

# A sensitivity analysis of the PAWN sensitivity index

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## 1 Preliminary functions

```
# PRELIMINARY FUNCTIONS -----

# Install the development version of the pawnr package
devtools::install_github("arnalduy/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",
              "gggridges"))

# Create custom theme
theme_AP <- function() {
  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))
}

# 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

# 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

```

# CONSTRUCT SAMPLE MATRICES -----
A <- B <- list()
for(i in k) {
  # For Sobol' STi
  A[[i]] <- mclapply(N, function(N) sobol_matrices(n = floor(N / (i + 1)), k = i), mc.cores = n)
  # For PAWN
  B[[i]] <- mclapply(N, function(N) randtoolbox::sobol(n = N, dim = i))
}

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

names(A) <- models
names(B) <- models

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

for(i in names(B)) {

```

```

names(B[[i]]) <- N
}

```

## 2.2 Model output

```

# COMPUTE MODEL OUTPUT -----

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

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

names(Y.pawn) <- models
for(i in names(Y.pawn)) {
  names(Y.pawn[[i]]) <- N
}

# PLOT MODEL UNCERTAINTY -----

lapply(models, function(models) Y.pawn[[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") +

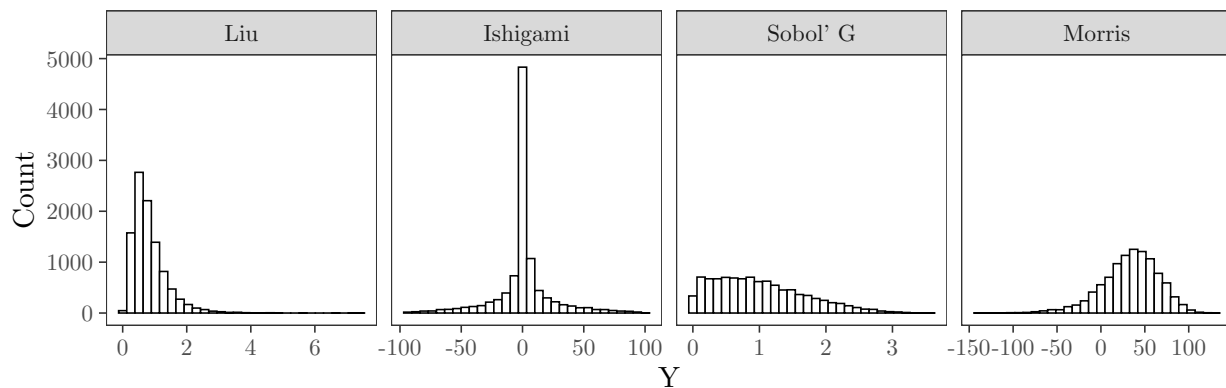
```

```

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))

```

## `stat\_bin()` using `bins = 30`. Pick better value with `binwidth`.



## 2.3 Sobol' indices

```

# COMPUTE SOBOLE' 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 = floor(as.numeric(j) / (length(params[[i]]) + 1)),
                                   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 = floor(as.numeric(j) / (length(params[[i]]) + 1)),
                                          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:= "$S_{Ti}~*$"] %>%
  .[, .(model, N, parameters, original, low.ci, high.ci, diff, method, sensitivity)]
```

## 2.4 PAWN

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

```
pawn.indices <- pawn.ci <- list()
for(i in names(B)) {
  for(j in names(B[[i]])) {
    pawn.indices[[i]][[j]] <- pawn_generic(data = B[[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.pawn)) {
  for(j in names(Y.pawn[[i]])) {
    pawn.index.dummy[[i]][[j]] <- pawn_dummy(Y = Y.pawn[[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"]

# EXPORT SOBOLO' AND PAWN CONVERGENCE RATES -----

fwrite(sobol.convergence, "sobol.convergence.csv")
fwrite(pawn.convergence, "pawn.convergence.csv")

```

## 2.5 Plot convergence

```

# PLOT CONVERGENCE -----

sobol.convergence[sensitivity == "STi"] %>%
  .[, sensitivity:= NULL] %>%
  .[, method:= factor(method, levels = c("PAWN", "$S_{Ti}~*$"))] %>%
  rbind(., pawn.convergence) %>%
  ggplot(., aes(N, diff,
                group = parameters,
                color = parameters)) +

```

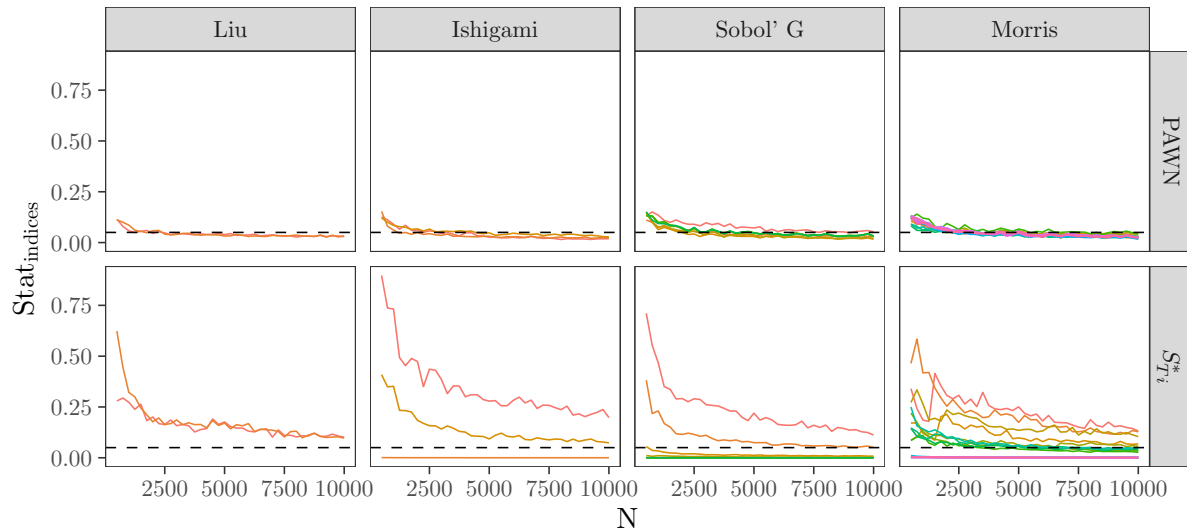
```

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))

```

Model inputs

— X1	— X5	— X9	— X13	— X17
— X2	— X6	— X10	— X14	— X18
— X3	— X7	— X11	— X15	— X19
— X4	— X8	— X12	— X16	— X20



*# PLOT CONVERGENCE (SHOWING THE RANGE OF SAMPLES USED) -----*

```

sobol.convergence[sensitivity == "STi"] %>%
[, sensitivity:= NULL] %>%
rbind(., pawn.convergence) %>%
[, method:= factor(method, levels = c("PAWN", "$S_{Ti}~*${}"))] %>%
ggplot(., aes(N, diff,
              group = parameters,
              color = parameters)) +
geom_line() +
annotate("rect",

```



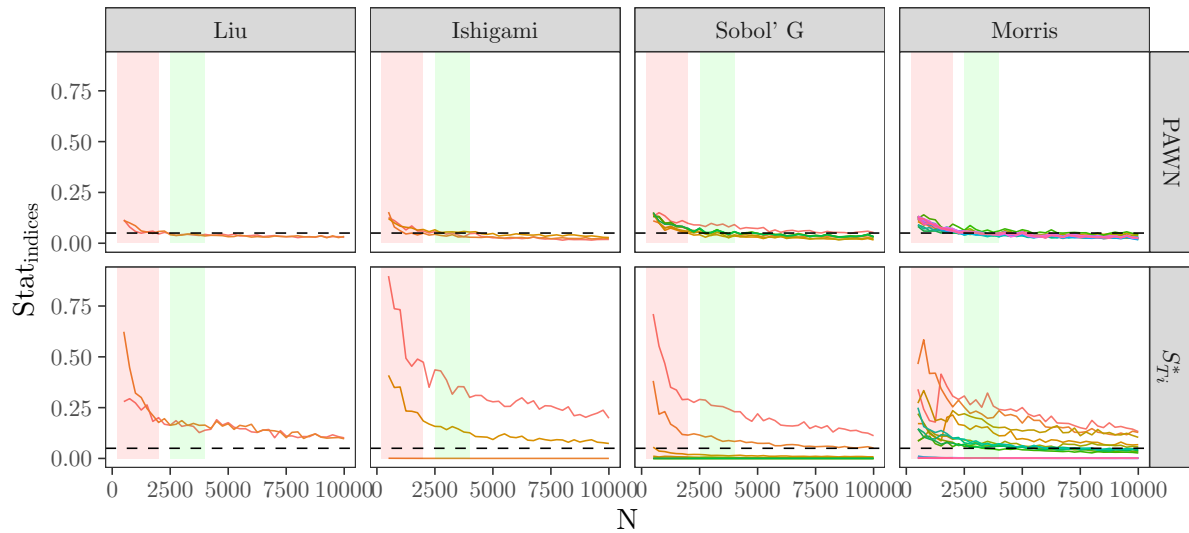
```

    xmin = 200,
    xmax = 2000,
    ymin = 0,
    ymax = Inf,
    alpha = 0.1,
    fill="red") +
  annotate("rect", xmin = 2500,
    xmax = 4000,
    ymin = 0,
    ymax = Inf,
    alpha = 0.1,
    fill="green") +
  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))

```

Model inputs

X1	X5	X9	X13	X17
X2	X6	X10	X14	X18
X3	X7	X11	X15	X19
X4	X8	X12	X16	X20



```

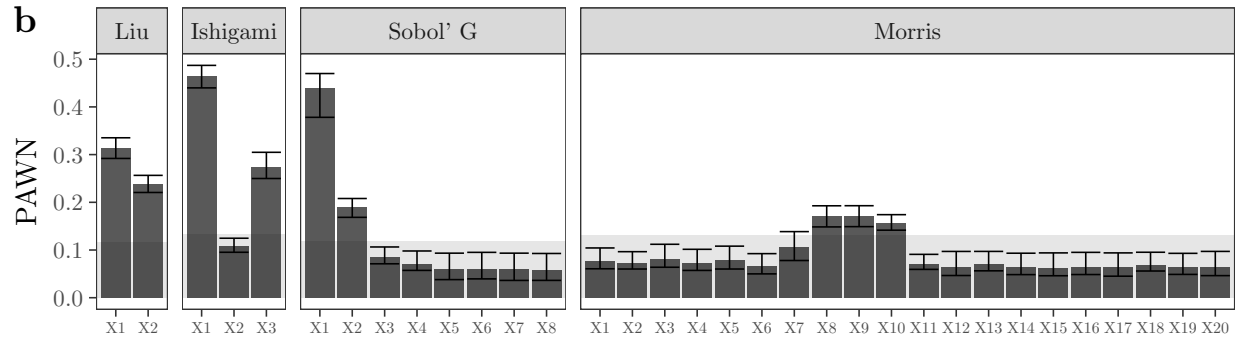
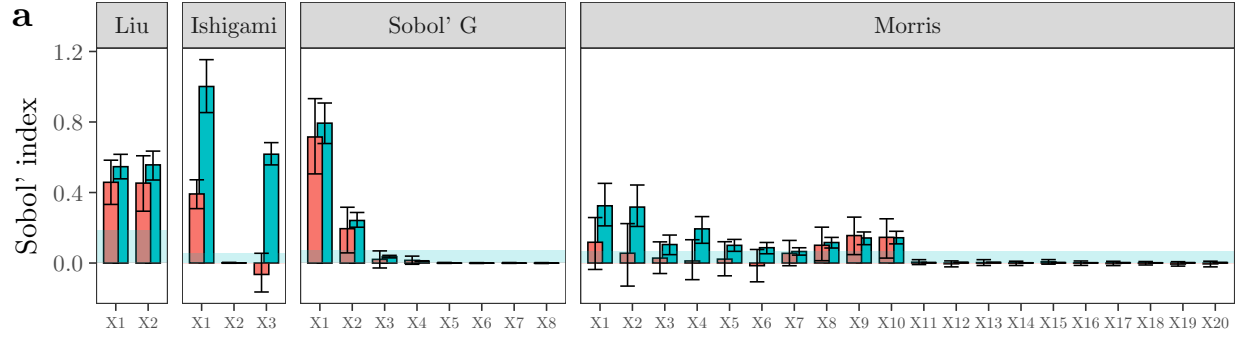
# PLOT SOBOL' AND PAWN INDICES -----

# 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"))

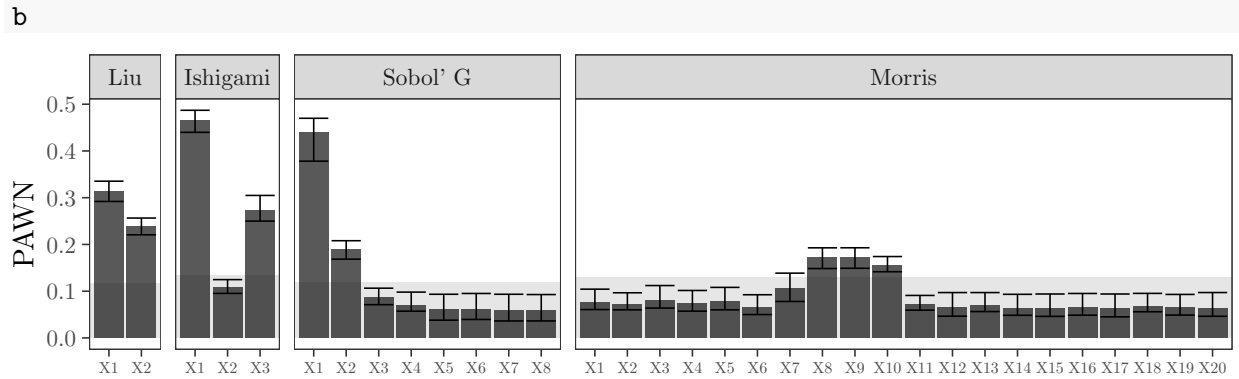
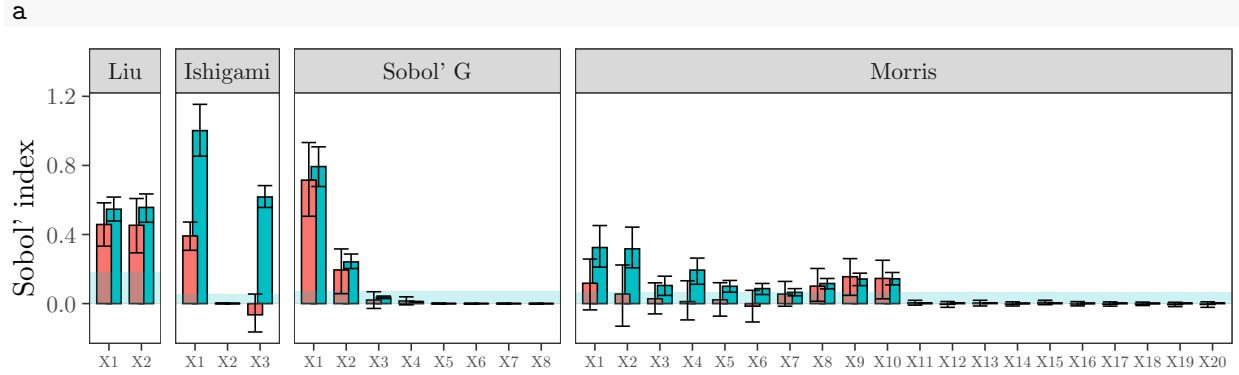
# PAWN indices
b <- pawn.convergence[N==4000] %>%
  plot_pawn(.) +
  geom_rect(data = pawn.index.dummy[N==4000],
            aes(ymin = 0,
                ymax = high.ci,
                xmin = -Inf,
                xmax = Inf),
            fill = "black",
            alpha = 0.1,
            inherit.aes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

```

Sobol' indices ■  $S_i$  ■  $S_{T_i}$



# PLOT SOBO' AND PAWN INDICES (INDIVIDUAL PLOTS) -----



## 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:= .(mapapply(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 -----

# 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

```

# 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"))]

# 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: $max \\in \\in \\theta$ Morris  X1-X3    0.940
##  3: $max \\in \\in \\theta$ Morris  X1-X4    0.890
##  4: $max \\in \\in \\theta$ Morris  X1-X5    0.887
##  5: $max \\in \\in \\theta$ 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
```

```
# Export results
```

```
rbindlist(final.overlap) %>%
  fwrite(., "pawn.overlap.csv")
```

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

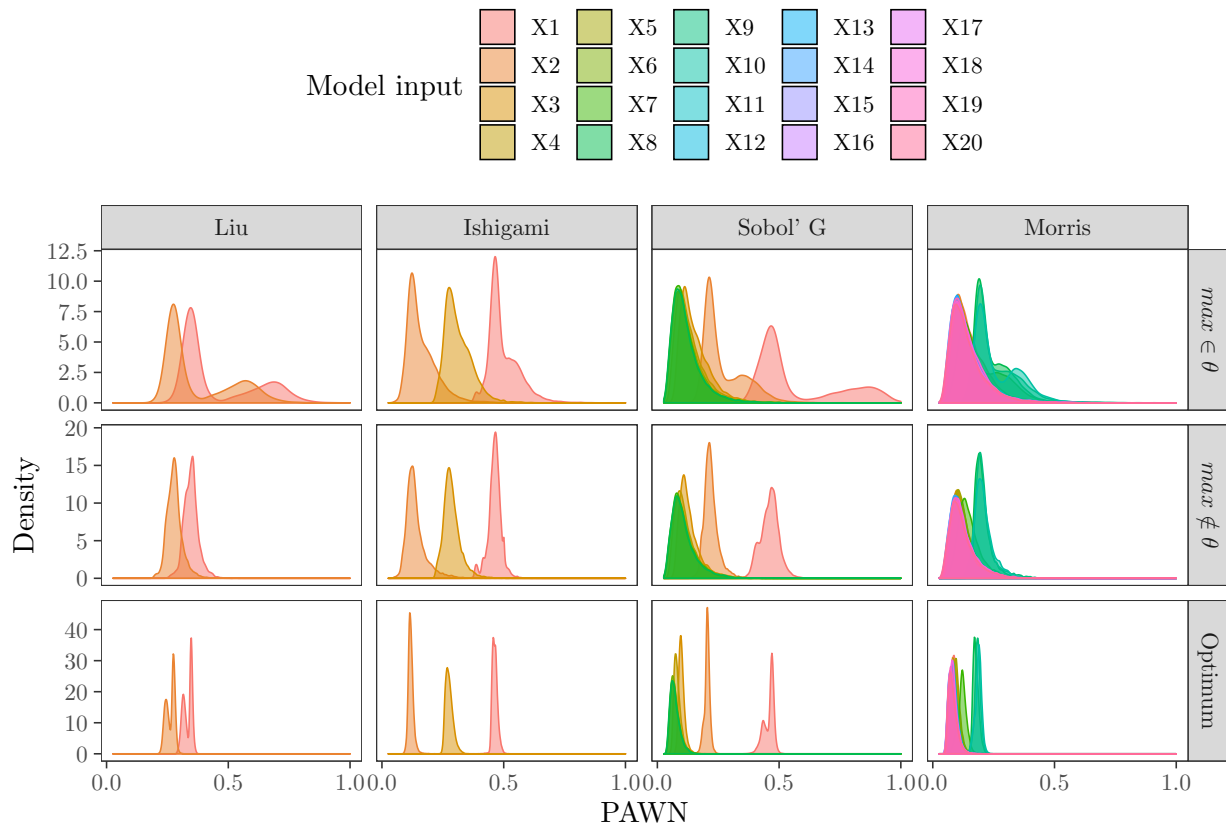
```
plot.uncertainty.pawn <- ggplot(AB.pawn, aes(value,
                                              fill = parameter,
                                              color = parameter)) +
  geom_density(alpha = 0.5,
               position = "identity") +
  facet_grid(setting~Model,
             scales = "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")

# 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)]

# 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"))]

# EXPORT DATA -----

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

# PLOT AGGREGATED SOBOLO' 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 SOBOLO' 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 SOBOLO' AND SUM OF SOBOLO' -----

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

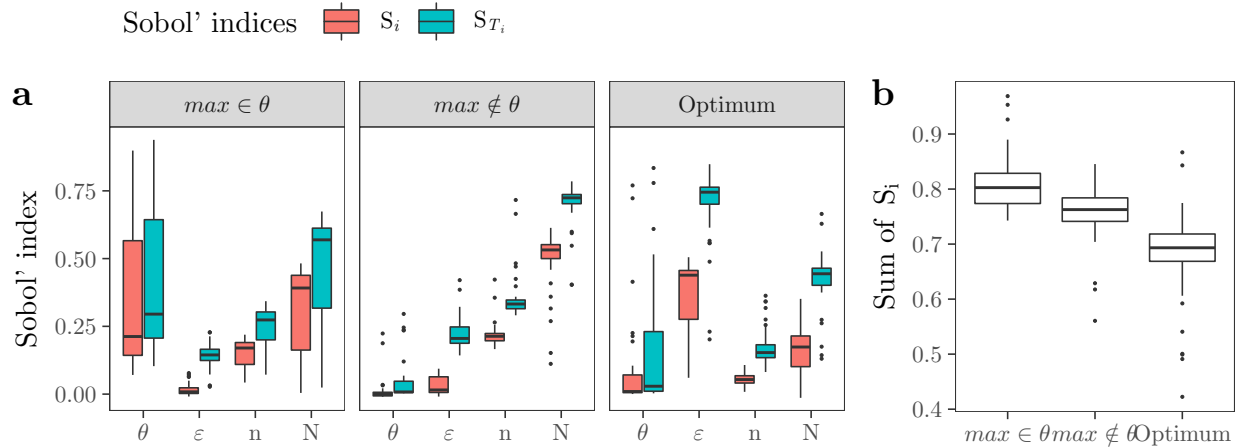
bottom <- plot_grid(a, b,
                   ncol = 2,
                   align = "hv",
                   labels = "auto",
                   rel_widths = c(2.2, 1))

## 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  $T_i$ 
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 = floor(N / (k + 1)), 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)]

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

```

```
print(n)
```

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

#### 4.4 Run the model

```

# 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)

# 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 -----

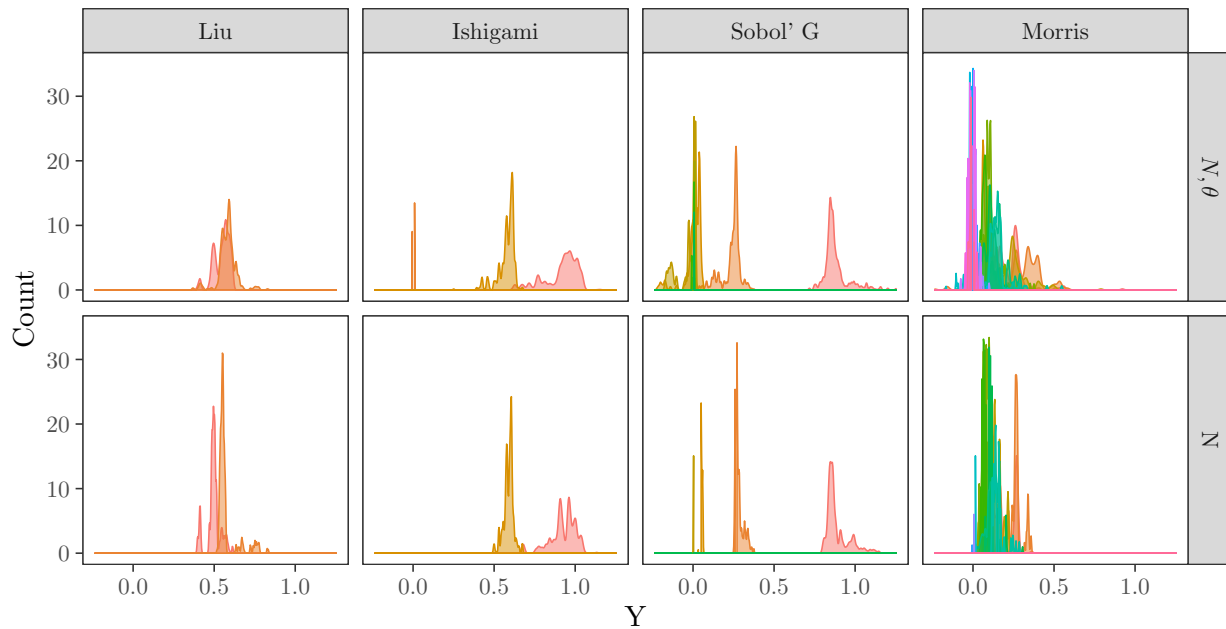
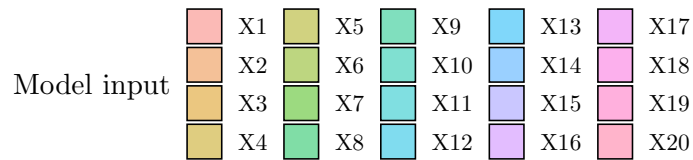
AB.sobol %>%
  ggplot(., aes(value,

```

```

    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  0.555
## 2:      N      Liu X1-X2  0.091
##
## [[2]]
##      setting      Model    rn overlap
## 1: $N,\\theta$ Ishigami X1-X2  0.000
## 2: $N,\\theta$ Ishigami X1-X3  0.025
## 3: $N,\\theta$ Ishigami X2-X3  0.000
## 4:      N      Ishigami X1-X2  0.000
## 5:      N      Ishigami X1-X3  0.012
## 6:      N      Ishigami X2-X3  0.000
##
## [[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	0.017
## 9:	\$N,\\theta\$	Sobol'	G X2-X4	0.012
## 10:	\$N,\\theta\$	Sobol'	G X2-X5	0.001
## 11:	\$N,\\theta\$	Sobol'	G X2-X6	0.001
## 12:	\$N,\\theta\$	Sobol'	G X2-X7	0.001
## 13:	\$N,\\theta\$	Sobol'	G X2-X8	0.001
## 14:	\$N,\\theta\$	Sobol'	G X3-X4	0.625
## 15:	\$N,\\theta\$	Sobol'	G X3-X5	0.069
## 16:	\$N,\\theta\$	Sobol'	G X3-X6	0.072
## 17:	\$N,\\theta\$	Sobol'	G X3-X7	0.067
## 18:	\$N,\\theta\$	Sobol'	G X3-X8	0.049
## 19:	\$N,\\theta\$	Sobol'	G X4-X5	0.084
## 20:	\$N,\\theta\$	Sobol'	G X4-X6	0.096
## 21:	\$N,\\theta\$	Sobol'	G X4-X7	0.071
## 22:	\$N,\\theta\$	Sobol'	G X4-X8	0.050
## 23:	\$N,\\theta\$	Sobol'	G X5-X6	0.351
## 24:	\$N,\\theta\$	Sobol'	G X5-X7	0.480
## 25:	\$N,\\theta\$	Sobol'	G X5-X8	0.594
## 26:	\$N,\\theta\$	Sobol'	G X6-X7	0.351
## 27:	\$N,\\theta\$	Sobol'	G X6-X8	0.299
## 28:	\$N,\\theta\$	Sobol'	G X7-X8	0.472
## 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	0.054
## 52:		N	Sobol' G X5-X7	0.353
## 53:		N	Sobol' G X5-X8	0.567
## 54:		N	Sobol' G X6-X7	0.027

```
## 55:          N Sobol' G X6-X8    0.068
## 56:          N Sobol' G X7-X8    0.244
##          setting      Model      rn overlap
##
## [[4]]
##          setting      Model      rn overlap
## 1: $N,\\theta$ Morris    X1-X2    0.259
## 2: $N,\\theta$ Morris    X1-X3    0.088
## 3: $N,\\theta$ Morris    X1-X4    0.570
## 4: $N,\\theta$ Morris    X1-X5    0.148
## 5: $N,\\theta$ Morris    X1-X6    0.169
## ---
## 376:         N Morris X17-X19    0.505
## 377:         N Morris X17-X20    0.375
## 378:         N Morris X18-X19    0.046
## 379:         N Morris X18-X20    0.143
## 380:         N Morris X19-X20    0.284
```

```
# Export results
```

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

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

```
a <- ggplot(AB.pawn, aes(value, parameter, fill = parameter)) +
  geom_density_ridges(rel_min_height = 0.01, alpha = 0.2, scale = 5) +
  facet_grid(Model ~ setting,
             scales = "free",
             space = "free_y") +
  labs(x = "PAWN",
       y = "") +
  theme_AP() +
  theme(axis.text.y = element_text(size = 6),
        legend.position = "none")

b <- ggplot(AB.sobol[!setting == "N"], aes(value, parameter, fill = parameter)) +
  geom_density_ridges(rel_min_height = 0.01, alpha = 0.2, scale = 5) +
  facet_grid(Model ~ setting,
             scales = "free",
             space = "free_y") +
  labs(x = "$S_{Ti}^{~*}$",
       y = "") +
  theme_AP() +
  theme(legend.position = "none",
        axis.text.y=element_blank(),
        axis.ticks.y = element_blank())

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

```
scale_fill_discrete(name = "Model input"))
```

```
## Picking joint bandwidth of 0.0194
## Picking joint bandwidth of 0.00344
## Picking joint bandwidth of 0.00231
## Picking joint bandwidth of 0.00717
## Picking joint bandwidth of 0.0035
## Picking joint bandwidth of 0.00151
## Picking joint bandwidth of 0.00924
## Picking joint bandwidth of 0.00498
## Picking joint bandwidth of 0.00209
## Picking joint bandwidth of 0.00841
## Picking joint bandwidth of 0.00538
## Picking joint bandwidth of 0.00191
```

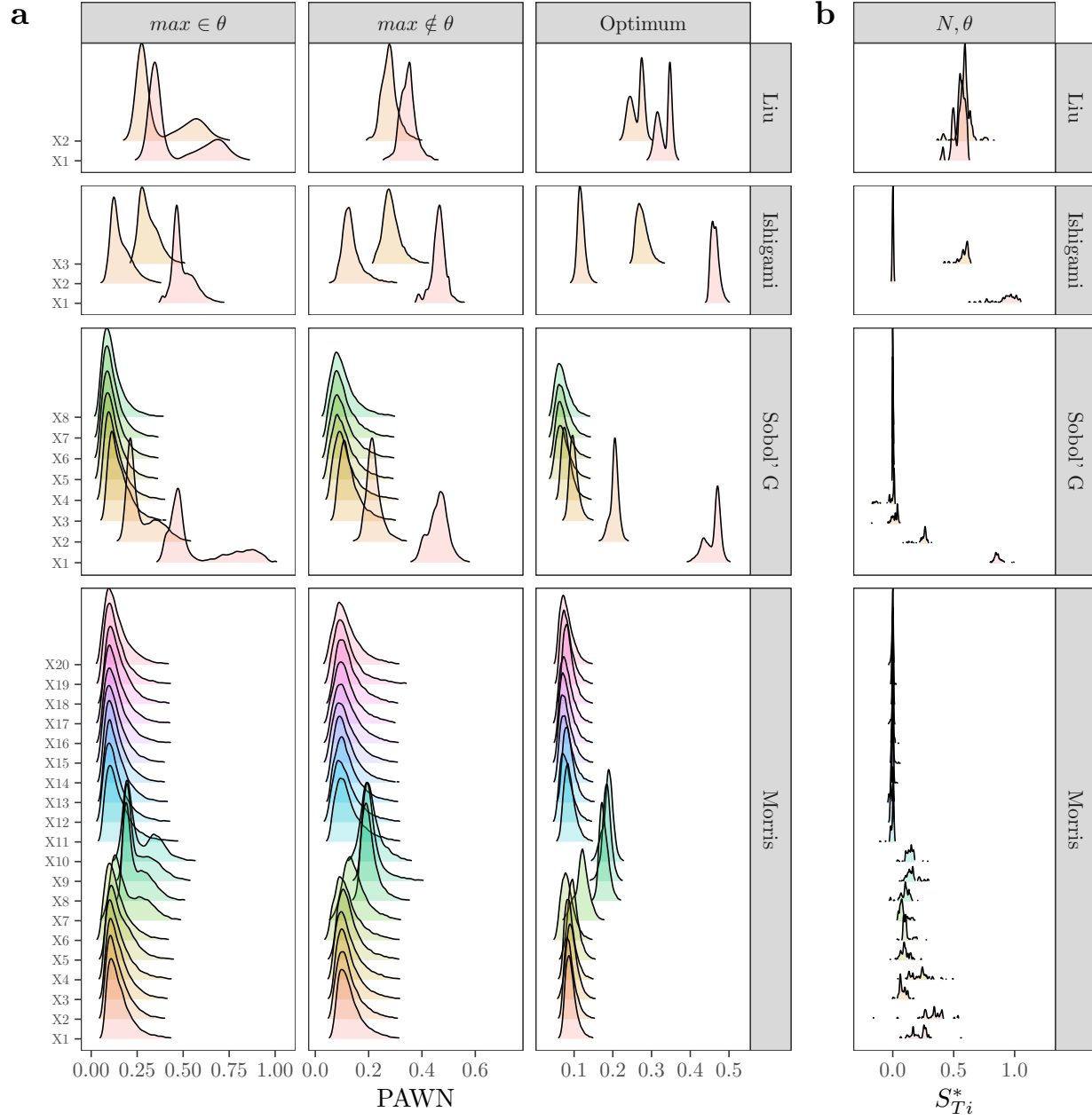
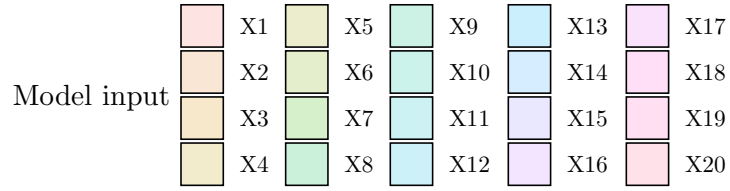
```
bottom <- plot_grid(a, b,
  ncol = 2,
  labels = "auto",
  align = "h",
  rel_widths = c(1, 0.38))
```

```
## Picking joint bandwidth of 0.0194
## Picking joint bandwidth of 0.00344
## Picking joint bandwidth of 0.00231
## Picking joint bandwidth of 0.00717
## Picking joint bandwidth of 0.0035
## Picking joint bandwidth of 0.00151
## Picking joint bandwidth of 0.00924
## Picking joint bandwidth of 0.00498
## Picking joint bandwidth of 0.00209
## Picking joint bandwidth of 0.00841
## Picking joint bandwidth of 0.00538
## Picking joint bandwidth of 0.00191
## Picking joint bandwidth of 0.00551
## Picking joint bandwidth of 0.00476
## Picking joint bandwidth of 0.00219
```



## Picking joint bandwidth of 0.00344

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



## 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
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)
```

[illegible]

# 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)]

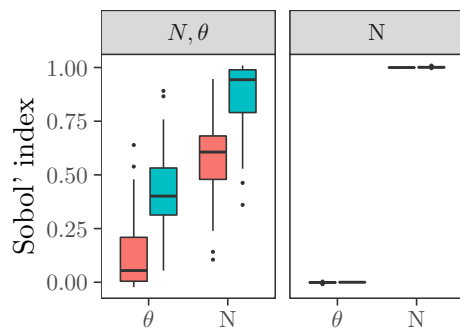
# EXPORT DATA -----

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))

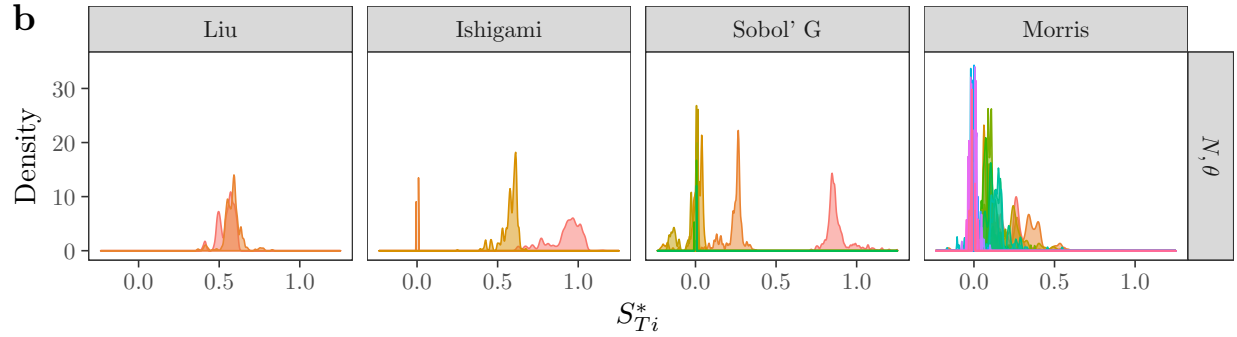
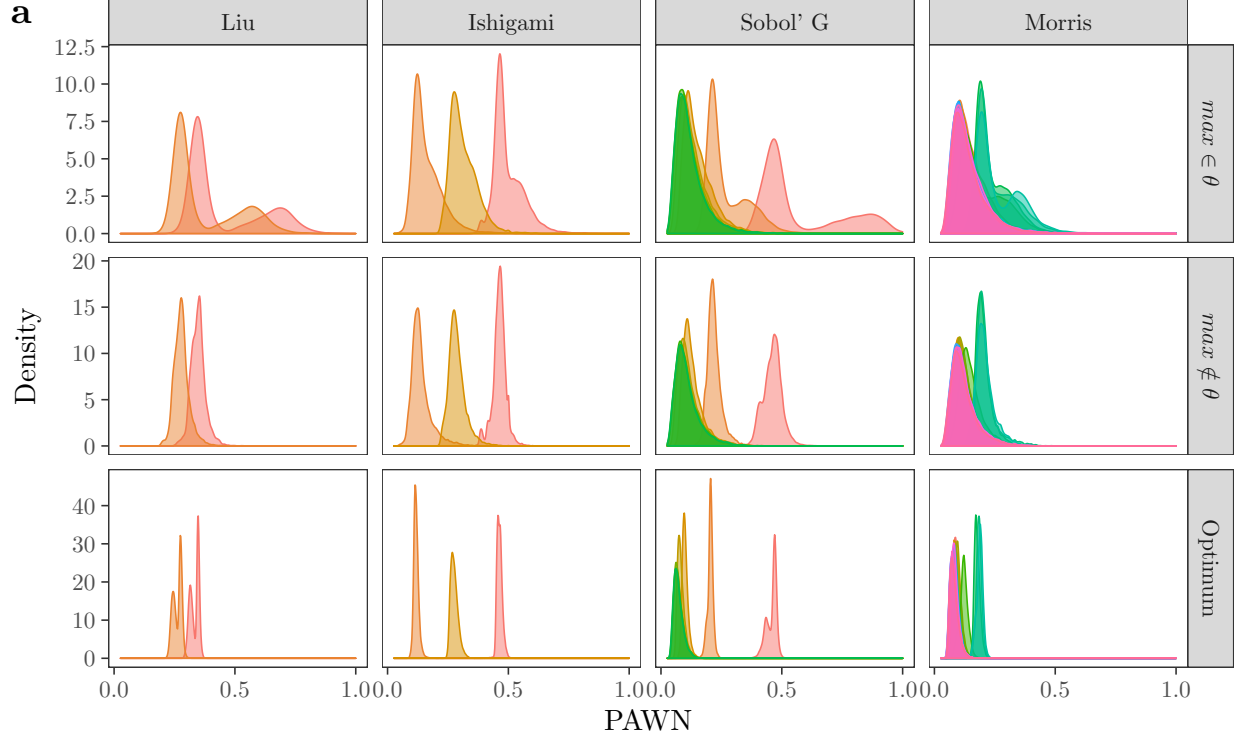
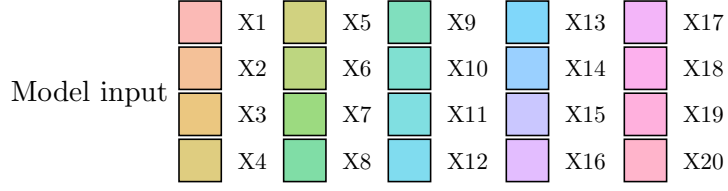
# Get legend
legend <- get_legend(a + theme(legend.position = "top"))

# 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.

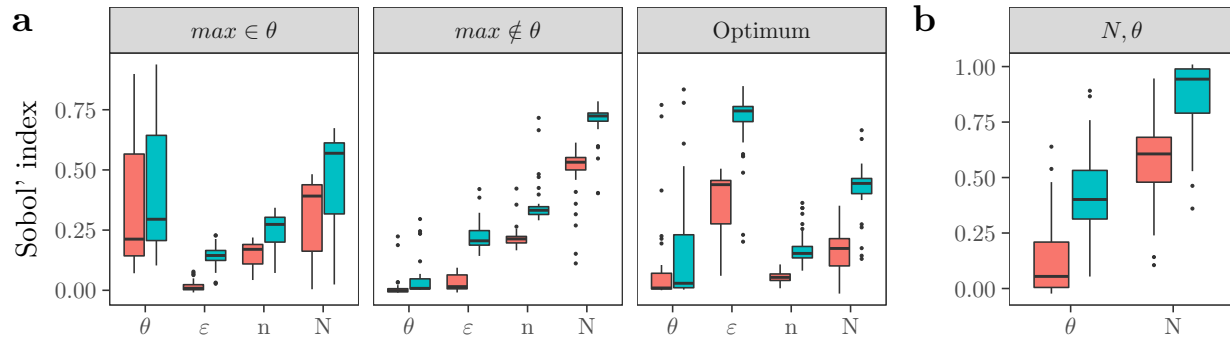
plot_grid(legend, bottom,
          ncol = 1,
          align = "hv",
          rel_heights = c(0.21, 1))

## 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.
```

Sobol' indices ■  $S_i$  ■  $S_{T_i}$



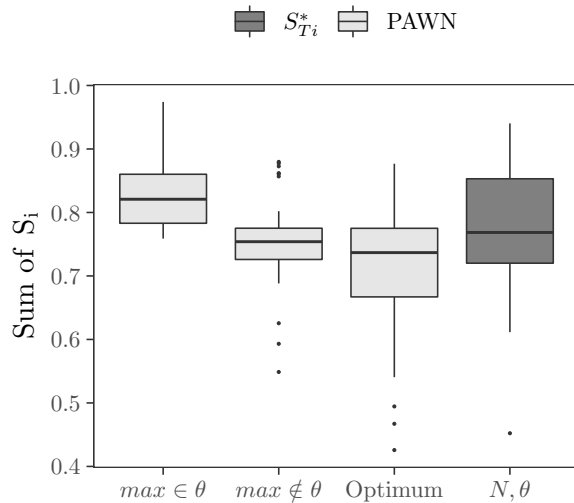
# PLOT AGGREGATED SUM OF SI -----

```
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 SOBOLO' 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' index") +
      theme(legend.position = "none")
  }
}

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

# PLOT SOBOLO' INDICES FOR LIU, ISHIGAMI AND SOBOLO' 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.
```

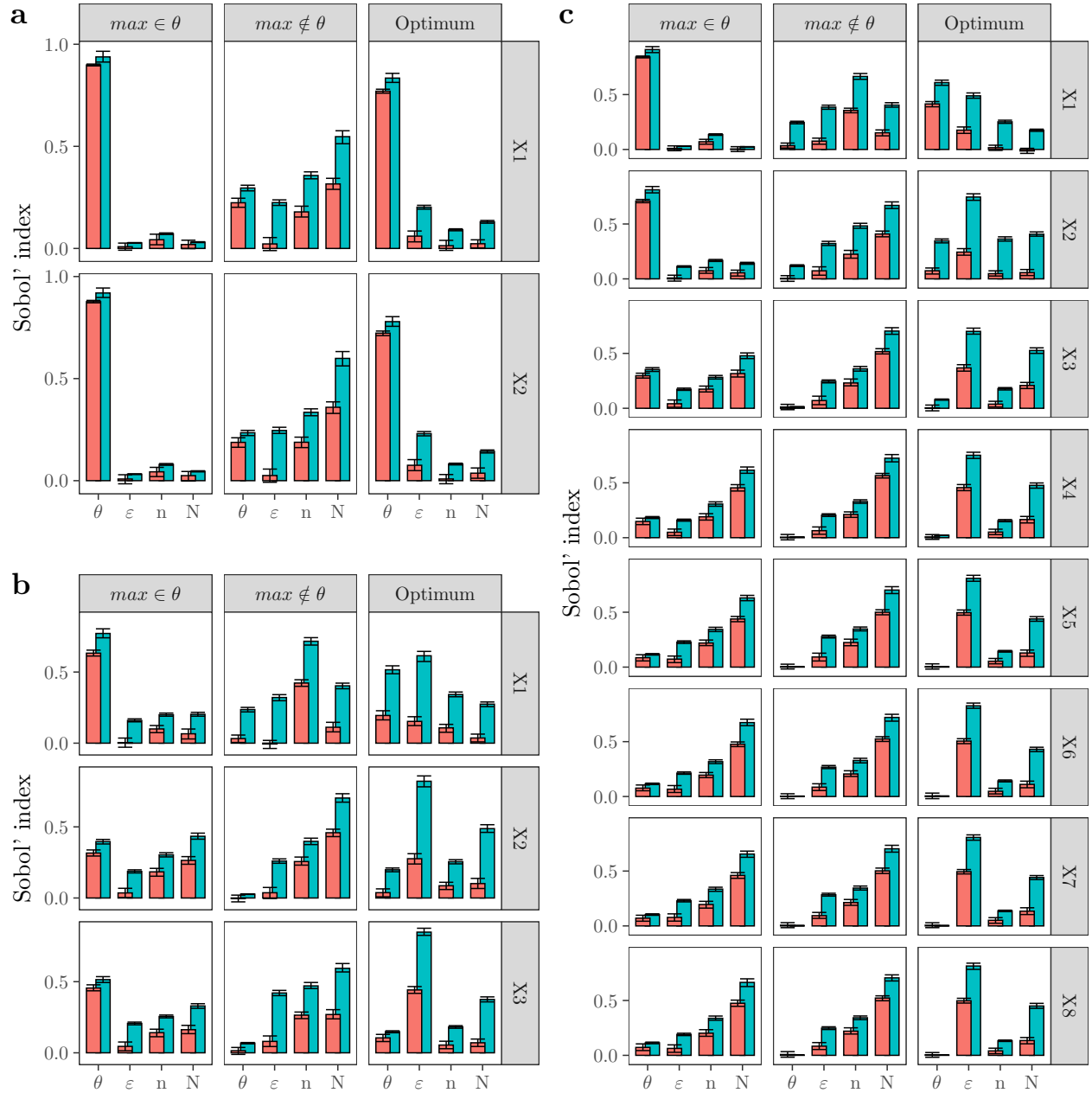
```
## Warning: Graphs cannot be horizontally aligned unless the axis parameter is
```

## set. Placing graphs unaligned.

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

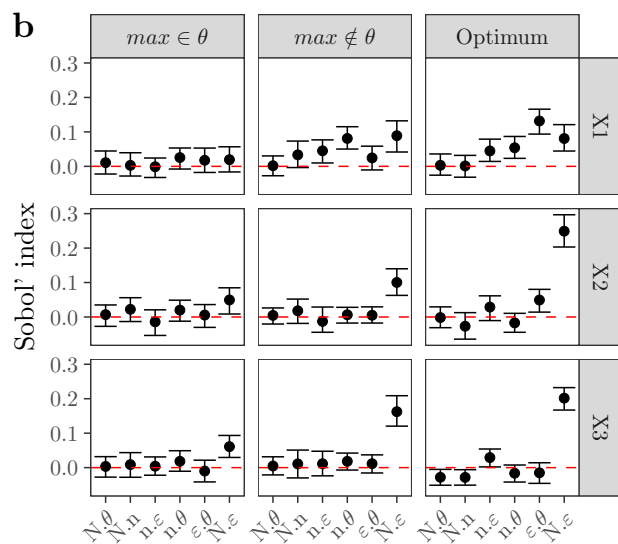
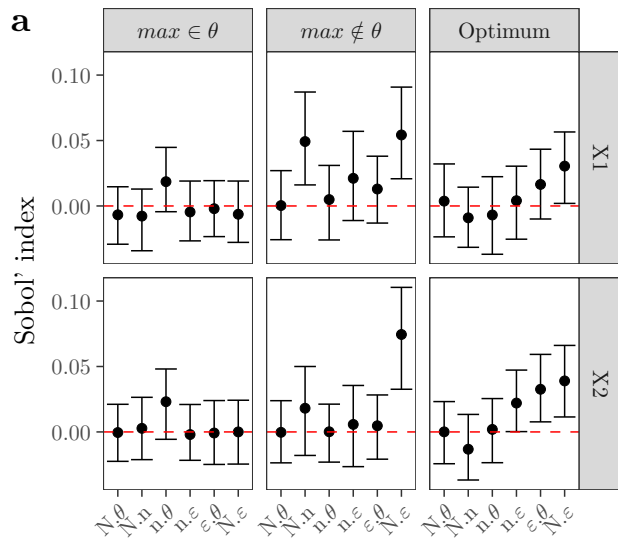
```
plot_grid(legend, all[[1]],
          ncol = 1,
          rel_heights = c(0.1, 1))
```

Sobol' indices ■  $S_i$  ■  $S_{T_i}$

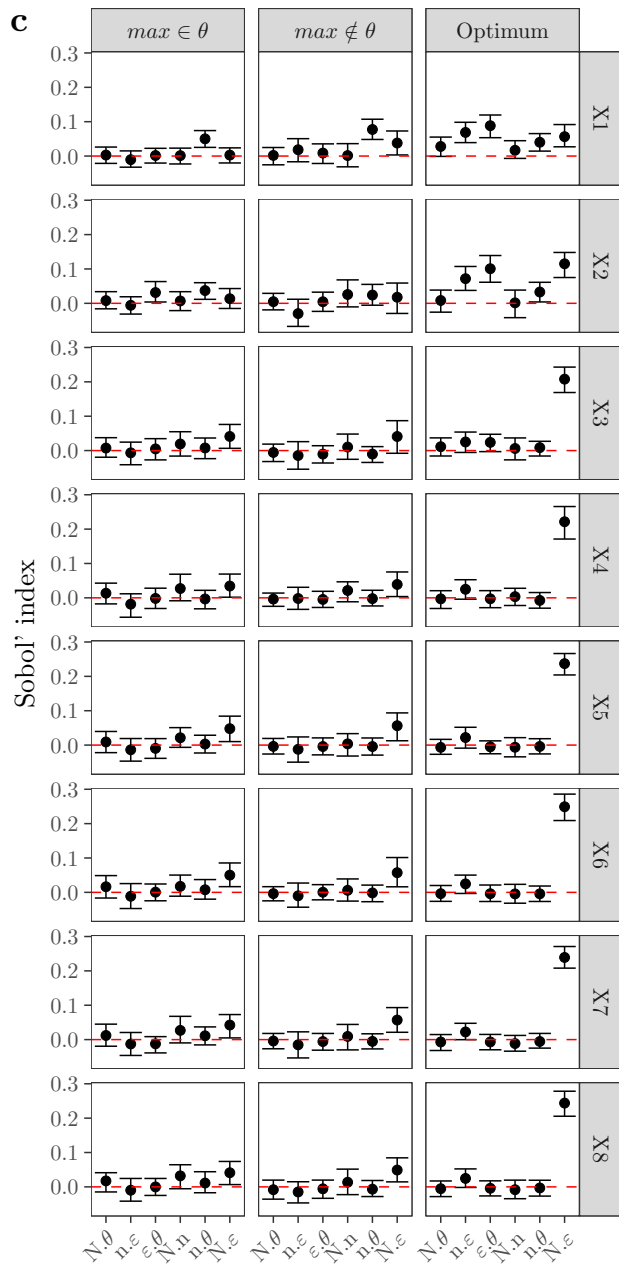


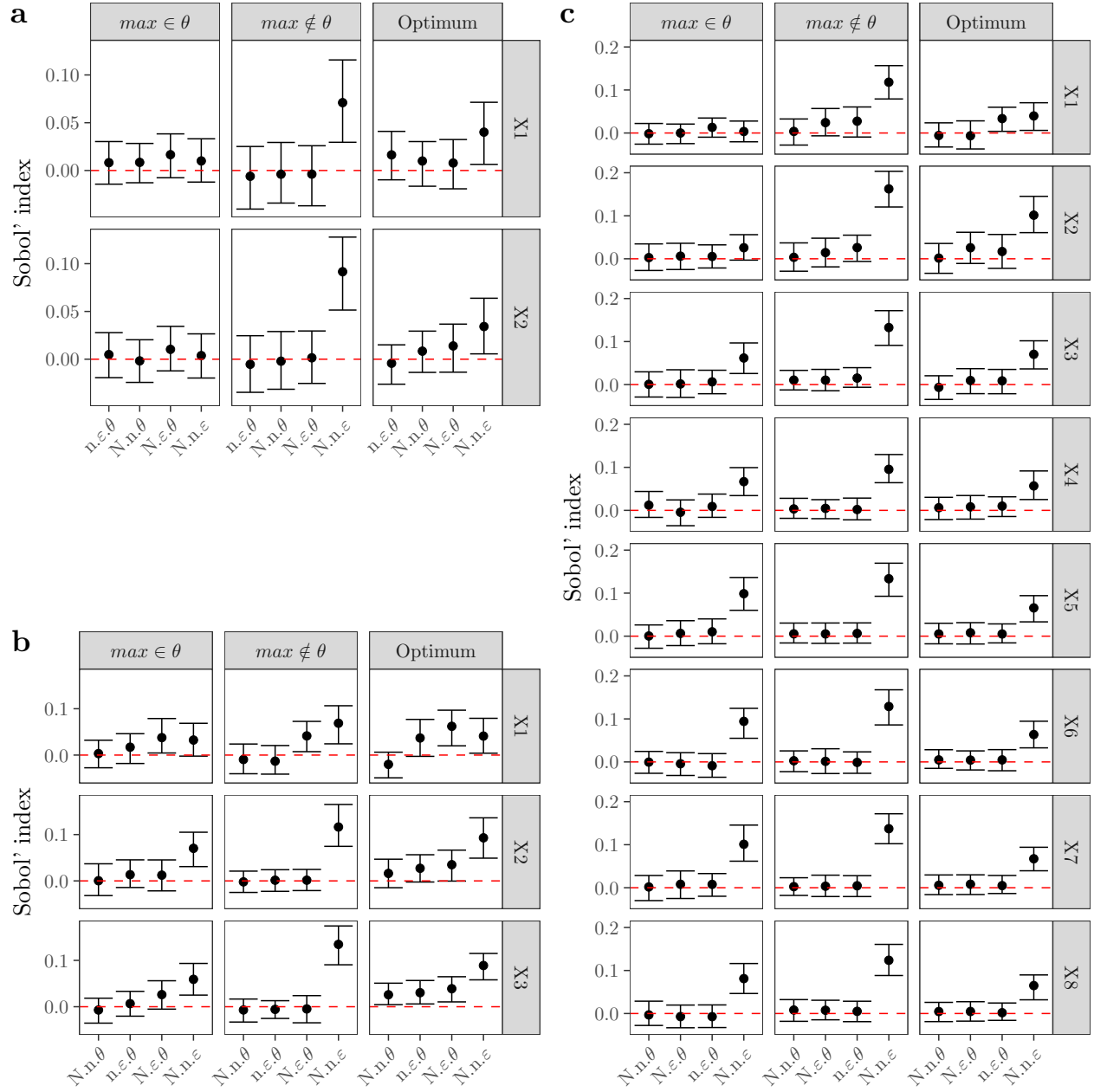
```
lapply(2:3, function(x) all[x])
```

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



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

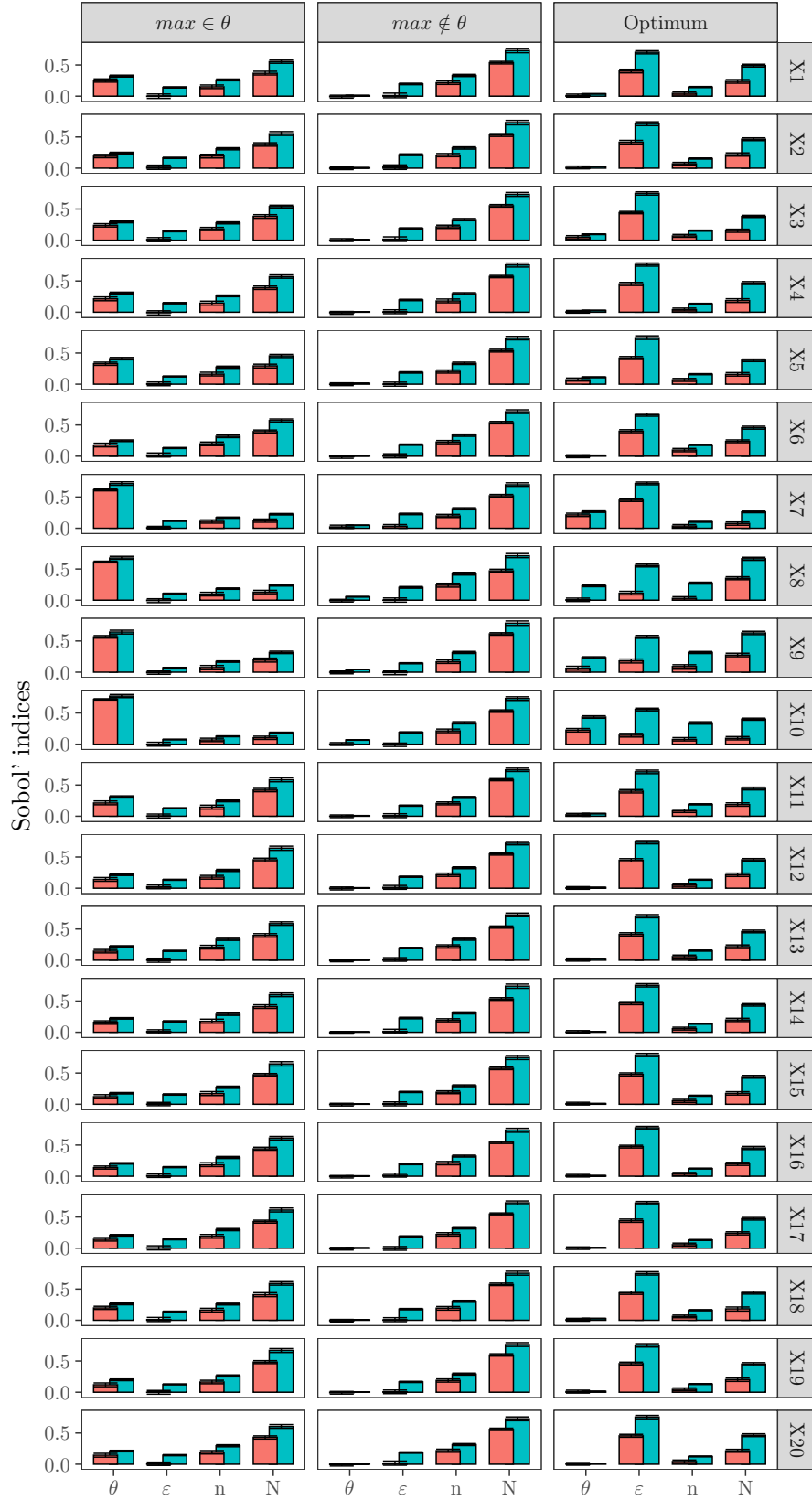




*# PLOT SOBOB' INDICES FOR THE MORRIS FUNCTION* -----

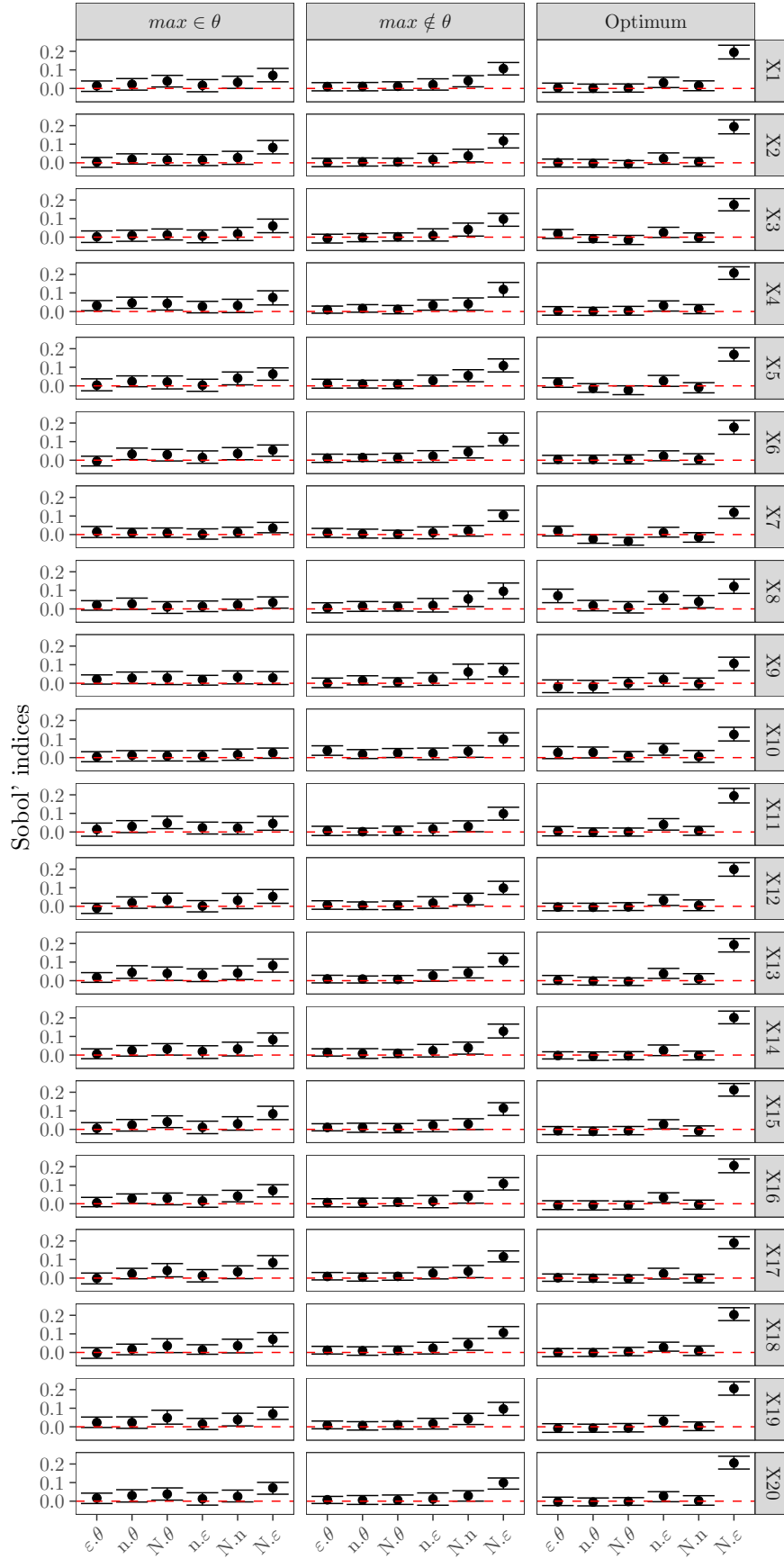
```
plot_grid(legend, gg[[4]][[1]],
          ncol = 1,
          rel_heights = c(0.07, 1))
```

Sobol' indices ■  $S_i$  ■  $S_{T_i}$



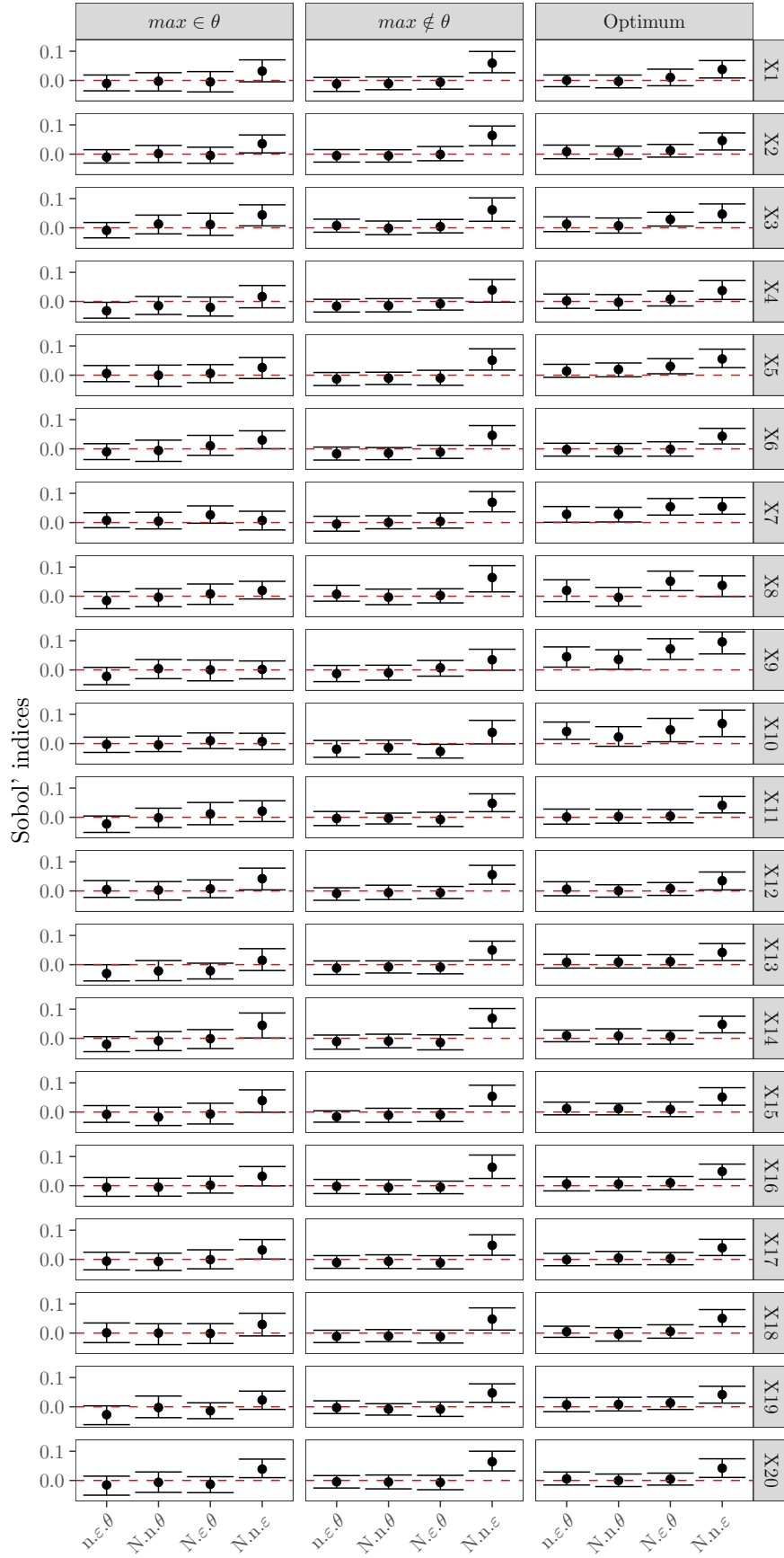
```
lapply(2:3, function(x) gg[[4]][[x]])
```

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



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





```

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

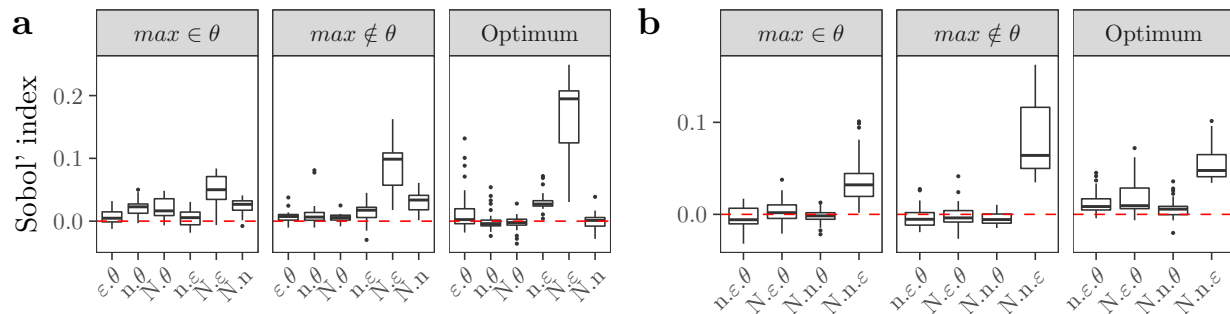
gg <- list()
second.third <- c("Sij", "Sijk")
for(i in second.third) {
  gg[[i]] <- final.pawn.ci[sensitivity == i] %>%
    ggplot(., aes(parameters, original)) +
    geom_boxplot(outlier.size = 0.2) +
    labs(x = NULL,
         y = "Sobol' index") +
    scale_fill_discrete(name = "Sobol' indices",
                        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")

```



```

# 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' index") +
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) +

```

```

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.

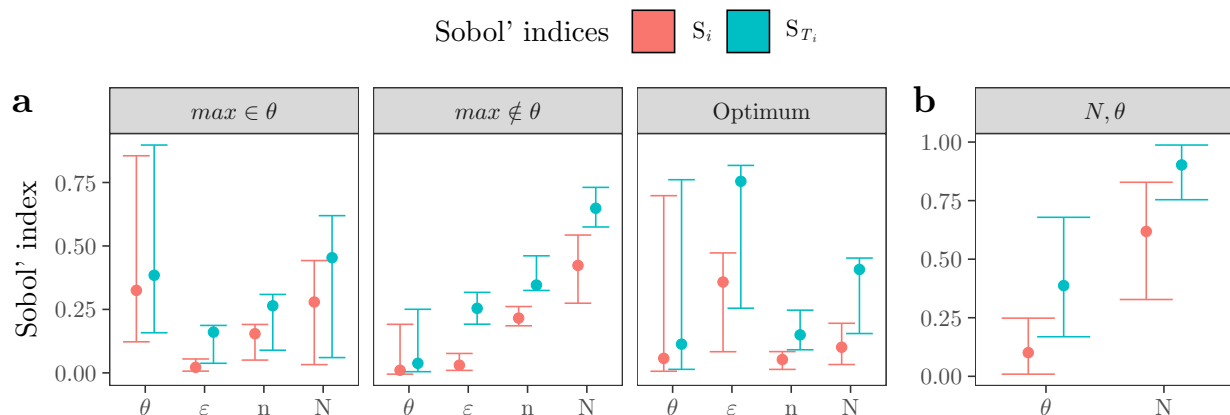
```

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.



```

# PLOT DESIGN PARAMETERS FOR SOBOLE: ALL FUNCTIONS -----
tmp <- final.sobol[!setting == "N"] %>%
  split(., .$Model)

```

```

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' index") +
    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)

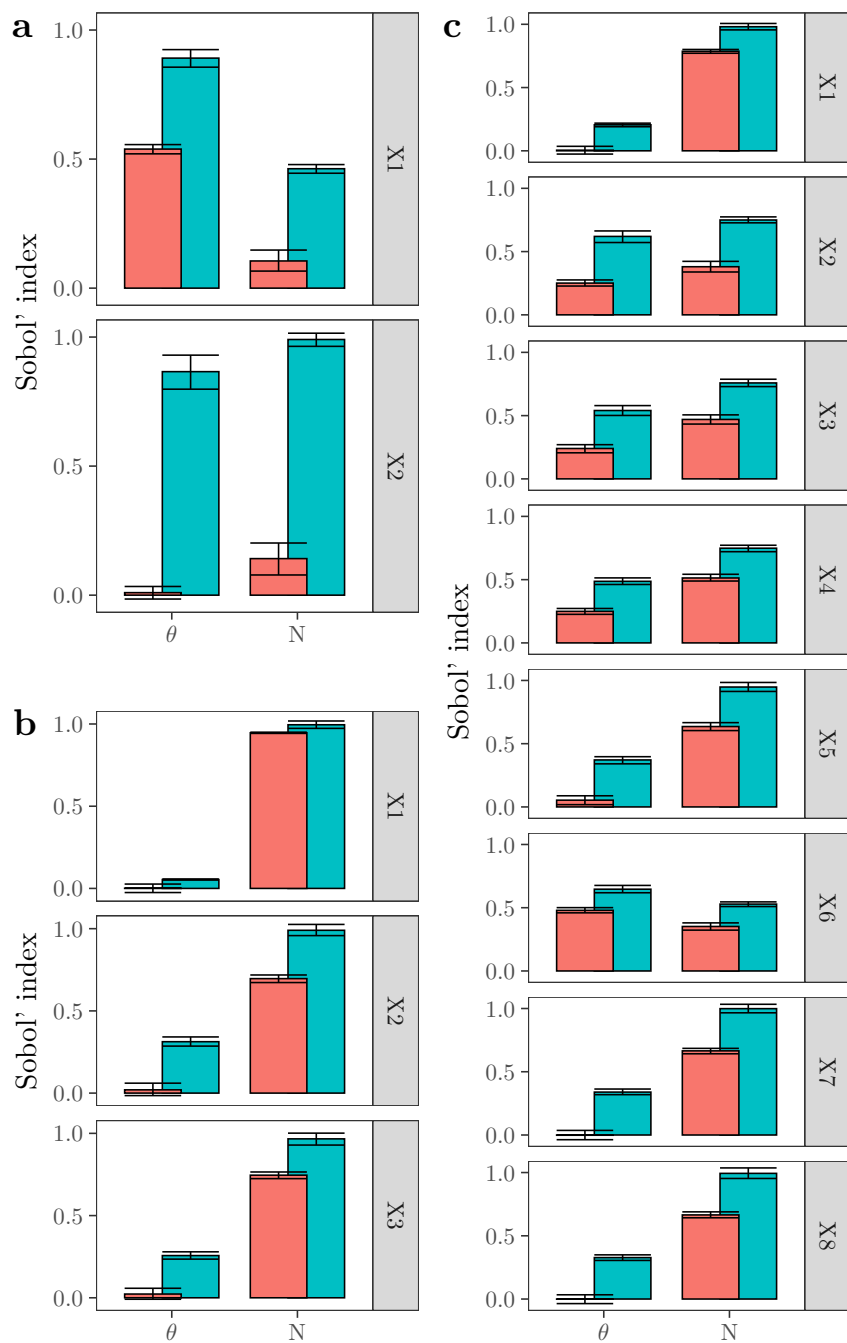
## Warning: Graphs cannot be horizontally aligned unless the axis parameter is
## set. Placing graphs unaligned.

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

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

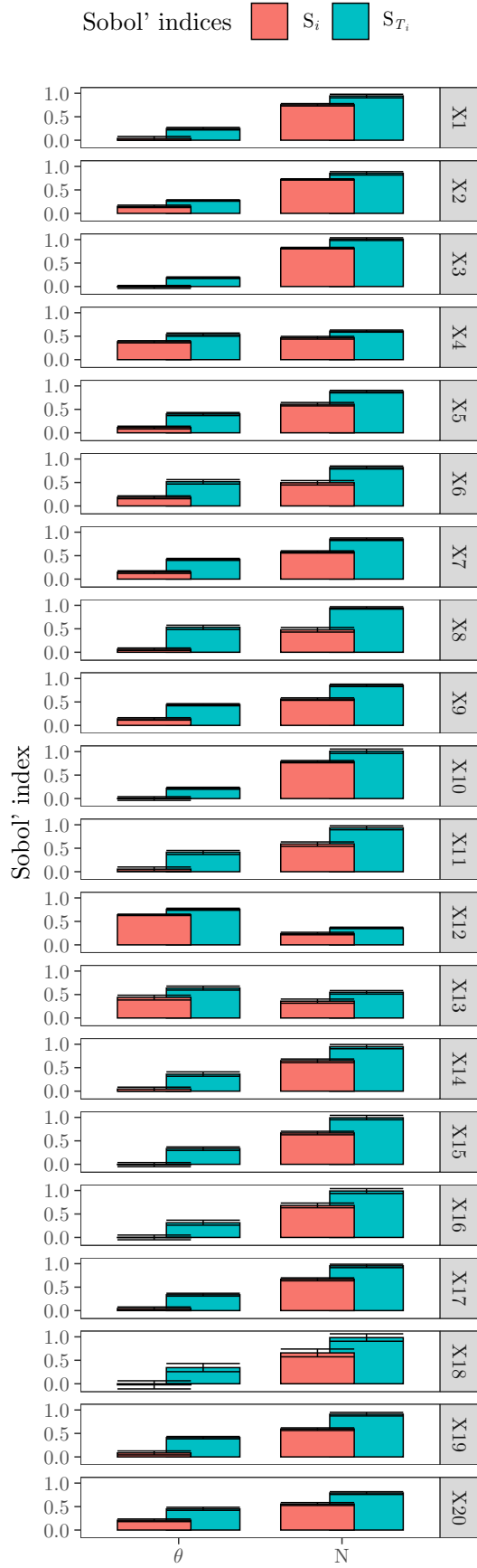
```

Sobol' indices ■  $S_i$  ■  $S_{T_i}$



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

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



## 6 Session information

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

```
sessionInfo()
```

```
## R version 3.6.1 (2019-07-05)
## Platform: x86_64-apple-darwin15.6.0 (64-bit)
## Running under: macOS Catalina 10.15.2
##
## 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 ggridges_0.5.1 wesanderson_0.3.6
## [4] sensobol_0.2.1 pawnr_0.0.0.9000 overlapping_1.5.4
## [7] testthat_2.2.1 cowplot_1.0.0 scales_1.0.0
## [10] doParallel_1.0.15 iterators_1.0.12 foreach_1.4.7
## [13] boot_1.3-23 sensitivity_1.16.2 randtoolbox_1.30.0
## [16] rngWELL_0.10-5 data.table_1.12.2 forcats_0.4.0
## [19] stringr_1.4.0 dplyr_0.8.3 purrr_0.3.2
## [22] readr_1.3.1 tidyr_1.0.0 tibble_2.1.3
## [25] ggplot2_3.2.1 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_0.3.5
## [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_0.4.0 bibtex_0.4.2
## [31] sessioninfo_1.1.1 htmlwidgets_1.5.1 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]	plyr_1.8.4	pkgbuild_1.0.5	grid_3.6.1
## [49]	crayon_1.3.4	lattice_0.20-38	haven_2.1.1
## [52]	hms_0.5.1	zeallot_0.1.0	knitr_1.25
## [55]	ps_1.3.0	pillar_1.4.2	reshape2_1.4.3
## [58]	codetools_0.2-16	pkgload_1.0.2	glue_1.3.1
## [61]	evaluate_0.14	remotes_2.1.0	modelr_0.1.5
## [64]	vctr_0.2.0	Rdpack_0.11-0	cellranger_1.1.0
## [67]	gtable_0.3.0	assertthat_0.2.1	xfun_0.9
## [70]	broom_0.5.2	filehash_2.4-2	tinytex_0.16
## [73]	memoise_1.1.0	ellipsis_0.3.0	