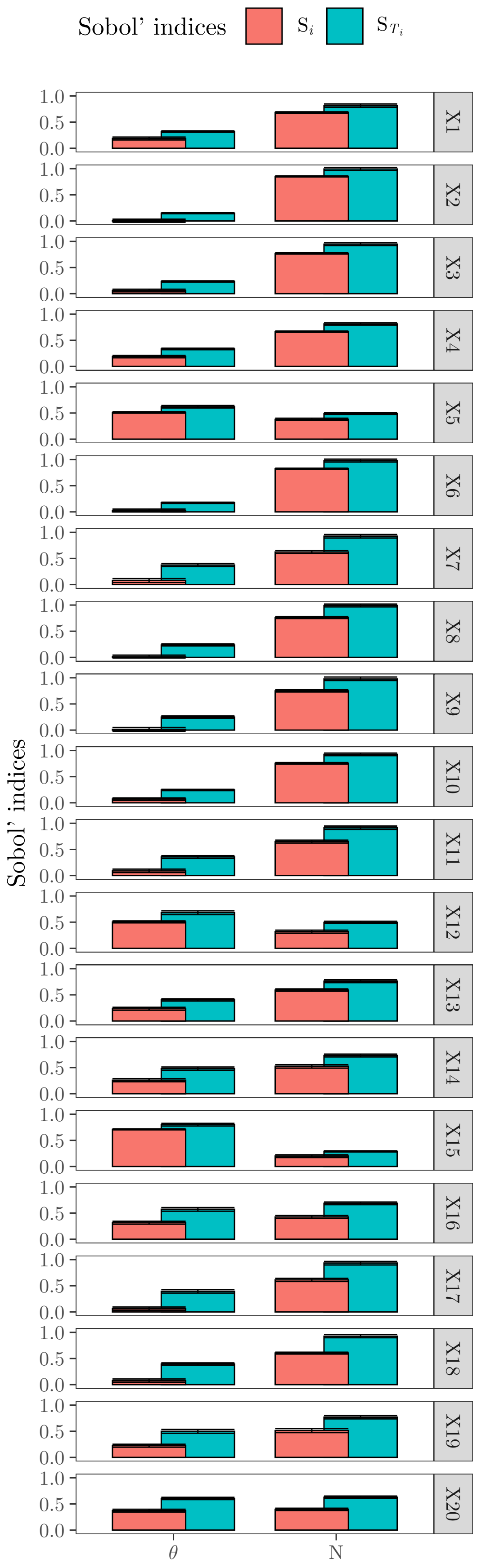
```r
gg <- list()
for(i in names(tmp)) {
    gg[[i]] <- plot_sobol(tmp[[i]], type = 1) +
      scale_y_continuous(breaks = pretty_breaks(n = 3)) +
      facet_grid(model.input ~.) +
      labs(x = "",
           y = "Sobol' indices") +
      theme(legend.position = "none")
}

# Extract legend
legend <- get_legend(gg[[1]] + theme(legend.position = "top"))

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

left <- plot_grid(gg[[1]], gg[[2]],
                  labels = c("a", "b"),
                  align = "h",
                  ncol = 1)
```

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

```r
all <- plot_grid(left, gg[[3]],
                 labels = c("", "c"),
                 ncol = 2)

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



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

plot_grid(legend, gg[[4]],
          ncol = 1,
          rel_heights = c(0.07, 1))
```


Sobol' indices
S_i
S_{T_i}
Sobol' indices
1.0
0.5
0.0
X1
X2
X3
X4
X5
X6
X7
X8
X9
X10
X11
X12
X13
X14
X15
X16
X17
X18
X19
X20
θ
N

6 Session information

```r
# SESSION INFORMATION ---------------------------------------------------------

sessionInfo()
```

```
## R version 3.6.1 (2019-07-05)
## Platform: x86_64-apple-darwin15.6.0 (64-bit)
## Running under: macOS Mojave 10.14.6
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/3.6/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/3.6/Resources/lib/libRlapack.dylib
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
## [1] parallel  stats     graphics  grDevices utils     datasets  methods
## [8] base
##
## other attached packages:
##  [1] checkpoint_0.4.7   wesanderson_0.3.6  sensobol_0.2.1
##  [4] pawnr_0.0.0.9000   overlapping_1.5.4  testthat_2.2.1
##  [7] cowplot_1.0.0      scales_1.0.0       doParallel_1.0.15
## [10] iterators_1.0.12   foreach_1.4.7      boot_1.3-23
## [13] sensitivity_1.16.1 randtoolbox_1.30.0 rngWELL_0.10-5
## [16] data.table_1.12.2  forcats_0.4.0      stringr_1.4.0
## [19] dplyr_0.8.3        purrr_0.3.2        readr_1.3.1
## [22] tidyr_1.0.0        tibble_2.1.3       ggplot2_3.2.1
## [25] tidyverse_1.2.1
##
## loaded via a namespace (and not attached):
##  [1] nlme_3.1-141      fs_1.3.1          usethis_1.5.1
##  [4] lubridate_1.7.4   devtools_2.2.0    httr_1.4.1
##  [7] rprojroot_1.3-2   tools_3.6.1       backports_1.1.4
## [10] R6_2.4.0          DT_0.9            lazyeval_0.2.2
## [13] colorspace_1.4-1  withr_2.1.2       tidyselect_0.2.5
## [16] prettyunits_1.0.2 processx_3.4.1    curl_4.1
## [19] compiler_3.6.1    cli_1.1.0         rvest_0.3.4
## [22] xml2_1.2.2        desc_1.2.0        labeling_0.3
## [25] callr_3.3.2       digest_0.6.21     rmarkdown_1.15
## [28] pkgconfig_2.0.3   htmltools_0.3.6   bibtex_0.4.2
## [31] sessioninfo_1.1.1 htmlwidgets_1.3   rlang_0.4.0
## [34] readxl_1.3.1      rstudioapi_0.10   generics_0.0.2
## [37] tikzDevice_0.12.3 jsonlite_1.6      magrittr_1.5
## [40] Rcpp_1.0.2        munsell_0.5.0     lifecycle_0.1.0
## [43] stringi_1.4.3     yaml_2.2.0        gbRd_0.4-11
## [46] pkgbuild_1.0.5    grid_3.6.1        crayon_1.3.4
## [49] lattice_0.20-38   haven_2.1.1       hms_0.5.1
## [52] zeallot_0.1.0     knitr_1.25        ps_1.3.0
## [55] pillar_1.4.2      codetools_0.2-16  pkgload_1.0.2
## [58] glue_1.3.1        evaluate_0.14     remotes_2.1.0
## [61] modelr_0.1.5      vctrs_0.2.0       Rdpack_0.11-0
## [64] cellranger_1.1.0  gtable_0.3.0      assertthat_0.2.1
## [67] xfun_0.9          broom_0.5.2       filehash_2.4-2
## [70] tinytex_0.16      memoise_1.1.0     ellipsis_0.3.0
```