

A sensitivity analysis of the PAWN sensitivity index

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Contents

1	Preliminary functions	2
2	Check convergence of Sobol' indices and PAWN	2
2.1	Sample matrix	3
2.2	Model output	3
2.3	Sobol' indices	4
2.4	PAWN	6
2.5	Plot convergence	7
3	Sensitivity of PAWN to its design parameters	10
3.1	The model	10
3.2	Settings	11
3.3	Sample matrix	12
3.4	Run the model	13
3.5	Uncertainty analysis	14
3.6	Sensitivity analysis	25
4	Sensitivity of Sobol' indices to its design parameters	28
4.1	The model	28
4.2	Settings	29
4.3	Sample matrix	29
4.4	Run the model	30
4.5	Uncertainty analysis	31
4.6	Sensitivity analysis	41
5	Extra plots	44

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"))

# 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(detectedCores() * 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 <- 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

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

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

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

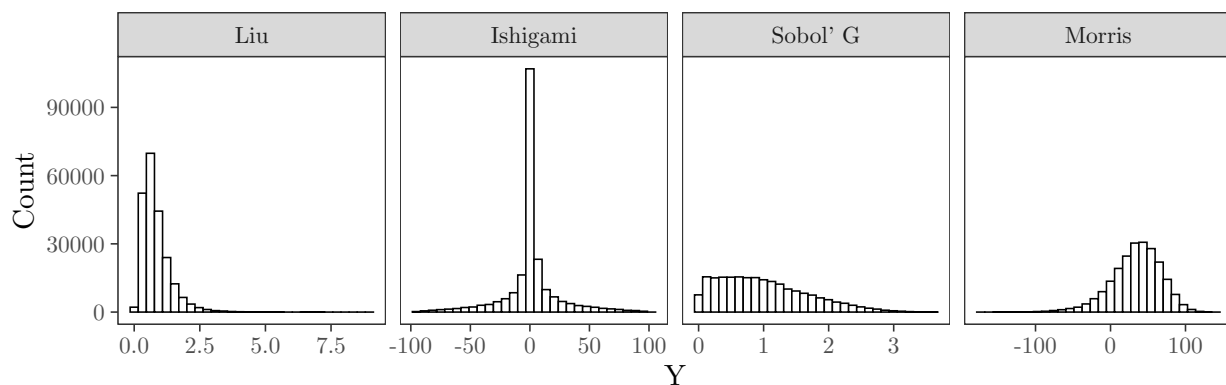
```
}
```

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

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

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

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



2.3 Sobol' indices

```
# COMPUTE 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 = as.numeric(j),
                                  type = "saltelli",
                                  R = R,
                                  parallel = "multicore",
                                  ncpus = n_cores)
    out.ci[[i]][[j]] <- sobol_ci(out[[i]][[j]],
                                 params = params[[i]],
                                 type = type,
                                 conf = conf)
  }
}

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

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

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

# SOBOL' CONVERGENCE -----

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

```

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

2.4 PAWN

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

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

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

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

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

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

# PAWN CONVERGENCE -----

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

```

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

```

2.5 Plot convergence

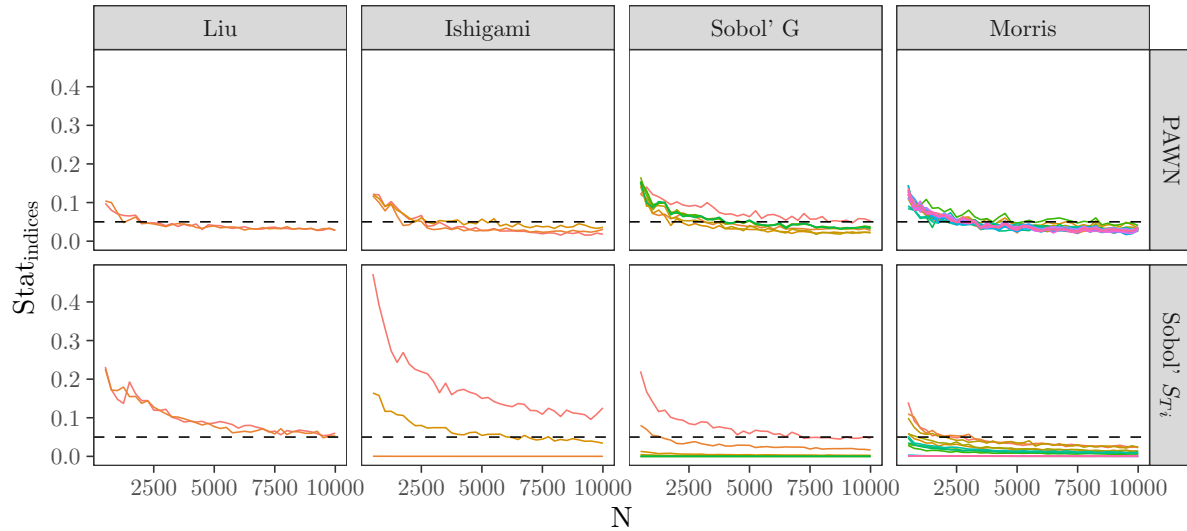
```

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

```

Model inputs

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



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

# Sobol' indices
a <- plot_sobol(sobol.convergence[N==max(N)],
               dummy = sobol.dummy.final[N==max(N)]) +
  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==max(N)] %>%
  plot_pawn(.) +
  geom_rect(data = pawn.index.dummy[N==max(N)],
           aes(ymin = 0,
               ymax = high.ci,
               xmin = -Inf,
               xmax = Inf),
           fill = "black",
           alpha = 0.1,
```



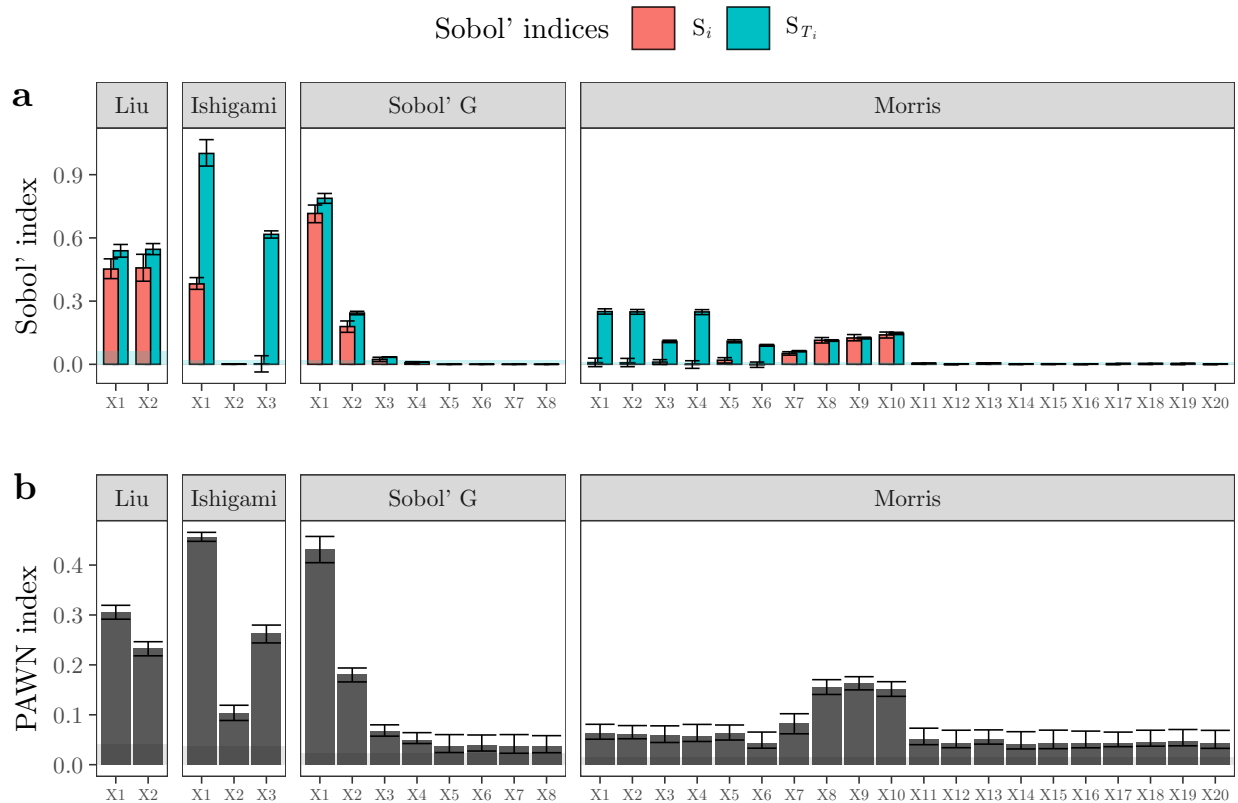
```

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

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

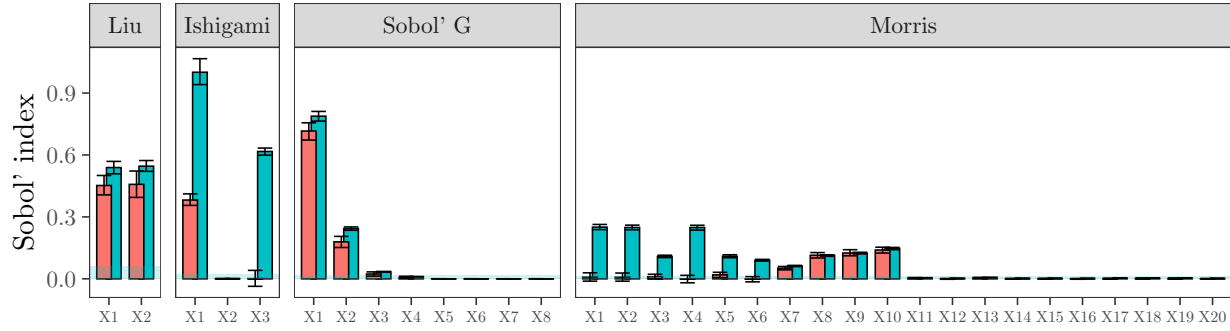
plot_grid(legend, bottom,
          labels = c("", ""),
          ncol = 1,
          align = "",
          rel_heights = c(0.1, 1))

```

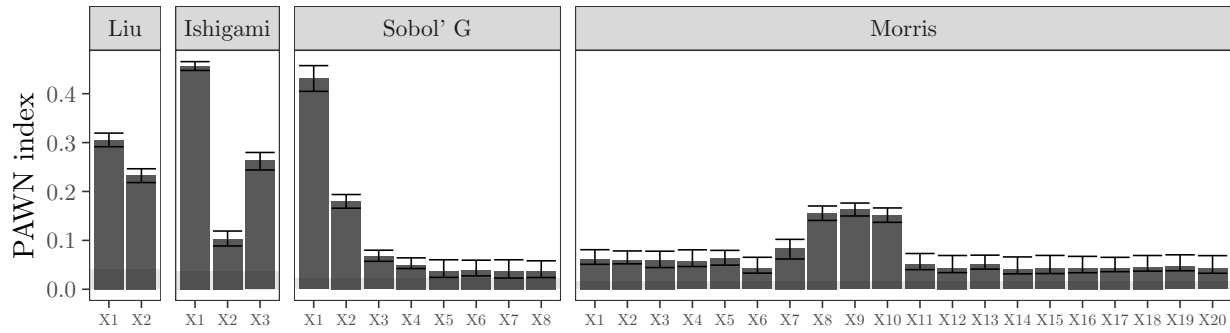


PLOT SOBO' AND PAWN INDICES (INDIVIDUAL PLOTS) -----

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 -----

```

```

# Set sample size
n <- 2 ^ 12

# 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
##          ---
## 786428: optimum      4 2500 16      864     2
## 786429: optimum      4 3500 18      364     1
## 786430: optimum      4 3000 17      114     2
## 786431: optimum      4 2000 19      614     1
## 786432: optimum      4 2000 17      372     1

```

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 ^ 12))], 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  0.268
## 2:    $max \\notin \\theta$ Liu X1-X2  0.126
## 3:           Optimum   Liu X1-X2  0.012
##
## [[2]]
##           setting   Model    rn overlap
## 1:    $max \\in \\theta$ Ishigami X1-X2  0.009
## 2:    $max \\in \\theta$ Ishigami X1-X3  0.052
## 3:    $max \\in \\theta$ Ishigami X2-X3  0.094
## 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  0.040
## 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   0.106
##  2:    $max \\in \\theta$ Sobol' G X1-X3   0.011
##  3:    $max \\in \\theta$ Sobol' G X1-X4   0.012
##  4:    $max \\in \\theta$ Sobol' G X1-X5   0.007
##  5:    $max \\in \\theta$ Sobol' G X1-X6   0.008
##  6:    $max \\in \\theta$ Sobol' G X1-X7   0.007
##  7:    $max \\in \\theta$ Sobol' G X1-X8   0.009
##  8:    $max \\in \\theta$ Sobol' G X2-X3   0.196
##  9:    $max \\in \\theta$ Sobol' G X2-X4   0.141
## 10:    $max \\in \\theta$ Sobol' G X2-X5   0.109
## 11:    $max \\in \\theta$ Sobol' G X2-X6   0.109
## 12:    $max \\in \\theta$ Sobol' G X2-X7   0.102
## 13:    $max \\in \\theta$ Sobol' G X2-X8   0.104
## 14:    $max \\in \\theta$ Sobol' G X3-X4   0.703
## 15:    $max \\in \\theta$ Sobol' G X3-X5   0.589
## 16:    $max \\in \\theta$ Sobol' G X3-X6   0.569
## 17:    $max \\in \\theta$ Sobol' G X3-X7   0.543
## 18:    $max \\in \\theta$ Sobol' G X3-X8   0.545
## 19:    $max \\in \\theta$ Sobol' G X4-X5   0.836
## 20:    $max \\in \\theta$ Sobol' G X4-X6   0.808
## 21:    $max \\in \\theta$ Sobol' G X4-X7   0.778
## 22:    $max \\in \\theta$ Sobol' G X4-X8   0.778
## 23:    $max \\in \\theta$ Sobol' G X5-X6   0.954
## 24:    $max \\in \\theta$ Sobol' G X5-X7   0.921
## 25:    $max \\in \\theta$ Sobol' G X5-X8   0.916
## 26:    $max \\in \\theta$ Sobol' G X6-X7   0.947
## 27:    $max \\in \\theta$ Sobol' G X6-X8   0.953
## 28:    $max \\in \\theta$ Sobol' G X7-X8   0.954
## 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   0.088
## 38: $max \\notin \\theta$ Sobol' G X2-X5   0.075
## 39: $max \\notin \\theta$ Sobol' G X2-X6   0.077
## 40: $max \\notin \\theta$ Sobol' G X2-X7   0.075
## 41: $max \\notin \\theta$ Sobol' G X2-X8   0.075
## 42: $max \\notin \\theta$ Sobol' G X3-X4   0.644
## 43: $max \\notin \\theta$ Sobol' G X3-X5   0.567
## 44: $max \\notin \\theta$ Sobol' G X3-X6   0.547
## 45: $max \\notin \\theta$ Sobol' G X3-X7   0.525
## 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 0.824
## 49: $max \\notin \\theta$ Sobol' G X4-X7 0.800
## 50: $max \\notin \\theta$ Sobol' G X4-X8 0.794
## 51: $max \\notin \\theta$ Sobol' G X5-X6 0.951
## 52: $max \\notin \\theta$ Sobol' G X5-X7 0.926
## 53: $max \\notin \\theta$ Sobol' G X5-X8 0.919
## 54: $max \\notin \\theta$ Sobol' G X6-X7 0.953
## 55: $max \\notin \\theta$ Sobol' G X6-X8 0.954
## 56: $max \\notin \\theta$ Sobol' G X7-X8 0.957
## 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 0.001
## 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 0.278
## 71:          Optimum Sobol' G X3-X5 0.190
## 72:          Optimum Sobol' G X3-X6 0.182
## 73:          Optimum Sobol' G X3-X7 0.183
## 74:          Optimum Sobol' G X3-X8 0.172
## 75:          Optimum Sobol' G X4-X5 0.545
## 76:          Optimum Sobol' G X4-X6 0.528
## 77:          Optimum Sobol' G X4-X7 0.520
## 78:          Optimum Sobol' G X4-X8 0.493
## 79:          Optimum Sobol' G X5-X6 0.956
## 80:          Optimum Sobol' G X5-X7 0.945
## 81:          Optimum Sobol' G X5-X8 0.907
## 82:          Optimum Sobol' G X6-X7 0.953
## 83:          Optimum Sobol' G X6-X8 0.922
## 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 0.937
## 3: $max \\in \\theta$ Morris  X1-X4 0.889
## 4: $max \\in \\theta$ Morris  X1-X5 0.888
## 5: $max \\in \\theta$ Morris  X1-X6 0.814
## ---

```

```
## 566:          Optimum Morris X17-X19    0.880
## 567:          Optimum Morris X17-X20    0.963
## 568:          Optimum Morris X18-X19    0.751
## 569:          Optimum Morris X18-X20    0.679
## 570:          Optimum Morris X19-X20    0.888
```

```
lapply(par.overlap, function(x) final.overlap[[4]][rn %like% x])
```

```
## [[1]]
##           setting Model      rn overlap
## 1: $max \\in \\theta$ Morris  X1-X2    0.907
## 2: $max \\in \\in \\theta$ Morris  X1-X3    0.937
## 3: $max \\in \\in \\theta$ Morris  X1-X4    0.889
## 4: $max \\in \\in \\theta$ Morris  X1-X5    0.888
## 5: $max \\in \\in \\theta$ Morris  X1-X6    0.814
```

```
## ---
## 458:          Optimum Morris X17-X19    0.880
## 459:          Optimum Morris X17-X20    0.963
## 460:          Optimum Morris X18-X19    0.751
## 461:          Optimum Morris X18-X20    0.679
## 462:          Optimum Morris X19-X20    0.888
```

```
##
## [[2]]
##           setting Model      rn overlap
## 1: $max \\in \\in \\theta$ Morris  X1-X2    0.907
## 2: $max \\in \\in \\theta$ Morris  X1-X20    0.776
## 3: $max \\in \\in \\theta$ Morris  X2-X3    0.957
## 4: $max \\in \\in \\theta$ Morris  X2-X4    0.936
## 5: $max \\in \\in \\theta$ Morris  X2-X5    0.846
```

```
## ---
## 107:          Optimum Morris X15-X20    0.955
## 108:          Optimum Morris X16-X20    0.972
## 109:          Optimum Morris X17-X20    0.963
## 110:          Optimum Morris X18-X20    0.679
## 111:          Optimum Morris X19-X20    0.888
```

```
##
## [[3]]
##           setting Model      rn overlap
## 1:  $max \\in \\in \\theta$ Morris  X1-X3    0.937
## 2:  $max \\in \\in \\theta$ Morris  X2-X3    0.957
## 3:  $max \\in \\in \\theta$ Morris  X3-X4    0.928
## 4:  $max \\in \\in \\theta$ Morris  X3-X5    0.871
## 5:  $max \\in \\in \\theta$ Morris  X3-X6    0.854
## 6:  $max \\in \\in \\theta$ Morris  X3-X7    0.643
## 7:  $max \\in \\in \\theta$ Morris  X3-X8    0.236
## 8:  $max \\in \\in \\theta$ Morris  X3-X9    0.224
## 9:  $max \\in \\in \\theta$ Morris  X3-X10   0.251
## 10: $max \\in \\in \\theta$ Morris  X3-X11   0.900
```

## 11:	\$max \\in \\theta\$	Morris	X3-X12	0.805
## 12:	\$max \\in \\theta\$	Morris	X3-X13	0.877
## 13:	\$max \\in \\theta\$	Morris	X3-X14	0.845
## 14:	\$max \\in \\theta\$	Morris	X3-X15	0.805
## 15:	\$max \\in \\theta\$	Morris	X3-X16	0.844
## 16:	\$max \\in \\theta\$	Morris	X3-X17	0.841
## 17:	\$max \\in \\theta\$	Morris	X3-X18	0.932
## 18:	\$max \\in \\theta\$	Morris	X3-X19	0.819
## 19:	\$max \\in \\theta\$	Morris	X3-X20	0.818
## 20:	\$max \\notin \\theta\$	Morris	X1-X3	0.917
## 21:	\$max \\notin \\theta\$	Morris	X2-X3	0.961
## 22:	\$max \\notin \\theta\$	Morris	X3-X4	0.934
## 23:	\$max \\notin \\theta\$	Morris	X3-X5	0.914
## 24:	\$max \\notin \\theta\$	Morris	X3-X6	0.853
## 25:	\$max \\notin \\theta\$	Morris	X3-X7	0.590
## 26:	\$max \\notin \\theta\$	Morris	X3-X8	0.134
## 27:	\$max \\notin \\theta\$	Morris	X3-X9	0.123
## 28:	\$max \\notin \\theta\$	Morris	X3-X10	0.160
## 29:	\$max \\notin \\theta\$	Morris	X3-X11	0.885
## 30:	\$max \\notin \\theta\$	Morris	X3-X12	0.803
## 31:	\$max \\notin \\theta\$	Morris	X3-X13	0.882
## 32:	\$max \\notin \\theta\$	Morris	X3-X14	0.826
## 33:	\$max \\notin \\theta\$	Morris	X3-X15	0.793
## 34:	\$max \\notin \\theta\$	Morris	X3-X16	0.828
## 35:	\$max \\notin \\theta\$	Morris	X3-X17	0.835
## 36:	\$max \\notin \\theta\$	Morris	X3-X18	0.909
## 37:	\$max \\notin \\theta\$	Morris	X3-X19	0.807
## 38:	\$max \\notin \\theta\$	Morris	X3-X20	0.809
## 39:	Optimum	Morris	X1-X3	0.800
## 40:	Optimum	Morris	X2-X3	0.726
## 41:	Optimum	Morris	X3-X4	0.745
## 42:	Optimum	Morris	X3-X5	0.783
## 43:	Optimum	Morris	X3-X6	0.527
## 44:	Optimum	Morris	X3-X7	0.247
## 45:	Optimum	Morris	X3-X8	0.006
## 46:	Optimum	Morris	X3-X9	0.008
## 47:	Optimum	Morris	X3-X10	0.007
## 48:	Optimum	Morris	X3-X11	0.701
## 49:	Optimum	Morris	X3-X12	0.444
## 50:	Optimum	Morris	X3-X13	0.626
## 51:	Optimum	Morris	X3-X14	0.456
## 52:	Optimum	Morris	X3-X15	0.426
## 53:	Optimum	Morris	X3-X16	0.444
## 54:	Optimum	Morris	X3-X17	0.450
## 55:	Optimum	Morris	X3-X18	0.595
## 56:	Optimum	Morris	X3-X19	0.478
## 57:	Optimum	Morris	X3-X20	0.442
##	setting	Model	rn overlap	

```

##
## [[4]]
##          setting Model      rn overlap
##  1:    $max \\in \\theta$ Morris X1-X4  0.889
##  2:    $max \\in \\theta$ Morris X2-X4  0.936
##  3:    $max \\in \\theta$ Morris X3-X4  0.928
##  4:    $max \\in \\theta$ Morris X4-X5  0.870
##  5:    $max \\in \\theta$ Morris X4-X6  0.904
##  6:    $max \\in \\theta$ Morris X4-X7  0.636
##  7:    $max \\in \\theta$ Morris X4-X8  0.235
##  8:    $max \\in \\theta$ Morris X4-X9  0.225
##  9:    $max \\in \\theta$ Morris X4-X10 0.251
## 10:    $max \\in \\theta$ Morris X4-X11 0.947
## 11:    $max \\in \\theta$ Morris X4-X12 0.853
## 12:    $max \\in \\theta$ Morris X4-X13 0.921
## 13:    $max \\in \\theta$ Morris X4-X14 0.876
## 14:    $max \\in \\theta$ Morris X4-X15 0.851
## 15:    $max \\in \\theta$ Morris X4-X16 0.890
## 16:    $max \\in \\theta$ Morris X4-X17 0.889
## 17:    $max \\in \\theta$ Morris X4-X18 0.964
## 18:    $max \\in \\theta$ Morris X4-X19 0.865
## 19:    $max \\in \\theta$ Morris X4-X20 0.863
## 20: $max \\notin \\theta$ Morris X1-X4  0.870
## 21: $max \\notin \\theta$ Morris X2-X4  0.943
## 22: $max \\notin \\theta$ Morris X3-X4  0.934
## 23: $max \\notin \\theta$ Morris X4-X5  0.867
## 24: $max \\notin \\theta$ Morris X4-X6  0.893
## 25: $max \\notin \\theta$ Morris X4-X7  0.574
## 26: $max \\notin \\theta$ Morris X4-X8  0.134
## 27: $max \\notin \\theta$ Morris X4-X9  0.124
## 28: $max \\notin \\theta$ Morris X4-X10 0.160
## 29: $max \\notin \\theta$ Morris X4-X11 0.929
## 30: $max \\notin \\theta$ Morris X4-X12 0.845
## 31: $max \\notin \\theta$ Morris X4-X13 0.923
## 32: $max \\notin \\theta$ Morris X4-X14 0.872
## 33: $max \\notin \\theta$ Morris X4-X15 0.835
## 34: $max \\notin \\theta$ Morris X4-X16 0.873
## 35: $max \\notin \\theta$ Morris X4-X17 0.876
## 36: $max \\notin \\theta$ Morris X4-X18 0.950
## 37: $max \\notin \\theta$ Morris X4-X19 0.850
## 38: $max \\notin \\theta$ Morris X4-X20 0.849
## 39:          Optimum Morris X1-X4  0.893
## 40:          Optimum Morris X2-X4  0.958
## 41:          Optimum Morris X3-X4  0.745
## 42:          Optimum Morris X4-X5  0.586
## 43:          Optimum Morris X4-X6  0.646
## 44:          Optimum Morris X4-X7  0.200
## 45:          Optimum Morris X4-X8  0.005

```

```

## 46:          Optimum Morris  X4-X9    0.007
## 47:          Optimum Morris  X4-X10   0.006
## 48:          Optimum Morris  X4-X11   0.905
## 49:          Optimum Morris  X4-X12   0.541
## 50:          Optimum Morris  X4-X13   0.801
## 51:          Optimum Morris  X4-X14   0.556
## 52:          Optimum Morris  X4-X15   0.515
## 53:          Optimum Morris  X4-X16   0.541
## 54:          Optimum Morris  X4-X17   0.545
## 55:          Optimum Morris  X4-X18   0.779
## 56:          Optimum Morris  X4-X19   0.592
## 57:          Optimum Morris  X4-X20   0.536
##           setting  Model      rn overlap
##
## [[5]]
##           setting  Model      rn overlap
## 1:    $max \\in \\theta$ Morris  X1-X5    0.888
## 2:    $max \\in \\theta$ Morris  X2-X5    0.846
## 3:    $max \\in \\theta$ Morris  X3-X5    0.871
## 4:    $max \\in \\theta$ Morris  X4-X5    0.870
## 5:    $max \\in \\theta$ Morris  X5-X6    0.806
## 6:    $max \\in \\theta$ Morris  X5-X7    0.687
## 7:    $max \\in \\theta$ Morris  X5-X8    0.289
## 8:    $max \\in \\theta$ Morris  X5-X9    0.278
## 9:    $max \\in \\theta$ Morris  X5-X10   0.307
## 10:   $max \\in \\theta$ Morris  X5-X11   0.860
## 11:   $max \\in \\theta$ Morris  X5-X12   0.753
## 12:   $max \\in \\theta$ Morris  X5-X13   0.808
## 13:   $max \\in \\theta$ Morris  X5-X14   0.771
## 14:   $max \\in \\theta$ Morris  X5-X15   0.751
## 15:   $max \\in \\theta$ Morris  X5-X16   0.794
## 16:   $max \\in \\theta$ Morris  X5-X17   0.786
## 17:   $max \\in \\theta$ Morris  X5-X18   0.867
## 18:   $max \\in \\theta$ Morris  X5-X19   0.763
## 19:   $max \\in \\theta$ Morris  X5-X20   0.768
## 20: $max \\notin \\theta$ Morris  X1-X5    0.950
## 21: $max \\notin \\theta$ Morris  X2-X5    0.909
## 22: $max \\notin \\theta$ Morris  X3-X5    0.914
## 23: $max \\notin \\theta$ Morris  X4-X5    0.867
## 24: $max \\notin \\theta$ Morris  X5-X6    0.794
## 25: $max \\notin \\theta$ Morris  X5-X7    0.632
## 26: $max \\notin \\theta$ Morris  X5-X8    0.137
## 27: $max \\notin \\theta$ Morris  X5-X9    0.126
## 28: $max \\notin \\theta$ Morris  X5-X10   0.163
## 29: $max \\notin \\theta$ Morris  X5-X11   0.833
## 30: $max \\notin \\theta$ Morris  X5-X12   0.748
## 31: $max \\notin \\theta$ Morris  X5-X13   0.823
## 32: $max \\notin \\theta$ Morris  X5-X14   0.763

```

```

## 33: $max \\notin \\theta$ Morris X5-X15 0.740
## 34: $max \\notin \\theta$ Morris X5-X16 0.782
## 35: $max \\notin \\theta$ Morris X5-X17 0.784
## 36: $max \\notin \\theta$ Morris X5-X18 0.852
## 37: $max \\notin \\theta$ Morris X5-X19 0.752
## 38: $max \\notin \\theta$ Morris X5-X20 0.757
## 39: Optimum Morris X1-X5 0.640
## 40: Optimum Morris X2-X5 0.573
## 41: Optimum Morris X3-X5 0.783
## 42: Optimum Morris X4-X5 0.586
## 43: Optimum Morris X5-X6 0.419
## 44: Optimum Morris X5-X7 0.282
## 45: Optimum Morris X5-X8 0.006
## 46: Optimum Morris X5-X9 0.009
## 47: Optimum Morris X5-X10 0.008
## 48: Optimum Morris X5-X11 0.548
## 49: Optimum Morris X5-X12 0.354
## 50: Optimum Morris X5-X13 0.491
## 51: Optimum Morris X5-X14 0.365
## 52: Optimum Morris X5-X15 0.341
## 53: Optimum Morris X5-X16 0.354
## 54: Optimum Morris X5-X17 0.360
## 55: Optimum Morris X5-X18 0.464
## 56: Optimum Morris X5-X19 0.378
## 57: Optimum Morris X5-X20 0.355
##      setting Model      rn overlap
##
## [[6]]
##      setting Model      rn overlap
## 1:  $max \\in \\theta$ Morris X1-X6 0.814
## 2:  $max \\in \\theta$ Morris X2-X6 0.865
## 3:  $max \\in \\theta$ Morris X3-X6 0.854
## 4:  $max \\in \\theta$ Morris X4-X6 0.904
## 5:  $max \\in \\theta$ Morris X5-X6 0.806
## 6:  $max \\in \\theta$ Morris X6-X7 0.587
## 7:  $max \\in \\theta$ Morris X6-X8 0.213
## 8:  $max \\in \\theta$ Morris X6-X9 0.204
## 9:  $max \\in \\theta$ Morris X6-X10 0.230
## 10: $max \\in \\theta$ Morris X6-X11 0.930
## 11: $max \\in \\theta$ Morris X6-X12 0.924
## 12: $max \\in \\theta$ Morris X6-X13 0.936
## 13: $max \\in \\theta$ Morris X6-X14 0.928
## 14: $max \\in \\theta$ Morris X6-X15 0.931
## 15: $max \\in \\theta$ Morris X6-X16 0.959
## 16: $max \\in \\theta$ Morris X6-X17 0.969
## 17: $max \\in \\theta$ Morris X6-X18 0.905
## 18: $max \\in \\theta$ Morris X6-X19 0.931
## 19: $max \\in \\theta$ Morris X6-X20 0.947

```

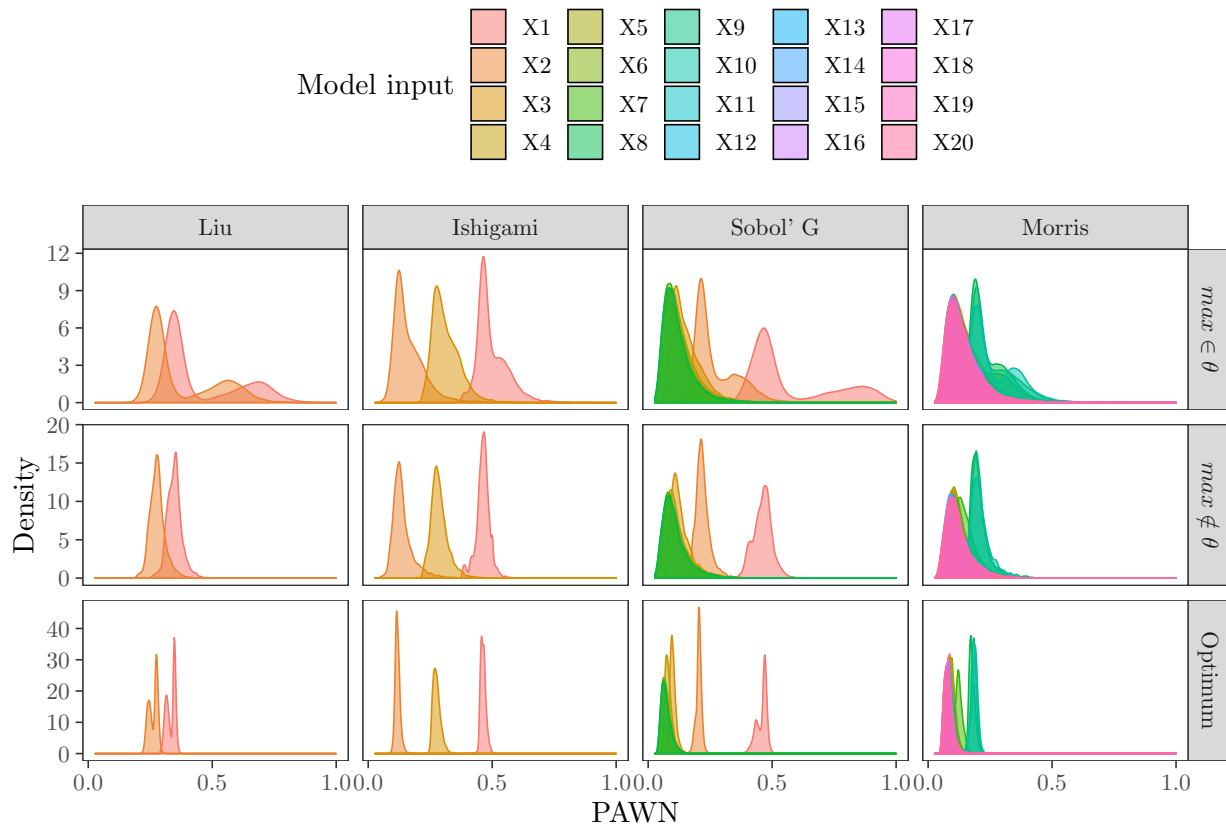
```
## 20: $max \\notin \\theta$ Morris X1-X6 0.792
## 21: $max \\notin \\theta$ Morris X2-X6 0.862
## 22: $max \\notin \\theta$ Morris X3-X6 0.853
## 23: $max \\notin \\theta$ Morris X4-X6 0.893
## 24: $max \\notin \\theta$ Morris X5-X6 0.794
## 25: $max \\notin \\theta$ Morris X6-X7 0.537
## 26: $max \\notin \\theta$ Morris X6-X8 0.128
## 27: $max \\notin \\theta$ Morris X6-X9 0.119
## 28: $max \\notin \\theta$ Morris X6-X10 0.153
## 29: $max \\notin \\theta$ Morris X6-X11 0.937
## 30: $max \\notin \\theta$ Morris X6-X12 0.932
## 31: $max \\notin \\theta$ Morris X6-X13 0.946
## 32: $max \\notin \\theta$ Morris X6-X14 0.940
## 33: $max \\notin \\theta$ Morris X6-X15 0.921
## 34: $max \\notin \\theta$ Morris X6-X16 0.943
## 35: $max \\notin \\theta$ Morris X6-X17 0.966
## 36: $max \\notin \\theta$ Morris X6-X18 0.913
## 37: $max \\notin \\theta$ Morris X6-X19 0.933
## 38: $max \\notin \\theta$ Morris X6-X20 0.943
## 39: Optimum Morris X1-X6 0.589
## 40: Optimum Morris X2-X6 0.663
## 41: Optimum Morris X3-X6 0.527
## 42: Optimum Morris X4-X6 0.646
## 43: Optimum Morris X5-X6 0.419
## 44: Optimum Morris X6-X7 0.170
## 45: Optimum Morris X6-X8 0.005
## 46: Optimum Morris X6-X9 0.006
## 47: Optimum Morris X6-X10 0.006
## 48: Optimum Morris X6-X11 0.713
## 49: Optimum Morris X6-X12 0.843
## 50: Optimum Morris X6-X13 0.795
## 51: Optimum Morris X6-X14 0.862
## 52: Optimum Morris X6-X15 0.808
## 53: Optimum Morris X6-X16 0.840
## 54: Optimum Morris X6-X17 0.848
## 55: Optimum Morris X6-X18 0.797
## 56: Optimum Morris X6-X19 0.896
## 57: Optimum Morris X6-X20 0.836
## setting Model rn overlap
```

```
# 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 ^ 12,
                                                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 SOBOL' INDICES -----

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

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

```

```

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

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

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

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

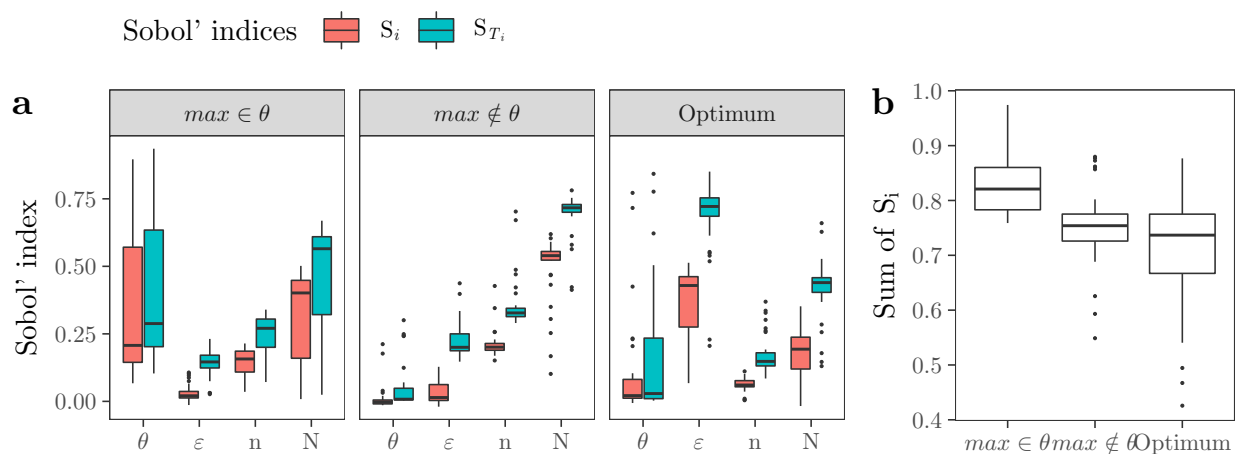
bottom <- plot_grid(a, b,
                    ncol = 2,
                    align = "hv",
                    labels = "auto",
                    rel_widths = c(2.2, 1))

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

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

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

```



4 Sensitivity of Sobol' indices to its design parameters

4.1 The model

```
# THE MODEL -----

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

sobol_matrix <- function(n, k) {
  df <- randtoolbox::sobol(n = n, dim = k * 2)
  A <- df[, 1:k]
  B <- df[, (k + 1) : (k * 2)]
  out <- scrambled_sobol(A = A, B = B)
  return(out)
}

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

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

```

}

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

# The model
model_sobol <- function(Model, N, k, Theta) {
  data <- sobol_matrix(n = N, k = k)
  if(Model == 1) {
    Y <- liu_Mapply(data)
  } else if(Model == 2) {
    Y <- sensobol::ishigami_Mapply(data)
  } else if(Model == 3) {
    Y <- sensobol::sobol_Fun(data)
  } else {
    Y <- sensitivity::morris.fun(data)
  }
  out <- sobol_Ti(Y, params = paste("X", 1:k, sep = ""), type = Theta)
  return(out)
}

```

4.2 Settings

```

# DEFINE SETTINGS -----

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

```

4.3 Sample matrix

```

# CREATION OF THE MATRICES -----

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

```

```

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

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

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

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

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
##      ---
## 131068:          N      4  650  jansen 20
## 131069:          N      4 1550  jansen 20
## 131070:          N      4 1100  jansen 20
## 131071:          N      4  200  jansen 20
## 131072:          N      4  200  jansen 20

```

```
print(n)
```

```
## [1] 4096
```

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 ^ 12))], 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)]
}

```

```

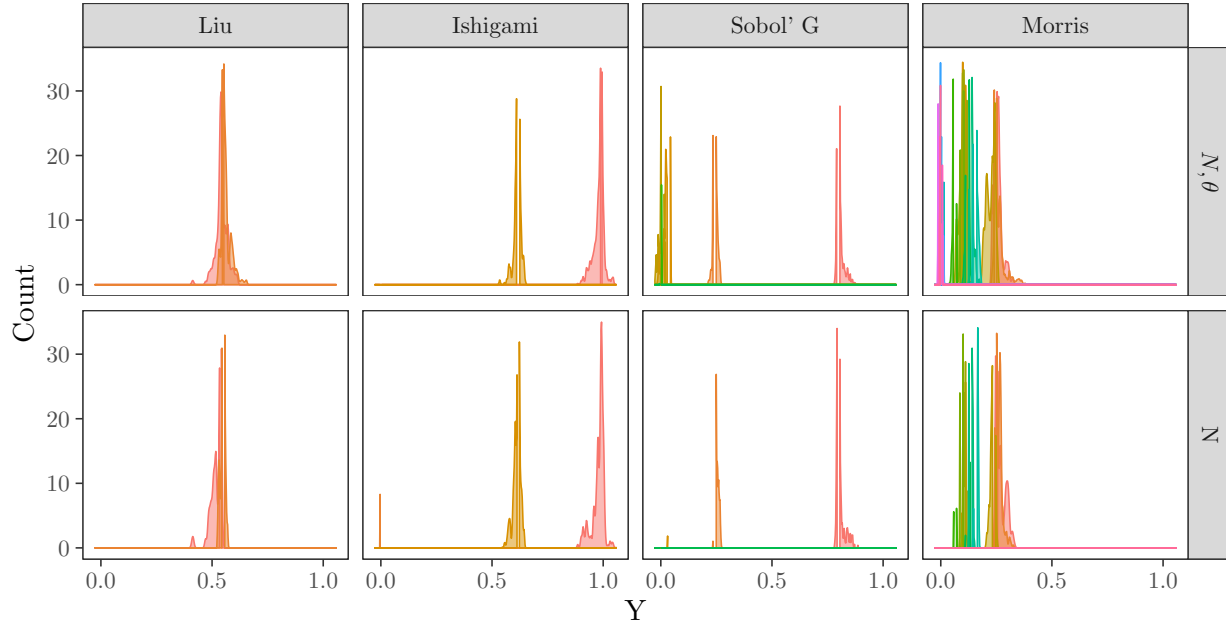
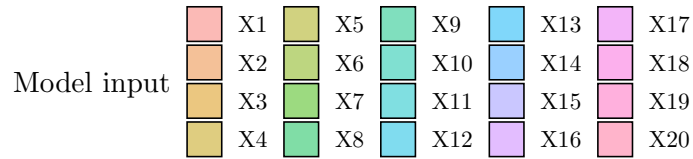
# EXPORT AB MATRIX FOR SOBOL' -----

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  0.348
## 2:      N      Liu X1-X2  0.193
##
## [[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  0.035
## 15: $N,\\theta$ Sobol' G X3-X5  0.001
## 16: $N,\\theta$ Sobol' G X3-X6  0.002
## 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  0.037
## 21: $N,\\theta$ Sobol' G X4-X7  0.027
## 22: $N,\\theta$ Sobol' G X4-X8  0.026
## 23: $N,\\theta$ Sobol' G X5-X6  0.780
## 24: $N,\\theta$ Sobol' G X5-X7  0.208
## 25: $N,\\theta$ Sobol' G X5-X8  0.674
## 26: $N,\\theta$ Sobol' G X6-X7  0.260
```

```

## 27: $N,\\theta$ Sobol' G X6-X8 0.595
## 28: $N,\\theta$ Sobol' G X7-X8 0.227
## 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 0.374
## 52:      N Sobol' G X5-X7 0.615
## 53:      N Sobol' G X5-X8 0.685
## 54:      N Sobol' G X6-X7 0.270
## 55:      N Sobol' G X6-X8 0.264
## 56:      N Sobol' G X7-X8 0.695
##      setting      Model      rn overlap
##
## [[4]]
##      setting      Model      rn overlap
## 1: $N,\\theta$ Morris   X1-X2 0.458
## 2: $N,\\theta$ Morris   X1-X3 0.000
## 3: $N,\\theta$ Morris   X1-X4 0.292
## 4: $N,\\theta$ Morris   X1-X5 0.000
## 5: $N,\\theta$ Morris   X1-X6 0.000
## ---
## 376:      N Morris X17-X19 0.063
## 377:      N Morris X17-X20 0.000
## 378:      N Morris X18-X19 0.028
## 379:      N Morris X18-X20 0.000
## 380:      N Morris X19-X20 0.000

```

```
lapply(par.overlap, function(x) final.overlap[[4]][rn %like% x])
```

```

## [[1]]
##      setting  Model      rn overlap
##  1: $N,\\theta$ Morris  X1-X2   0.458
##  2: $N,\\theta$ Morris  X1-X3   0.000
##  3: $N,\\theta$ Morris  X1-X4   0.292
##  4: $N,\\theta$ Morris  X1-X5   0.000
##  5: $N,\\theta$ Morris  X1-X6   0.000
##  ---
## 304:          N Morris X17-X19  0.063
## 305:          N Morris X17-X20  0.000
## 306:          N Morris X18-X19  0.028
## 307:          N Morris X18-X20  0.000
## 308:          N Morris X19-X20  0.000
##
## [[2]]
##      setting  Model      rn overlap
##  1: $N,\\theta$ Morris  X1-X2   0.458
##  2: $N,\\theta$ Morris  X1-X20  0.000
##  3: $N,\\theta$ Morris  X2-X3   0.000
##  4: $N,\\theta$ Morris  X2-X4   0.261
##  5: $N,\\theta$ Morris  X2-X5   0.000
##  6: $N,\\theta$ Morris  X2-X6   0.000
##  7: $N,\\theta$ Morris  X2-X7   0.000
##  8: $N,\\theta$ Morris  X2-X8   0.000
##  9: $N,\\theta$ Morris  X2-X9   0.000
## 10: $N,\\theta$ Morris  X2-X10  0.000
## 11: $N,\\theta$ Morris  X2-X11  0.000
## 12: $N,\\theta$ Morris  X2-X12  0.000
## 13: $N,\\theta$ Morris  X2-X13  0.000
## 14: $N,\\theta$ Morris  X2-X14  0.000
## 15: $N,\\theta$ Morris  X2-X15  0.000
## 16: $N,\\theta$ Morris  X2-X16  0.000
## 17: $N,\\theta$ Morris  X2-X17  0.000
## 18: $N,\\theta$ Morris  X2-X18  0.000
## 19: $N,\\theta$ Morris  X2-X19  0.000
## 20: $N,\\theta$ Morris  X2-X20  0.000
## 21: $N,\\theta$ Morris  X3-X20  0.000
## 22: $N,\\theta$ Morris  X4-X20  0.000
## 23: $N,\\theta$ Morris  X5-X20  0.000
## 24: $N,\\theta$ Morris  X6-X20  0.000
## 25: $N,\\theta$ Morris  X7-X20  0.000
## 26: $N,\\theta$ Morris  X8-X20  0.000
## 27: $N,\\theta$ Morris  X9-X20  0.000
## 28: $N,\\theta$ Morris  X10-X20 0.000
## 29: $N,\\theta$ Morris  X11-X20 0.076
## 30: $N,\\theta$ Morris  X12-X20 0.224
## 31: $N,\\theta$ Morris  X13-X20 0.003
## 32: $N,\\theta$ Morris  X14-X20 0.565

```

```

## 33: $N,\\theta$ Morris X15-X20 0.355
## 34: $N,\\theta$ Morris X16-X20 0.289
## 35: $N,\\theta$ Morris X17-X20 0.298
## 36: $N,\\theta$ Morris X18-X20 0.261
## 37: $N,\\theta$ Morris X19-X20 0.394
## 38:      N Morris   X1-X2 0.554
## 39:      N Morris  X1-X20 0.000
## 40:      N Morris   X2-X3 0.000
## 41:      N Morris   X2-X4 0.131
## 42:      N Morris   X2-X5 0.000
## 43:      N Morris   X2-X6 0.000
## 44:      N Morris   X2-X7 0.000
## 45:      N Morris   X2-X8 0.000
## 46:      N Morris   X2-X9 0.000
## 47:      N Morris  X2-X10 0.000
## 48:      N Morris  X2-X11 0.000
## 49:      N Morris  X2-X12 0.000
## 50:      N Morris  X2-X13 0.000
## 51:      N Morris  X2-X14 0.000
## 52:      N Morris  X2-X15 0.000
## 53:      N Morris  X2-X16 0.000
## 54:      N Morris  X2-X17 0.000
## 55:      N Morris  X2-X18 0.000
## 56:      N Morris  X2-X19 0.000
## 57:      N Morris  X2-X20 0.000
## 58:      N Morris  X3-X20 0.000
## 59:      N Morris  X4-X20 0.000
## 60:      N Morris  X5-X20 0.000
## 61:      N Morris  X6-X20 0.000
## 62:      N Morris  X7-X20 0.000
## 63:      N Morris  X8-X20 0.000
## 64:      N Morris  X9-X20 0.000
## 65:      N Morris X10-X20 0.000
## 66:      N Morris X11-X20 0.000
## 67:      N Morris X12-X20 0.312
## 68:      N Morris X13-X20 0.000
## 69:      N Morris X14-X20 0.516
## 70:      N Morris X15-X20 0.235
## 71:      N Morris X16-X20 0.617
## 72:      N Morris X17-X20 0.000
## 73:      N Morris X18-X20 0.000
## 74:      N Morris X19-X20 0.000
##      setting  Model      rn overlap
##
## [[3]]
##      setting  Model      rn overlap
##  1: $N,\\theta$ Morris  X1-X3  0.000
##  2: $N,\\theta$ Morris  X2-X3  0.000

```

```

## 3: $N,\\theta$ Morris X3-X4 0.000
## 4: $N,\\theta$ Morris X3-X5 0.521
## 5: $N,\\theta$ Morris X3-X6 0.189
## 6: $N,\\theta$ Morris X3-X7 0.000
## 7: $N,\\theta$ Morris X3-X8 0.153
## 8: $N,\\theta$ Morris X3-X9 0.006
## 9: $N,\\theta$ Morris X3-X10 0.001
## 10: $N,\\theta$ Morris X3-X11 0.000
## 11: $N,\\theta$ Morris X3-X12 0.000
## 12: $N,\\theta$ Morris X3-X13 0.000
## 13: $N,\\theta$ Morris X3-X14 0.000
## 14: $N,\\theta$ Morris X3-X15 0.000
## 15: $N,\\theta$ Morris X3-X16 0.000
## 16: $N,\\theta$ Morris X3-X17 0.000
## 17: $N,\\theta$ Morris X3-X18 0.000
## 18: $N,\\theta$ Morris X3-X19 0.000
## 19: $N,\\theta$ Morris X3-X20 0.000
## 20: N Morris X1-X3 0.000
## 21: N Morris X2-X3 0.000
## 22: N Morris X3-X4 0.000
## 23: N Morris X3-X5 0.098
## 24: N Morris X3-X6 0.034
## 25: N Morris X3-X7 0.000
## 26: N Morris X3-X8 0.011
## 27: N Morris X3-X9 0.000
## 28: N Morris X3-X10 0.000
## 29: N Morris X3-X11 0.000
## 30: N Morris X3-X12 0.000
## 31: N Morris X3-X13 0.000
## 32: N Morris X3-X14 0.000
## 33: N Morris X3-X15 0.000
## 34: N Morris X3-X16 0.000
## 35: N Morris X3-X17 0.000
## 36: N Morris X3-X18 0.000
## 37: N Morris X3-X19 0.000
## 38: N Morris X3-X20 0.000
##      setting Model      rn overlap
##
## [[4]]
##      setting Model      rn overlap
## 1: $N,\\theta$ Morris X1-X4 0.292
## 2: $N,\\theta$ Morris X2-X4 0.261
## 3: $N,\\theta$ Morris X3-X4 0.000
## 4: $N,\\theta$ Morris X4-X5 0.000
## 5: $N,\\theta$ Morris X4-X6 0.000
## 6: $N,\\theta$ Morris X4-X7 0.000
## 7: $N,\\theta$ Morris X4-X8 0.000
## 8: $N,\\theta$ Morris X4-X9 0.000

```

```

## 9: $N,\\theta$ Morris X4-X10 0.001
## 10: $N,\\theta$ Morris X4-X11 0.000
## 11: $N,\\theta$ Morris X4-X12 0.000
## 12: $N,\\theta$ Morris X4-X13 0.000
## 13: $N,\\theta$ Morris X4-X14 0.000
## 14: $N,\\theta$ Morris X4-X15 0.000
## 15: $N,\\theta$ Morris X4-X16 0.000
## 16: $N,\\theta$ Morris X4-X17 0.000
## 17: $N,\\theta$ Morris X4-X18 0.000
## 18: $N,\\theta$ Morris X4-X19 0.000
## 19: $N,\\theta$ Morris X4-X20 0.000
## 20:      N Morris X1-X4 0.107
## 21:      N Morris X2-X4 0.131
## 22:      N Morris X3-X4 0.000
## 23:      N Morris X4-X5 0.000
## 24:      N Morris X4-X6 0.000
## 25:      N Morris X4-X7 0.000
## 26:      N Morris X4-X8 0.000
## 27:      N Morris X4-X9 0.000
## 28:      N Morris X4-X10 0.000
## 29:      N Morris X4-X11 0.000
## 30:      N Morris X4-X12 0.000
## 31:      N Morris X4-X13 0.000
## 32:      N Morris X4-X14 0.000
## 33:      N Morris X4-X15 0.000
## 34:      N Morris X4-X16 0.000
## 35:      N Morris X4-X17 0.000
## 36:      N Morris X4-X18 0.000
## 37:      N Morris X4-X19 0.000
## 38:      N Morris X4-X20 0.000
##      setting Model      rn overlap
##
## [[5]]
##      setting Model      rn overlap
## 1: $N,\\theta$ Morris X1-X5 0.000
## 2: $N,\\theta$ Morris X2-X5 0.000
## 3: $N,\\theta$ Morris X3-X5 0.521
## 4: $N,\\theta$ Morris X4-X5 0.000
## 5: $N,\\theta$ Morris X5-X6 0.260
## 6: $N,\\theta$ Morris X5-X7 0.017
## 7: $N,\\theta$ Morris X5-X8 0.176
## 8: $N,\\theta$ Morris X5-X9 0.002
## 9: $N,\\theta$ Morris X5-X10 0.000
## 10: $N,\\theta$ Morris X5-X11 0.000
## 11: $N,\\theta$ Morris X5-X12 0.000
## 12: $N,\\theta$ Morris X5-X13 0.000
## 13: $N,\\theta$ Morris X5-X14 0.000
## 14: $N,\\theta$ Morris X5-X15 0.000

```

```

## 15: $N,\\theta$ Morris X5-X16 0.000
## 16: $N,\\theta$ Morris X5-X17 0.000
## 17: $N,\\theta$ Morris X5-X18 0.000
## 18: $N,\\theta$ Morris X5-X19 0.000
## 19: $N,\\theta$ Morris X5-X20 0.000
## 20:      N Morris X1-X5 0.000
## 21:      N Morris X2-X5 0.000
## 22:      N Morris X3-X5 0.098
## 23:      N Morris X4-X5 0.000
## 24:      N Morris X5-X6 0.026
## 25:      N Morris X5-X7 0.000
## 26:      N Morris X5-X8 0.534
## 27:      N Morris X5-X9 0.000
## 28:      N Morris X5-X10 0.000
## 29:      N Morris X5-X11 0.000
## 30:      N Morris X5-X12 0.000
## 31:      N Morris X5-X13 0.000
## 32:      N Morris X5-X14 0.000
## 33:      N Morris X5-X15 0.000
## 34:      N Morris X5-X16 0.000
## 35:      N Morris X5-X17 0.000
## 36:      N Morris X5-X18 0.000
## 37:      N Morris X5-X19 0.000
## 38:      N Morris X5-X20 0.000
##      setting Model      rn overlap
##
## [[6]]
##      setting Model      rn overlap
## 1: $N,\\theta$ Morris X1-X6 0.000
## 2: $N,\\theta$ Morris X2-X6 0.000
## 3: $N,\\theta$ Morris X3-X6 0.189
## 4: $N,\\theta$ Morris X4-X6 0.000
## 5: $N,\\theta$ Morris X5-X6 0.260
## 6: $N,\\theta$ Morris X6-X7 0.000
## 7: $N,\\theta$ Morris X6-X8 0.015
## 8: $N,\\theta$ Morris X6-X9 0.000
## 9: $N,\\theta$ Morris X6-X10 0.000
## 10: $N,\\theta$ Morris X6-X11 0.000
## 11: $N,\\theta$ Morris X6-X12 0.000
## 12: $N,\\theta$ Morris X6-X13 0.000
## 13: $N,\\theta$ Morris X6-X14 0.000
## 14: $N,\\theta$ Morris X6-X15 0.000
## 15: $N,\\theta$ Morris X6-X16 0.000
## 16: $N,\\theta$ Morris X6-X17 0.000
## 17: $N,\\theta$ Morris X6-X18 0.000
## 18: $N,\\theta$ Morris X6-X19 0.000
## 19: $N,\\theta$ Morris X6-X20 0.000
## 20:      N Morris X1-X6 0.000

```



```
## 21:      N Morris  X2-X6  0.000
## 22:      N Morris  X3-X6  0.034
## 23:      N Morris  X4-X6  0.000
## 24:      N Morris  X5-X6  0.026
## 25:      N Morris  X6-X7  0.000
## 26:      N Morris  X6-X8  0.000
## 27:      N Morris  X6-X9  0.000
## 28:      N Morris  X6-X10 0.000
## 29:      N Morris  X6-X11 0.000
## 30:      N Morris  X6-X12 0.000
## 31:      N Morris  X6-X13 0.000
## 32:      N Morris  X6-X14 0.000
## 33:      N Morris  X6-X15 0.000
## 34:      N Morris  X6-X16 0.000
## 35:      N Morris  X6-X17 0.000
## 36:      N Morris  X6-X18 0.000
## 37:      N Morris  X6-X19 0.000
## 38:      N Morris  X6-X20 0.000
##          setting  Model    rn overlap
```

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 ^ 12,
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)
    }
  }
}

```

```

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

# ARRANGE DATA -----

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

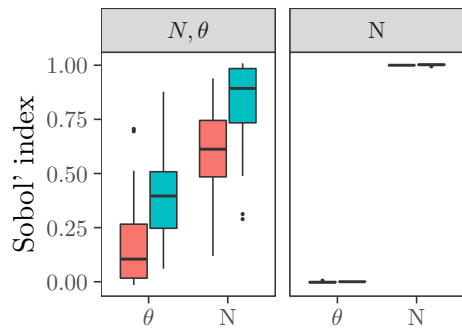
# EXPORT DATA -----

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

# PLOT SOBOL INDICES -----

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

```



5 Extra plots

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

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

b <- AB.sobol[!setting == "N"] %>%
  ggplot(., aes(value,
                fill = parameter,
                color = parameter)) +
  geom_density(alpha = 0.5,
              position = "identity") +
  facet_grid(setting~Model) +
  scale_fill_discrete(name = "Model input") +
  scale_color_discrete(guide = FALSE) +
  labs(x = expression(paste("Sobol'"~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))

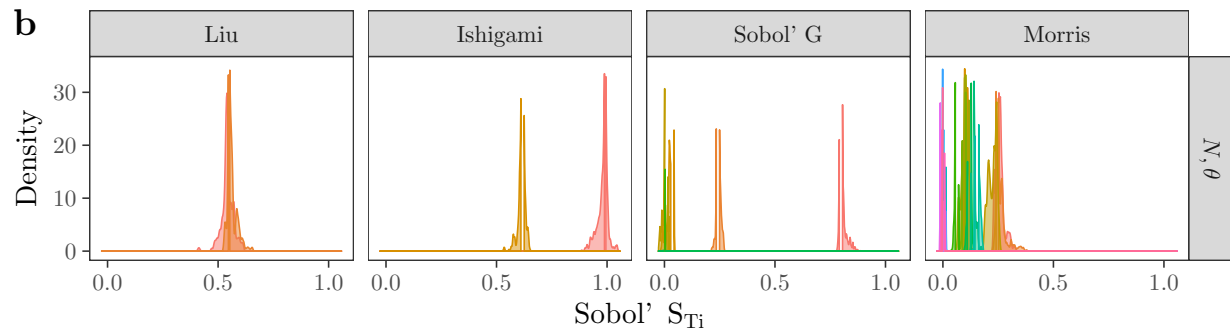
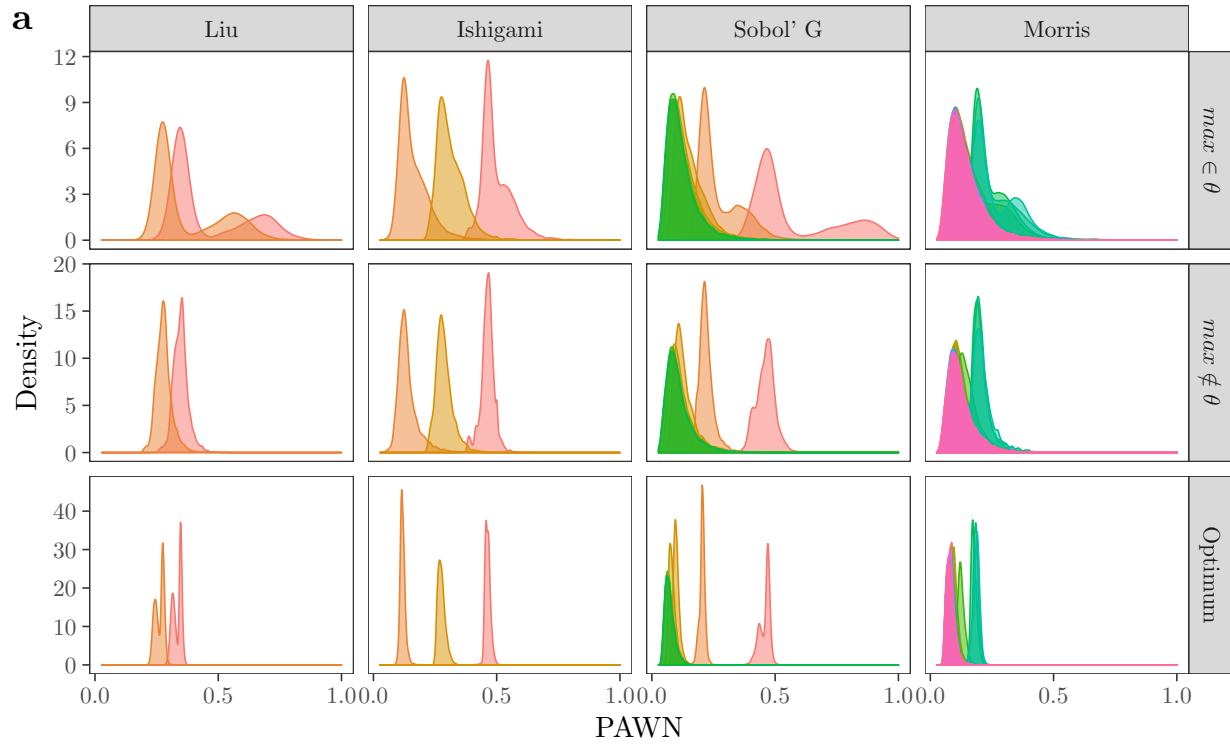
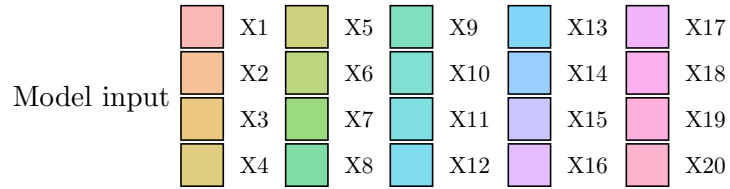
# Get legend
legend <- get_legend(a + theme(legend.position = "top"))

# 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 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"))

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")

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

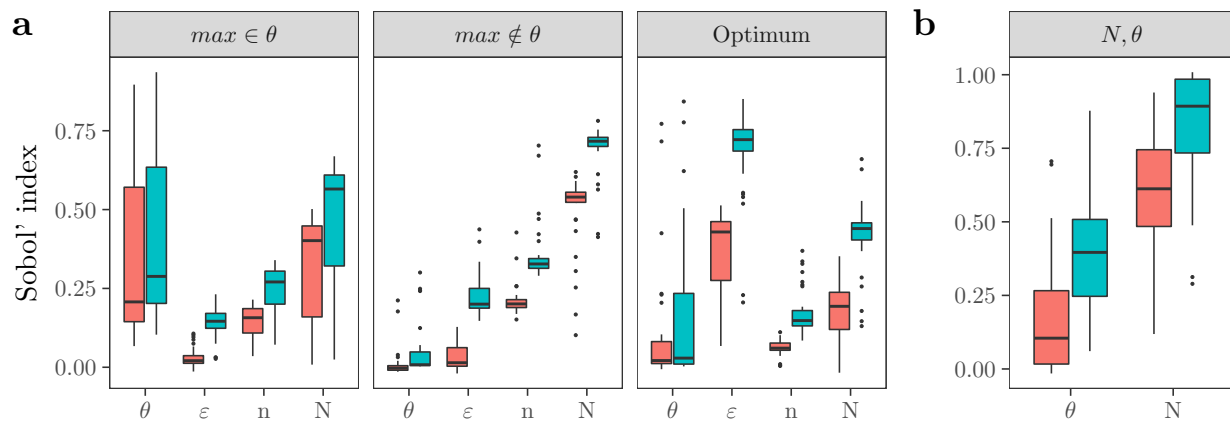
bottom <- plot_grid(a, b,
                    ncol = 2,
```

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

Sobol' indices  S_i  S_{T_i}



PLOT AGGREGATED SUM OF SI -----

```
a <- 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())

b <- final.sobol[sensitivity == "Si" & !setting == "N"] %>%
  .[, sum(original), .(Model, model.input, setting)] %>%
  ggplot(., aes(setting, V1)) +
  geom_boxplot(outlier.size = 0.2) +
  labs(x = "",
       y = "") +
  theme_bw() +
  theme(panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        axis.title.x=element_blank())
```

```
plot_grid(a, b,
          ncol = 2,
          labels = "auto",
          align = "hv",
          rel_widths = c(1, 0.4))
```

