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("arnaldpuy/pawnr", build_vignettes = TRUE)
# Function to read in all required packages in one go:
loadPackages <- function(x) {</pre>
  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",
               "ggridges"))
# Create custom theme
theme_AP <- function() {</pre>
  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 \leftarrow 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")</pre>
params <- lapply(k, function(x) paste("X", 1:x, sep = ""))</pre>
names(params) <- models</pre>
# Function to compute the Liu et al. function
liu <- function(X1, X2) {</pre>
  X1 / X2
}
liu_Mapply <- function(X) {</pre>
  X[, 1] \leftarrow qchisq(X[, 1], df = 10)
  X[, 2] \leftarrow 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))
}

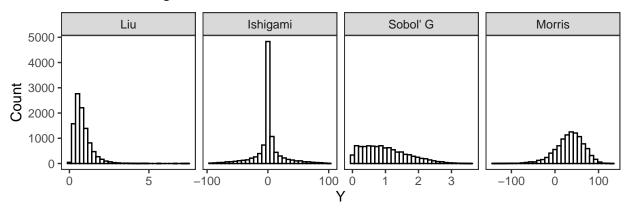
A <- A[!sapply(A, is.null)]
B <- B[!sapply(B, is.null)]
names(A) <- models
names(B) <- models
for(i in names(A)) {
    names(A[[i]]) <- N
}
for(i in names(B)) {</pre>
```

```
names(B[[i]]) <- N
}</pre>
```

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))</pre>
  } 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))</pre>
  } else {
    Y[[i]] <- lapply(A[[i]], function(x) sensitivity::morris.fun(x))
    Y.pawn[[i]] <- lapply(B[[i]], function(x) sensitivity::morris.fun(x))</pre>
 }
}
names(Y) <- models</pre>
for(i in names(Y)) {
  names(Y[[i]]) <- N</pre>
}
names(Y.pawn) <- models</pre>
for(i in names(Y.pawn)) {
  names(Y.pawn[[i]]) <- N</pre>
}
# PI.OT 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") +
```

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



2.3 Sobol' indices

```
# COMPUTE SOBOL' INDICES AND THEIR CONFIDENCE INTERVALS -
out <- out.ci <- list()</pre>
for(i in names(A)) {
  for(j in names(A[[i]])) {
    out[[i]][[j]] <- sobol_indices(Y[[i]][[j]],</pre>
                                     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]],</pre>
                                   params = params[[i]],
                                   type = type,
                                   conf = conf)
  }
```

```
# SOBOL INDICES AND CONFIDENCE INTERVALS OF DUMMY PARAMETER -----
sobol.dummy <- sobol.dummy.ci <- list()</pre>
for(i in names(A)) {
  for(j in names(A[[i]])) {
    sobol.dummy[[i]][[j]] <- sobol_dummy(Y[[i]][[j]],</pre>
                                          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]],</pre>
                                                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()</pre>
for(i in names(B)) {
 for(j in names(B[[i]]) ) {
   pawn.indices[[i]][[j]] <- pawn_generic(data = B[[i]][[j]],</pre>
                                           Y = Y.pawn[[i]][[j]],
                                           n = n,
                                            test = median,
```

R = R

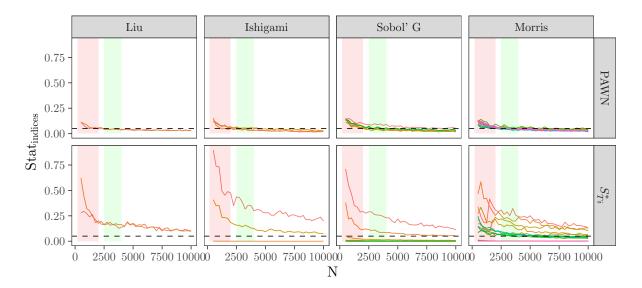
```
pawn.ci[[i]][[j]] <- pawn_ci(pawn.indices[[i]][[j]])</pre>
  }
}
# PAWN AND CONFIDENCE INTERVALS OF DUMMY PARAMETER --
pawn.index.dummy <- list()</pre>
for(i in names(Y.pawn)) {
  for(j in names(Y.pawn[[i]]) ) {
    pawn.index.dummy[[i]][[j]] <- pawn_dummy(Y = Y.pawn[[i]][[j]],</pre>
                                             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 SOBOL' AND PAWN CONVERGENCE RATES ----
fwrite(sobol.convergence, "sobol.convergence.csv")
fwrite(pawn.convergence, "pawn.convergence.csv")
```

2.5 Plot convergence

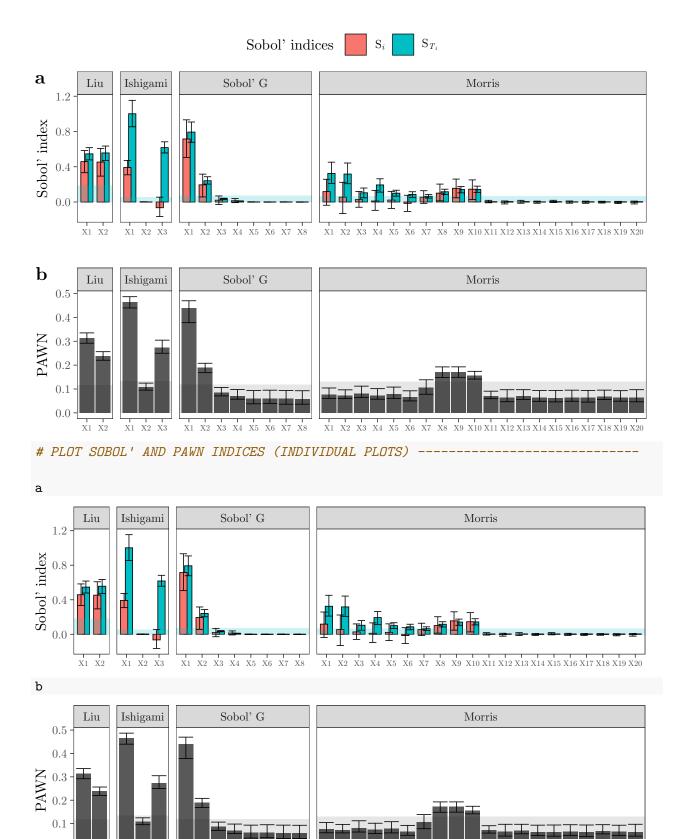
```
geom_line() +
  geom_hline(yintercept = 0.05,
             lty = 2) +
  scale_color_discrete(name = "Model inputs") +
  labs(y = expression(Stat[indices]),
       x = "N") +
  facet_grid(method~model) +
  theme bw() +
  theme(legend.position = "top",
        panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        legend.background = element_rect(fill = "transparent",
                                           color = NA),
        legend.key = element_rect(fill = "transparent",
                                  color = NA))
                               — X1 — X5 — X9 — X13 — X17
                                X2 — X6 — X10 — X14 — X18
                  Model inputs ___ x3 __ x7 __ x11 __ x15 __ x19
                               — X4 — X8 — X12 — X16 — X20
              Liu
                              Ishigami
                                                Sobol' G
                                                                   Morris
  0.75 -
  0.50
  0.25
Statindices 0.00 0.75
  0.50
                                                                               S_T^*
  0.25
         2500 5000 7500 10000
                          2500 5000 7500 10000
                                             2500 5000 7500 10000
                                                               2500 5000 7500 10000
                                         Ν
# 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))
```





```
# 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"))</pre>
# 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)
```



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

X1 X2 X3 X4 X5 X6 X7 X8

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))</pre>
# The model
model_pawn <- function(Model, N, n, epsilon, theta) {</pre>
  # 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)</pre>
  # Transform distribution:
 if(Model == 1) {
    ModelRun <- liu_Mapply
 } else if(Model == 2) {
    ModelRun <- sensobol::ishigami_Mapply</pre>
  } else if(Model == 3) {
    ModelRun <- sensobol::sobol_Fun</pre>
  } else {
    ModelRun <- sensitivity::morris.fun</pre>
  }
  # 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),</pre>
                   size = floor(nrow(data) / n),
                   # Without replacement
                   replace = FALSE)
  # Bind model inputs and model output
  dt <- data.table::data.table(cbind(data, Y))</pre>
  # Subset and obtain the unconditional model output
 Y_unc <- dt[index, Y]
```

```
# Create the intervals
 melted <- data.table::melt(dt,</pre>
                              measure.vars = 1:(ncol(dt) - 1),
                              variable.name = "parameters")
  # Compute PAWN indices
  out <- melted[order(parameters, value)][</pre>
    , .(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]</pre>
 } else if(theta == 2) {
    final <- out[, median(statistic), parameters][, V1]</pre>
  } else {
    final <- out[, max(statistic), parameters][, V1]</pre>
 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")</pre>
```

3.3 Sample matrix

```
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)</pre>
A <- list(tmp, max, copy(tmp))
# Name the slots
names(A) <- c("max", "no.max", "optimum")</pre>
# 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)
```

```
##
                              N n epsilon theta
            setting Model
##
         1:
                max
                         1 1100 12
                                        500
                                                2
##
         2:
                         1 1550 8
                                        750
                                                1
                max
         3:
                                        250
                                                3
##
                max
                         1 650 16
##
         4:
                max
                         1 875 10
                                        625
                                                1
##
         5:
                         1 1775 18
                                        125
##
## 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

```
# Define parallel computing
cl <- makeCluster(n_cores)</pre>
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]])</pre>
names(rowNumber) <- models</pre>
out <- list()</pre>
for(i in models) {
  out[[i]] <- Y.pawn[rowNumber[[i]]]</pre>
}
dt.models <- list()</pre>
for(i in seq_along(1:4)) {
  dt.models[[i]] <- cbind(A.pawn[Model == i], data.table(do.call(rbind, out[[i]])))</pre>
```

}

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$setting)
overlap.results <- mclapply(overlap.dt, function(x) {</pre>
  split(x, x$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) {</pre>
  cbind(y$0V) %>%
    data.frame() %>%
    setDT(., keep.rownames = TRUE)
  }))
pawn.overlap.results <- lapply(tmp, function(x)</pre>
  rbindlist(x, idcol = "Model")) %>%
  rbindlist(., idcol = "setting") %>%
  setnames(., ".", "overlap")
par.overlap <- paste("X", 1:6, sep = "")</pre>
```

```
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:
                                            0.013
                    Optimum
                               Liu X1-X2
##
## [[2]]
##
                     setting
                                Model
                                         rn overlap
## 1:
         $max \\in \\theta$ Ishigami X1-X2
                                               0.009
         $max \\in \\theta$ Ishigami X1-X3
## 2:
                                               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
          $max \\in \\theta$ Sobol' G X1-X2
##
   1:
                                                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
          $max \\in \\theta$ Sobol' G X2-X3
##
   8:
                                                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
```

```
Optimum Sobol' G X3-X5
## 71:
                                                0.191
## 72:
                      Optimum Sobol' G X3-X6
                                                0.183
## 73:
                                                0.184
                      Optimum Sobol' G X3-X7
## 74:
                      Optimum Sobol' G X3-X8
                                                0.174
## 75:
                      Optimum Sobol' G X4-X5
                                                0.542
## 76:
                      Optimum Sobol' G X4-X6
                                                0.523
## 77:
                      Optimum Sobol' G X4-X7
                                                0.516
## 78:
                      Optimum Sobol' G X4-X8
                                                0.490
## 79:
                      Optimum Sobol' G X5-X6
                                                0.957
## 80:
                      Optimum Sobol' G X5-X7
                                                0.947
## 81:
                      Optimum Sobol' G X5-X8
                                                0.907
## 82:
                      Optimum Sobol' G X6-X7
                                                0.953
## 83:
                      Optimum Sobol' G X6-X8
                                                0.919
## 84:
                      Optimum Sobol' G X7-X8
                                                0.954
##
                      setting
                                 Model
                                           rn overlap
##
## [[4]]
##
                    setting Model
                                        rn overlap
     1: $max \\in \\theta$ Morris
                                     X1-X2
                                              0.907
##
##
     2: $max \\in \\theta$ Morris
                                     X1-X3
                                              0.940
##
     3: $max \\in \\theta$ Morris
                                     X1-X4
                                              0.890
     4: $max \\in \\theta$ Morris
##
                                     X1-X5
                                              0.887
##
     5: $max \\in \\theta$ Morris
                                     X1-X6
                                              0.814
##
## 566:
                    Optimum Morris X17-X19
                                              0.884
## 567:
                    Optimum Morris X17-X20
                                              0.971
## 568:
                    Optimum Morris X18-X19
                                              0.756
## 569:
                    Optimum Morris X18-X20
                                              0.680
## 570:
                    Optimum Morris X19-X20
                                              0.890
# Export results
rbindlist(final.overlap) %>%
  fwrite(., "pawn.overlap.csv")
# PLOT UNCERTAINTY ----
plot.uncertainty.pawn <- ggplot(AB.pawn, aes(value,</pre>
                                               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
                                        X1
                                               X5
                                                      X9
                                                               X13
                                                                       X17
                                       X2
                                               X6
                                                      X10
                                                               X14
                                                                       X18
                      Model input
                                       X3
                                               X7
                                                      X11
                                                               X15
                                                                       X19
                                        X4
                                               X8
                                                      X12
                                                               X16
                                                                       X20
               Liu
                                  Ishigami
                                                       Sobol' G
                                                                             Morris
  12.5
  10.0 -
   7.5 - 
   5.0 -
   2.5
   0.0
    20
    15
                                                                                           max \notin \theta
    10
    5
     0
    40
                                                                                           Optimum
    30
    20
    10
                        1.00.0
                                              1.00.0
                                                                               0.5
                                                                                        1.0
      0.0
               0.5
                                    0.5
                                                                   1.00.0
                                             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],
```

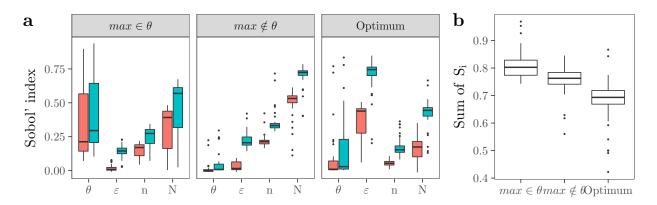
```
ifelse(Model == 2, models[2],
                            ifelse(Model == 3, models[3], models[4])))] %>%
  .[, model.input:= gsub("V", "X", model.input)] %>%
  .[, model.input:= factor(model.input,
                         levels = paste("X", 1:20, sep = ""))] %>%
  .[, Model:= factor(Model,
                     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,</pre>
                                                 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()</pre>
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]],</pre>
                                          params = parameters,
                                          type = type,
                                          conf = conf,
                                          second = TRUE,
                                          third = TRUE)
   }
 }
}
# Rearrange data
```

```
final.pawn.ci <- lapply(pawn.ci, function(x)</pre>
  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"))</pre>
# PLOT SUM OF SOBOL' SI -----
b <- final.pawn.ci[sensitivity == "Si"][</pre>
  , 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]))) +
```

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 $\begin{picture}(1,0) \put(0,0){\line(0,0){100}} \put(0,0){$



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)</pre>
```

```
for(i in 1:ncol(A)) {
    AB <- A
    AB[, i] \leftarrow B[, i]
    X \leftarrow rbind(X, AB)
  }
  AB \leftarrow rbind(A, X[((2*nrow(A)) + 1):nrow(X), ])
  return(AB)
}
sobol_matrix <- function(n, k) {</pre>
  df \leftarrow randtoolbox::sobol(n = n, dim = k * 2)
  A \leftarrow df[, 1:k]
  B \leftarrow 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) {</pre>
  n <- length(Y_A[!is.na(Y_A)])</pre>
  f0 \leftarrow (1 / n) * sum(Y_A)
  VY \leftarrow 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 \leftarrow ((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) {</pre>
  return(mapply(sobol_all,
                  MoreArgs = list(type = type),
                  d[, "Y_A"],
                  d[, "Y_AB"]))
}
sobol_Ti <- function(Y, params, type) {</pre>
  k <- length(params)</pre>
  p \leftarrow length(1:(length(Y) / (k + 1)))
  Y_A \leftarrow Y[1:p]
  Y_AB \leftarrow Y[(p + 1):length(Y)]
  parameters <- rep(params, each = length(Y_A))</pre>
```

```
vec <- cbind(Y_A, Y_AB)</pre>
  out <- data.table(vec, parameters)</pre>
  output <- out[, sobol_Ti_Mapply(.SD, type = type), parameters][, V1]</pre>
  return(output)
}
# The model
model_sobol <- function(Model, N, k, Theta) {</pre>
  data \leftarrow 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)</pre>
  return(out)
```

4.2 Settings

```
# DEFINE SETTINGS -----
# Set parameters
parameters.sobol <- c("N", "Theta")</pre>
```

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 \leftarrow copy(A)
A.DT <- list(A, N.only)
names(A.DT) <- c("N.Theta", "N")</pre>
A <- rbindlist(A.DT, idcol = "setting")
A.sobol \leftarrow 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
                    1 1775 sobol 2
##
        5: N.Theta
##
                      4 650 jansen 20
## 262140:
                 N
## 262141:
                 N
                      4 1550 jansen 20
                       4 1100 jansen 20
## 262142:
                 N
## 262143:
                       4 200 jansen 20
                 N
## 262144:
                       4 200 jansen 20
print(n)
```

[1] 8192

4.4 Run the model

```
# 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]])))
}</pre>
```

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))
                                                 Х9
                                                         X13
                                                                 X17
                                    X1
                                           X5
                                    X2
                                           X6
                                                  X10
                                                         X14
                                                                 X18
                    Model input
                                    X3
                                           X7
                                                 X11
                                                         X15
                                                                 X19
                                    X4
                                                  X12
                                                         X16
                                                                 X20
             Liu
                               Ishigami
                                                   Sobol' G
                                                                       Morris
  30
  20
  10
  30
  20
  10
                                               0.0
       0.0
                  1.0
                           0.0
                                 0.5
                                      1.0
                                                     0.5
                                                          1.0
                                                                        0.5
                                                                              1.0
             0.5
                                           Y
# CHECK OVERLAP --
overlap.dt <- split(AB.sobol, AB.sobol$setting)</pre>
```

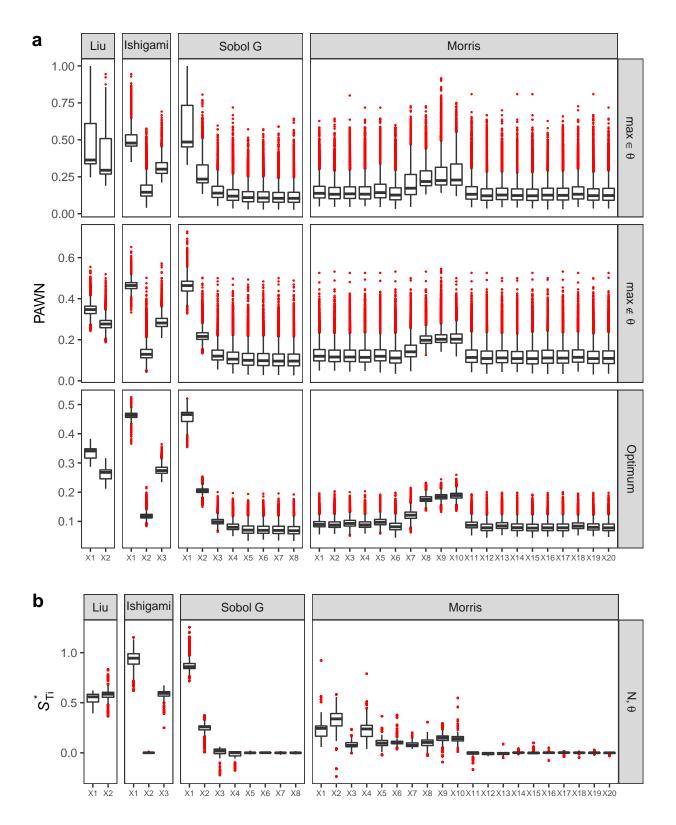
```
overlap.results <- mclapply(overlap.dt, function(x) {</pre>
  split(x, x$Model, drop = TRUE) %>%
    lapply(., function(x) split(x, x$parameter, drop = TRUE)) %>%
    lapply(., function(x) lapply(x, function(y) y[, value])) %>%
    lapply(., function(x) overlap(x))},
 mc.cores = n_cores)
tmp <- lapply(overlap.results, function(x) lapply(x, function(y) {</pre>
  cbind(y$0V) %>%
    data.frame() %>%
    setDT(., keep.rownames = TRUE)
}))
sobol.overlap.results <- lapply(tmp, function(x)</pre>
  rbindlist(x, idcol = "Model")) %>%
 rbindlist(., idcol = "setting") %>%
  setnames(., ".", "overlap")
par.overlap <- paste("X", 1:6, sep = "")</pre>
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
                                      0.069
## 15: $N, \\theta$ Sobol' G X3-X5
## 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
                 N Sobol' G X3-X7
## 45:
                                      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
##
                      Model
           setting
                               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 ----
AB.pawn <- fread("AB.pawn.csv")
AB.sobol <- fread("AB.sobol.csv")
AB.pawn.plot <- copy(AB.pawn)
AB.sobol.plot <- copy(AB.sobol)
AB.pawn.plot <- AB.pawn.plot[, setting:= ifelse(setting %in% "$max \\in \\theta$", "max %in% to
                          ifelse(setting %in% "$max \\notin \\theta$", "max %notin% theta", se
  .[, Model:= ifelse(Model %in% "Sobol' G", "Sobol~G", Model)] %>%
  .[, Model:= factor(Model, levels = c("Liu", "Ishigami", "Sobol~G", "Morris"))] %>%
  .[, parameter:= factor(parameter, levels = paste("X", 1:20, sep = ""))]
AB.sobol.plot <- AB.sobol.plot[, setting:= ifelse(setting %in% c("$N,\\theta$"), "list(N,theta
  .[, Model:= ifelse(Model %in% "Sobol' G", "Sobol~G", Model)] %>%
  .[, Model:= factor(Model, levels = c("Liu", "Ishigami", "Sobol~G", "Morris"))] %>%
  .[, parameter:= factor(parameter, levels = paste("X", 1:20, sep = ""))]
a <- ggplot(AB.pawn.plot, aes(parameter, value)) +
  geom_boxplot(outlier.colour = "red",
               outlier.size = 0.2) +
 facet_grid(setting ~ Model,
             scales = "free",
             space = "free_x",
             labeller = label_parsed) +
```

```
labs(y = "PAWN",
       x = "") +
  theme AP() +
  theme(axis.text.x = element_text(size = 6),
        legend.position = "none")
b <- ggplot(AB.sobol.plot[!setting == "N"], aes(parameter, value)) +
  geom_boxplot(outlier.colour = "red",
               outlier.size = 0.2) +
  facet_grid(setting ~ Model,
             scales = "free",
             space = "free_x",
             labeller = label_parsed) +
  labs(y = expression(italic(S)[Ti]^"*"),
       x = "") +
  theme_AP() +
  theme(axis.text.x = element_text(size = 6),
        legend.position = "none")
plot_grid(a, b,
          ncol = 1,
          labels = "auto",
          align = "h",
          rel_heights = c(1, 0.42))
```

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



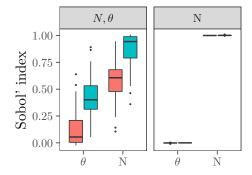
4.6 Sensitivity analysis

DATASET FOR SENSITIVITY ANALYSIS

```
full.dataset.sobol <- lapply(dt.models, function(x)</pre>
 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,</pre>
                                                       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()</pre>
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]],</pre>
                                        params = parameters.sobol,
                                        type = type,
                                        conf = conf)
   }
```

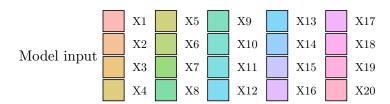
```
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to
                                     1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to
                                     1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to
                                     1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to
                                     1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
## [1] "All values of t are equal to 1 \n Cannot calculate confidence intervals"
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## [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"
# ARRANGE DATA -----
final.sobol <- lapply(out, function(x)</pre>
  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 ----
```

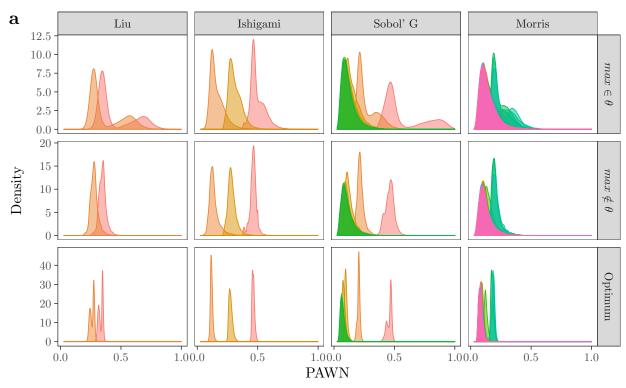
```
fwrite(final.sobol, "final.sobol.csv")
# PLOT SOBOL INDICES --
ggplot(final.sobol, aes(parameters, original,
                        fill = sensitivity)) +
  geom_boxplot(outlier.size = 0.2) +
 labs(x = "",
       y = "Sobol' index") +
  scale_fill_discrete(name = "Sobol' indices",
                      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")
```

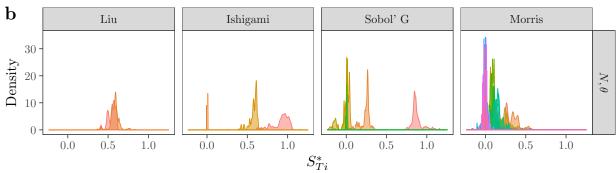


5 Extra plots

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







```
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"))</pre>
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)
```

Sobol' indices \square $S_i \square$ S_{T_i} b \mathbf{a} N, θ $max \in \theta$ $max \notin \theta$ Optimum 1.00 Sobol' index 0.750.750.50 0.500.25 0.250.00 0.00 # PLOT NEW AGGREGATED SOBOL' INDICES final.pawn.plot <- copy(final.pawn.ci)</pre> final.sobol.plot <- copy(final.sobol)</pre> paramets <- gsub(final.pawn.plot[, parameters], pattern ="\\", replacement="", fixed=TRUE) %>% gsub(., pattern ="\$", replacement="", fixed=TRUE) %>% gsub(., pattern =".", replacement="~", fixed=TRUE) final.pawn.plot <- final.pawn.plot[, setting:= ifelse(setting %in% "\$max \\in \\theta\$", "max " ifelse(setting %in% "\$max \\notin \\theta .[, model:= ifelse(model %in% "Sobol' G", "Sobol~G", model)] %>% .[, model:= factor(model, levels = c("Liu", "Ishigami", "Sobol~G", "Morris"))] %>% .[, parameters:= cbind(paramets)] paramets.sobol <- gsub(final.sobol.plot[, parameters], pattern ="\\", replacement="", fixed=TR</pre> gsub(., pattern ="\$", replacement="", fixed=TRUE) final.sobol.plot <- final.sobol.plot[, Model:= ifelse(Model %in% "Sobol' G", "Sobol~G", Model)] .[, Model:= factor(Model, levels = c("Liu", "Ishigami", "Sobol~G", "Morris"))] %% .[, parameters:= cbind(paramets.sobol)] %>% .[, setting:= ifelse(setting %in% "\$N,\\theta\$", "list(N, theta)", setting)] a <- final.pawn.plot[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)]),

scale_x_discrete(labels = c(expression(italic(n)),

expression(S[italic(T[i])]))) +

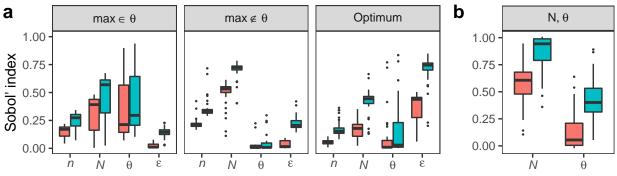
```
expression(italic(N)),
                              expression(theta),
                              expression(epsilon))) +
  scale_y_continuous(limits = c(0, 1)) +
  theme bw() +
  facet_wrap(~ setting,
             labeller = label_parsed) +
  theme(panel.grid.major = element_blank(),
        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"))</pre>
## Warning: Removed 27 rows containing non-finite values (stat_boxplot).
b <- final.sobol.plot[!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])]))) +
  scale_x_discrete(labels = c(expression(italic(N)),
                   expression(theta))) +
  facet_wrap(~ setting,
             labeller = label_parsed) +
  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: Removed 27 rows containing non-finite values (stat_boxplot).
- ## 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 \Longrightarrow $S_i \Longrightarrow S_{T_i}$



```
# PLOT AGGREGATED SUM OF SI
final.sobol2 <- setnames(final.sobol, "Model", "model")</pre>
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())
```

```
\downarrow S_{T_i}^* \rightleftharpoons PAWN
```

```
\begin{array}{c} 1.0 \\ 0.9 \\ \hline 0.8 \\ \hline 0.8 \\ 0.6 \\ \hline 0.5 \\ \hline 0.4 \\ \hline max \in \theta \quad max \notin \theta \quad \text{Optimum} \quad N, \theta \\ \end{array}
```

```
# ARRANGE TO PLOT SOBOL' INDICES FOR EACH FUNCTION ------
tmp <- split(final.pawn.ci, final.pawn.ci$model)</pre>
gg <- list()</pre>
for(i in names(tmp)) {
  for(j in 1:3) {
    gg[[i]][[j]] <- plot_sobol(tmp[[i]], type = j) +</pre>
      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"))</pre>
# PLOT SOBOL' INDICES FOR LIU, ISHIGAMI AND SOBOL' G -----
all <- lapply(1:3, function(x) {
  left <- plot_grid(gg[[1]][[x]], gg[[2]][[x]],</pre>
                    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.

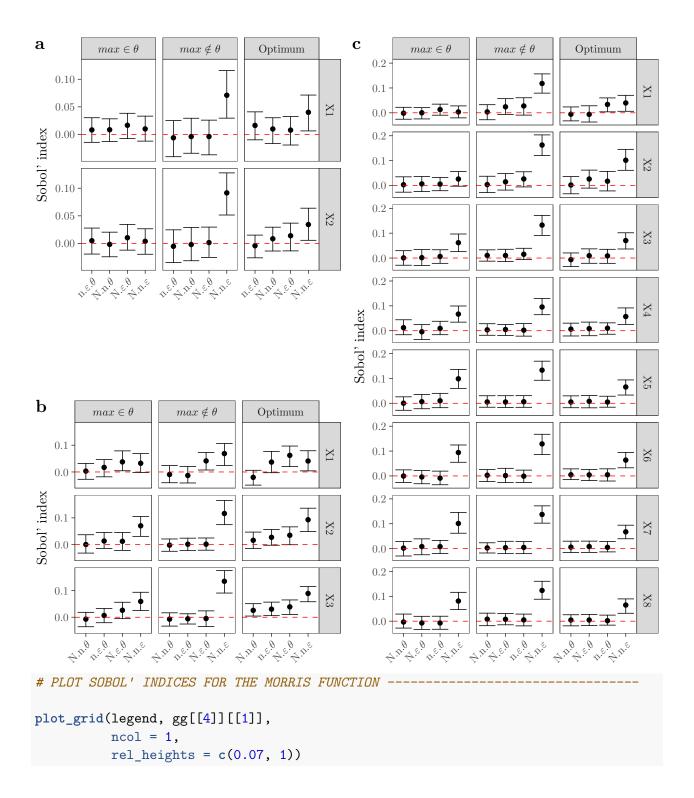
```
plot_grid(legend, all[[1]],
                    ncol = 1,
                    rel_heights = c(0.1, 1))
                                                           Sobol' indices
                                                                                    \mathbf{c}
               \max \in \theta
                                     \max \notin \theta
                                                           Optimum
                                                                                                                                               Optimum
                                                                                                   \max \in \theta
                                                                                                                          \max \notin \theta
     1.0
                                                                                         0.5
     0.5
                                                                             \times_1
                                                                                         0.0
Sobol' index
                                                                                         0.5
                                                                                         0.0
                                                                                         0.5
     0.5
                                                                             \chi_2
     0.0
                                                                                         0.5
                                                                                    Sobol' index

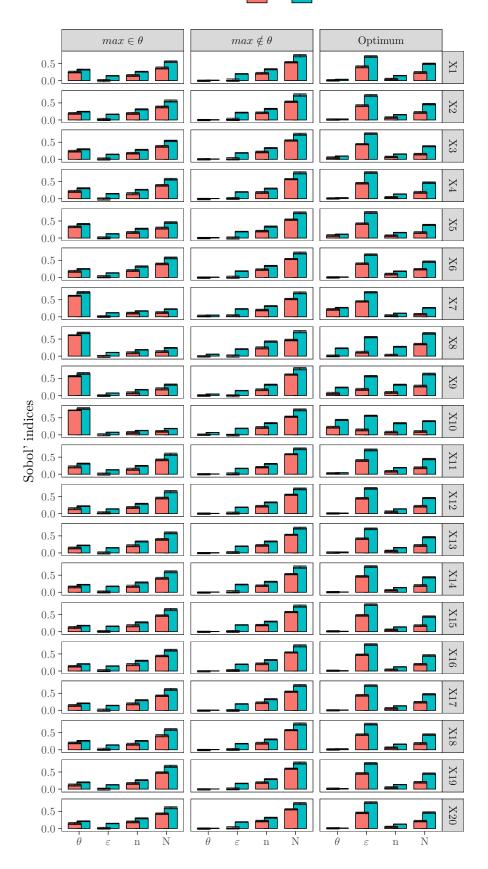
0.0

0.0
\mathbf{b}
               \max \in \theta
                                     \max \notin \theta
                                                           Optimum
                                                                                                                                                                 \chi_5
                                                                                         0.0
     0.5
                                                                             \times_1
                                                                                         0.5
Sobol' index
                                                                                         0.5
     0.5
                                                                             \chi_3
                                                                                         0.5
```

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

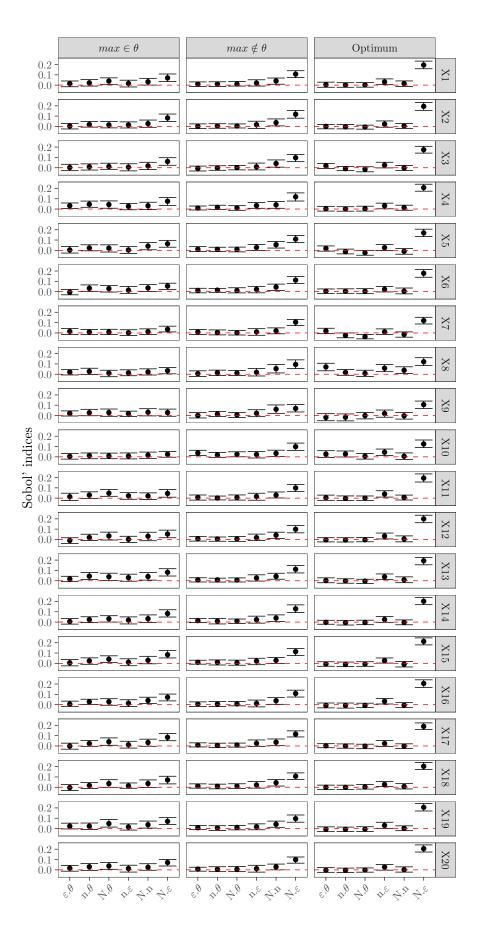
[[1]] ## [[1]][[1]] \mathbf{c} \mathbf{a} $max \in \theta$ $\max \notin \theta$ Optimum $\max \in \theta$ Optimum $\max \notin \theta$ 0.3 0.10 0.2 0.1 0.05 0.0 0.3 Sobol' index 0.00 0.2 0.1 0.10 0.0 0.3 0.05 0.2 X30.1 ᆂ┋┋ 0.3 0.2 0.1 Sobol' index 0.0 0.3 ፏ 0.2 χ_5 0.1 ▼▼▼₹₹ \mathbf{b} 0.0 $max \in \theta$ $\max \notin \theta$ Optimum 0.3 0.3 0.2 0.2 9X0.1 0.1 ▼▼▼▼ 0.0 0.0 Sobol' index 0.3 0.3 ፏ 0.2 0.2 χ_2 X7 0.1 0.1 0.3 0.3 Ŧ 0.2 0.2 χ_3 X8 0.1 0.1 ## ## ## [[2]] ## [[2]][[1]]





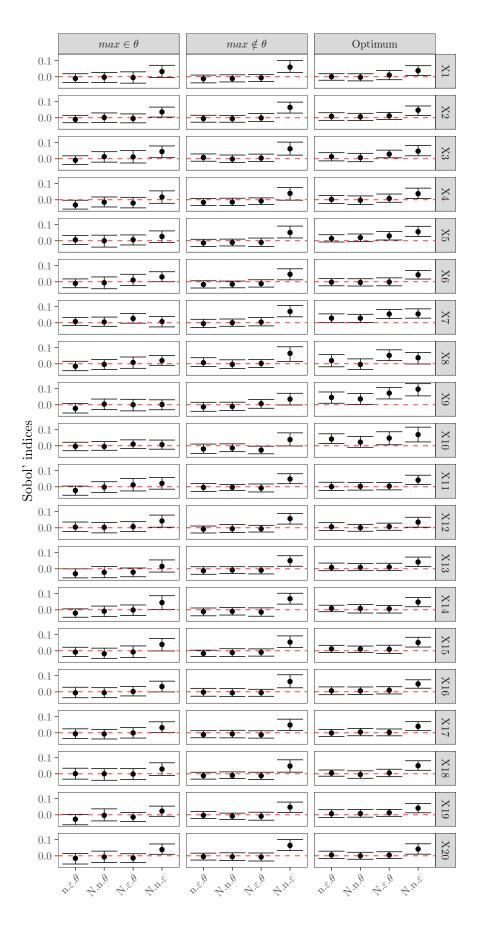
```
lapply(2:3, function(x) gg[[4]][[x]])
```

[[1]]



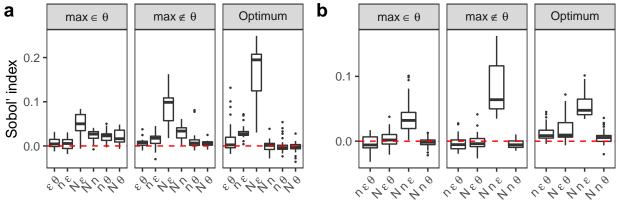
##

[[2]]



```
# MERGE SECOND AND THIRD-ORDER EFFECTS ----
gg <- list()</pre>
second.third <- c("Sij", "Sijk")</pre>
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")
                                             b
\mathbf{a}
         max \in \theta
                     max \notin \theta
                                  Optimum
                                                      max \in \theta
                                                                   max \notin \theta
                                                                               Optimum
Sobol' index
   0.2
                                                0.1
   0.1
# MERGE SECOND AND THIRD-ORDER EFFECTS
final.pawn.plot <- final.pawn.plot[, parameters:= gsub(parameters,</pre>
                                                             pattern = "varepsilon",
```

```
replacement = "epsilon",
                                                        fixed = TRUE)]
gg <- list()</pre>
second.third <- c("Sij", "Sijk")</pre>
for(i in second.third) {
  gg[[i]] <- final.pawn.plot[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)) +
    scale_x_discrete(labels = ggplot2:::parse_safe) +
    facet_wrap(~ setting,
               labeller = label_parsed) +
    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
```

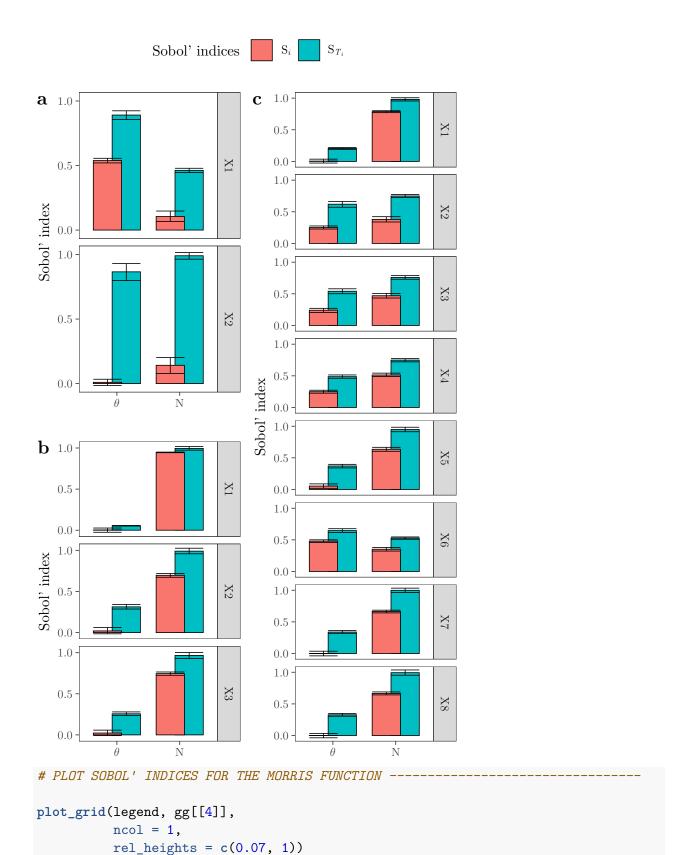
```
.[, .(Median = median(original)),
    by = .(setting, Model, sensitivity, parameters)] %>%
  # Compute the aggregated median and the percentiles
  .[, .(aggregated.median = median(Median),
        low.ci = quantile(Median, probs = 0.025),
        high.ci = quantile(Median, probs = 0.975)),
   by = .(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")
```

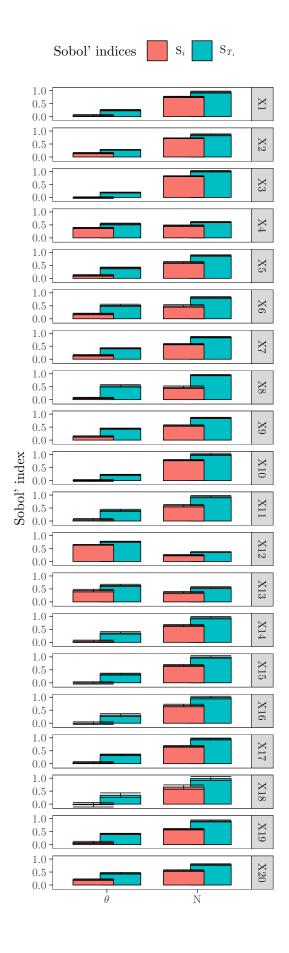
Warning: Graphs cannot be vertically aligned unless the axis parameter is ## set. Placing graphs unaligned.

Sobol' indices S_i S_{T_i}

```
b
\mathbf{a}
                                                                                                                                                   N, \theta
                        \max \in \theta
                                                            max \notin \theta
                                                                                                Optimum
                                                                                                                             1.00
      0.75
Sobol' index
                                                                                                                             0.75
      0.50
                                                                                                                             0.50
      0.25
                                                                                                                             0.25
      0.00
                                                                                                                             0.00
                                                                              Ń
                                                                                                                                                             Ń
```

```
# PLOT DESIGN PARAMETERS FOR SOBOL: ALL FUNCTIONS ---
tmp <- final.sobol[!setting == "N"] %>%
  split(., .$Model)
gg <- list()
for(i in names(tmp)) {
    gg[[i]] <- plot_sobol(tmp[[i]], type = 1) +</pre>
      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"))</pre>
# PLOT SOBOL' INDICES FOR LIU, ISHIGAMI AND SOBOL' G -----
left <- plot_grid(gg[[1]], gg[[2]],</pre>
                  labels = c("a", "b"),
                  align = "h",
                  ncol = 1
```





6 Session information

[43] yaml_2.2.0

```
# 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
           /Library/Frameworks/R.framework/Versions/3.6/Resources/lib/libRblas.0.dylib
## BLAS:
## 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
                           tidyr_1.0.0
## [22] readr_1.3.1
                                               tibble_2.1.3
                           tidyverse_1.2.1
## [25] ggplot2_3.2.1
##
## 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] jsonlite_1.6
                          magrittr_1.5
                                             Rcpp_1.0.2
## [40] munsell_0.5.0
                          lifecycle_0.1.0
                                             stringi_1.4.3
```

plyr_1.8.4

gbRd_0.4-11

```
## [46] pkgbuild_1.0.5
                          grid_3.6.1
                                            crayon_1.3.4
## [49] lattice_0.20-38
                          haven_2.1.1
                                            hms_0.5.1
## [52] zeallot_0.1.0
                          knitr_1.25
                                            ps_1.3.0
## [55] pillar_1.4.2
                          reshape2_1.4.3
                                            codetools_0.2-16
## [58] pkgload_1.0.2
                          glue_1.3.1
                                            evaluate_0.14
## [61] remotes_2.1.0
                          modelr_0.1.5
                                            vctrs_0.2.0
                          cellranger_1.1.0
                                            gtable_0.3.0
## [64] Rdpack_0.11-0
## [67] assertthat_0.2.1
                                            broom_0.5.2
                          xfun_0.9
## [70] memoise_1.1.0
                          ellipsis_0.3.0
```