Is VARS more intuitive and efficient than Sobol' indices?

R code

Arnald Puy

1 Presentation

This document presents the code workflow of the paper "Is VARS more intuitive and efficient than Sobol' indices?", by A. Puy, S. Lo Piano, and A. Saltelli, currently under review. The abstract is the following:

The Variogram Analysis of Response Surfaces (VARS) has been proposed by Razavi and Gupta in Water Resources Research as a new comprehensive framework in sensitivity analysis. According to the authors, VARS provides a more intuitive notion of sensitivity and it is much more computationally efficient than Sobol' indices. Here we review these arguments and critically compare the performance of VARS-TO, for total-order index, against the total-order Jansen estimator. We argue that, unlike classic variance-based methods, VARS lacks a clear definition of what is an "important" factor, and prove that the alleged computational superiority of VARS does not hold when its uncertain space is thoroughly explored. We conclude that while VARS enriches the spectrum of existing methods for sensitivity analysis, especially for a diagnostic use of mathematical models, it complements rather than substitutes classic estimators used in variance-based sensitivity analysis.

The results of the paper should be fully reproducible in any personal computer. Questions about the code or the computational design should be addressed to A. Puy (apuy@princeton.edu, arnald.puy@pm.me).

1.1 Preliminary functions

We start by creating a function to load all required libraries for the analysis in one go. We also set a checkpoint to ensure that our code is fully reproducible for anyone anytime. Finally, we design a short theme function for all the plots that will be produced in the analysis.

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

# 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)
    }
  }
```

```
}

# Install development version of sensobol
remotes::install_github("arnaldpuy/sensobol")

# Load the packages
loadPackages(c("tidyverse", "sensobol", "data.table", "parallel",
               "foreach", "doParallel", "pcaPP", "scales",
               "cowplot", "logitnorm", "benchmarkme", "Rfast"))

# Create custom theme
theme_AP <- function() {
  theme_bw() +
    theme(panel.grid.major = element_blank(),
          panel.grid.minor = element_blank(),
          legend.background = element_rect(fill = "transparent",
                                           color = NA),
          legend.key = element_rect(fill = "transparent",
                                    color = NA))
}

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

checkpoint("2020-07-26",
           R.version ="3.6.3",
           checkpointLocation = getwd())
```

2 The issue of efficiency

In this section we present the code that produces Figs.1 and 2 of the main manuscript.

2.1 Functions to plot

```
# DEFINE FUNCTIONS TO PLOT ----------------------------------------------------

fig1_fun <- list(
  "fun1" = function(x) x ^ 2,
  "fun2" = function(x) ifelse(x < 0, -x, x),
  "fun3" = function(x) ifelse(x < 0, - (x + 1) ^ 2 + 1, - (x - 1) ^ 2 + 1)
)

fig2_fun <- list(
  "fun1" = function(x) 1.11 * x ^ 2,
  "fun2" = function(x) x ^ 2 - 0.2 * cos(7 * pi * x)
)

fig3_fun <- list(
  "fun1" = function(x) x,
  "fun2" = function(x) ((-1) ^ as.integer(4 * x) * (0.125 - (x %% 0.25)) + 0.125),
  "fun3" = function(x) ((-1) ^ as.integer(32 * x) *
                          (0.03125 - 2 * (x %% 0.03125)) + 0.03125) / 2
)

fig4_fun <- list(
  "fun1" = function(x) -sin(pi * x) - 0.3 * sin(3.33 * pi * x),
  "fun2" = function(x) -0.76 * sin(pi * (x - 0.2)) - 0.315,
  "fun3" = function(x) -0.12 * sin(1.05 * pi * (x - 0.2)) -
    0.02 * sin(95.24 * pi * x) - 0.96,
  "fun4" = function(x) -0.12 * sin(1.05 * pi * (x - 0.2)) - 0.96,
  "fun5" = function(x) -0.05 * sin(pi * (x - 0.2)) - 1.02,
  "fun6" = function(x) -1.08
)

# FUNCTION TO PLOT THE FUNCTIONS ----------------------------------------------

plot_function <- function(fun, min, max) {
  gg <- ggplot(data.frame(x = runif(1000, min, max)), aes(x)) +
    map(1:length(fun), function(nn) {
      stat_function(fun = fun[[nn]],
                    geom = "line",
                    aes_(color = factor(names(fun[nn]))))
    }) +
    labs(color = "Function",
         x = expression(italic(x)),
         y = expression(italic(y))) +
```

```
    theme_AP()
  return(gg)
}
```

2.2 Plot Figures

```
# PLOT FUNCTIONS ------------------------------------------------------------

a <- plot_function(fun = fig1_fun, -1, 1) +
  scale_color_manual(labels = c("$f_1(x)$","$f_2(x)$", "$f_3(x)$"),
                     values = c("#F8766D", "#B79F00", "#00BA38")) +
  labs(x = "", y = "$y$") +
  theme(legend.position = "none")

b <- plot_function(fun = fig2_fun, -1, 1) +
  scale_color_manual(labels = c("$f_1(x)$","$f_2(x)$"),
                     values = c("#F8766D", "#B79F00")) +
  labs(x = "", y = "") +
  theme(legend.position = "none")

c <- plot_function(fun = fig3_fun, 0, 1) +
  scale_color_manual(labels = c("$f_1(x)$","$f_2(x)$", "$f_3(x)$"),
                     values = c("#F8766D", "#B79F00", "#00BA38")) +
  scale_x_continuous(breaks = scales::pretty_breaks(n = 3)) +
  labs(x = "$x$", y = "$y$") +
  theme(legend.position = "none")

d <- plot_function(fun = fig4_fun, 0, 1) +
  scale_color_discrete(labels = c("$f_1(x)$","$f_2(x)$", "$f_3(x)$",
                                  "$f_4(x)$","$f_5(x)$", "$f_6(x)$")) +
  scale_x_continuous(breaks = scales::pretty_breaks(n = 3)) +
  labs(x = "$x$", y = "") +
  theme(legend.position = "none")

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

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

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

```
# PLOT FIGURE LIU -----------------------------------------------------------

mat <- randtoolbox::sobol(n = 1000, dim = 2)
mat[, 1] <- qchisq(mat[, 1], df = 10)
mat[, 2] <- qchisq(mat[, 2], df = 13.978)

fig.5.tikz <- data.table(mat) %>%
```

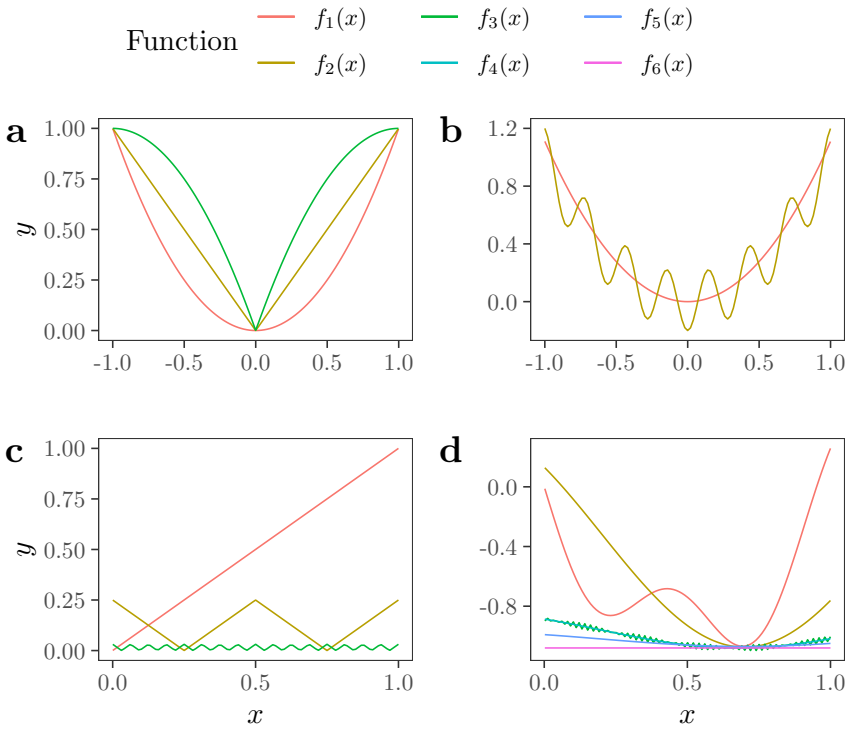


Figure 1: Examples of functions in Razavi and Gupta (2016). a) Unimodal functions with different structures. b) Multimodal versus unimodal function with identical variance. c) Functions covering different ranges in the response. d) A six-dimensional response surface. See Supplementary Materials for a mathematical description of all functions in all sub-plots.

```
  melt(., measure.vars = c("V1", "V2")) %>%
  ggplot(., aes(value, group = variable, colour = variable)) +
  geom_density() +
  labs(x = expression(italic(x)),
       y = "Density") +
  scale_color_discrete(name = "",
                       labels = c("$X_1 \\sim \\chi_{10} ^ {2}$",
                                  "$X_2 \\sim \\chi_{13.978} ^ {2}$")) +
  theme_AP() +
  theme(legend.text.align = 0,
        legend.position = c(0.93, 0.8))

# Fig.6
mat <- randtoolbox::sobol(n = 1000, dim = 2)
Y <- qchisq(mat[, 1], df = 10) / qchisq(mat[, 2], df = 13.978)
X1.fixed <- 10 / qchisq(mat[, 2], df = 13.978)
X2.fixed <- qchisq(mat[, 1], df = 10) / 13.978

fig.6.tikz <- cbind(Y, X1.fixed, X2.fixed) %>%
  data.table() %>%
  melt(., measure.vars = c("Y", "X1.fixed", "X2.fixed")) %>%
  ggplot(., aes(value, color = variable)) +
```

```
  geom_density() +
  scale_color_discrete(name = "", labels = c("Original PDF of Y",
                                             "$X_1$ fixed",
                                             "$X_2$ fixed")) +
  labs(x = expression(italic(y)),
       y = "") +
  theme_AP() +
  theme(legend.text.align = 0,
        legend.position = c(0.6, 0.8))

plot_grid(fig.5.tikz, fig.6.tikz, labels = "auto", align = "hv", ncol = 2)
```

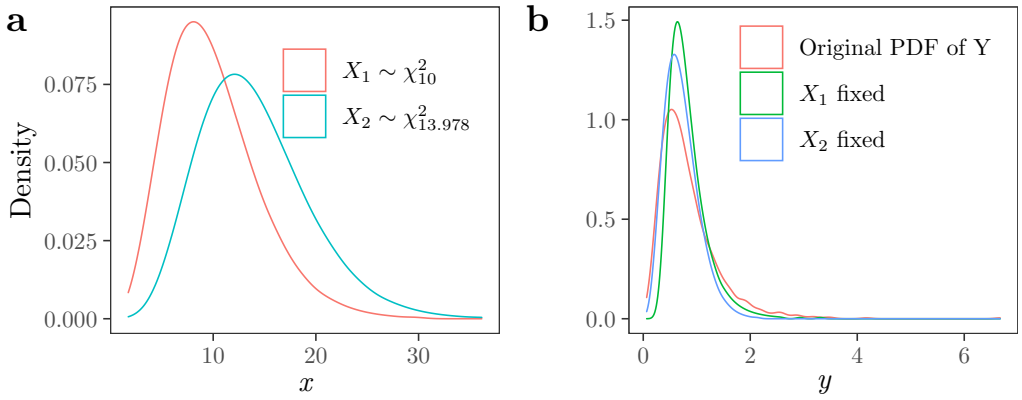


Figure 2: The highly skewed function of Liu, Chen, and Sudjianto (2006). a) Distribution of x_1 and x_2. b) Comparison of impacts of inputs.

3 The issue of efficiency

This section presents the code to compare the efficiency of VARS and the Jansen estimator (Jansen 1999). We first start by coding all the functions required to compute VARS:

The function `vars_matrices` creates the STAR-VARS sample matrix that VARS needs in order to compute VARS-TO. In our code, the sample matrix can be created with random numbers or with Sobol' Quasi Random Numbers (the default) (Sobol' 1967, @Sobol1976).

The function `vars_ti` allows to compute VARS-TO on the model output obtained from a STAR-VARS matrix. Our code pairs values separated by h (`method=one.step`) or separated by h, $2h$, $3h$,... (the default, `method=all.step`).

We also code the Jansen estimator (Jansen 1999) (`jansen_ti`), and a function to compute Savage scores (`savage_scores`) (Savage 1956). Finally, we code a function that allows to randomly transform the distribution of model inputs to normal, logitnormal or different beta distributions.

```
# CREATE STAR-VARS MATRICES ------------------------------------------------------

vars_matrices <- function(star.centers, params, h, method = "QRN") {
  out <- center <- sections <- A <- B <- AB <- X <- out <- list()
  if(method == "QRN") {
    mat <- randtoolbox::sobol(n = star.centers, dim = length(params))
  } else if(method == "R") {
    mat <- replicate(length(params), stats::runif(star.centers))
  } else {
    stop("method should be either QRN, R or LHS")
  }
  for(i in 1:nrow(mat)) {
    center[[i]] <- mat[i, ]
    sections[[i]] <- sapply(center[[i]], function(x) {
      all <- seq(x %% h, 1, h)
      non.zeros <- all[all!= 0]
    })
    B[[i]] <- sapply(1:ncol(mat), function(x)
      sections[[i]][, x][!sections[[i]][, x] %in% center[[i]][x]])
    A[[i]] <- matrix(center[[i]], nrow = nrow(B[[i]]),
                     ncol = length(center[[i]]), byrow = TRUE)
    X[[i]] <- rbind(A[[i]], B[[i]])
    for(j in 1:ncol(A[[i]])) {
      AB[[i]] <- A[[i]]
      AB[[i]][, j] <- B[[i]][, j]
      X[[i]] <- rbind(X[[i]], AB[[i]])
    }
    AB[[i]] <- X[[i]][(2 * nrow(B[[i]]) + 1):nrow(X[[i]]), ]
    out[[i]] <- rbind(unname(center[[i]]), AB[[i]])
  }
  return(do.call(rbind, out))
}
```

```r
# CREATE VARS FUNCTION ------------------------------------------------------

# Function to cut by size
CutBySize <- function(m, block.size, nb = ceiling(m / block.size)) {
  int <- m / nb
  upper <- round(1:nb * int)
  lower <- c(1, upper[-nb] + 1)
  size <- c(upper[1], diff(upper))
  cbind(lower, upper, size)
}

# VARS-TO algorithm
vars_ti <- function(Y, star.centers, params, h, method = "all.step") {
  n.cross.points <- length(params) * ((1 / h) - 1) + 1
  index.centers <- seq(1, length(Y), n.cross.points)
  mat <- matrix(Y[-index.centers], ncol = star.centers)
  indices <- CutBySize(nrow(mat), nb = length(params))
  out <- list()
  for(i in 1:nrow(indices)) {
    out[[i]] <- mat[indices[i, "lower"]:indices[i, "upper"], ]
  }
  if(method == "one.step") {
    d <- lapply(1:length(params), function(x)
      lapply(1:ncol(out[[x]]), function(j) {
        da <- c(out[[x]][, j][1],
                rep(out[[x]][, j][-c(1, length(out[[x]][, j]))], each = 2),
                out[[x]][, j][length(out[[x]][, j])])
      }))
  } else if(method == "all.step") {
    d <- lapply(1:length(params), function(x)
      lapply(1:ncol(out[[x]]), function(j) {
        da <- c(combn(out[[x]][, j], 2))
      }))
  } else {
    stop("method should be either one.step or all.step")
  }
  out <- lapply(d, function(x)
    lapply(x, function(y) matrix(y, nrow = length(y) / 2, byrow = TRUE)))
  variogr <- unlist(lapply(out, function(x) lapply(x, function(y)
    mean(0.5 * (y[, 1] - y[, 2]) ^ 2))) %>%
      lapply(., function(x) do.call(rbind, x)) %>%
      lapply(., mean))
  covariogr <- unlist(lapply(out, function(x)
    lapply(x, function(y) cov(y[, 1], y[, 2]))) %>%
      lapply(., function(x) Rfast::colmeans(do.call(rbind, x))))
  VY <- var(Y[index.centers])
  Ti <- (variogr + covariogr) / VY
```

```
  output <- data.table::data.table(Ti)
  output[, `:=`(parameters = params)]
  return(output)
}
```

```
# DEFINE JANSEN TOTAL-ORDER INDEX ----------------------------------------------

jansen_ti <- function(d, N, params) {
  m <- matrix(d, nrow = N)
  k <- length(params)
  Y_A <- m[, 1]
  Y_AB <- m[, -1]
  f0 <- (1 / length(Y_A)) * sum(Y_A)
  VY <- 1 / length(Y_A) * sum((Y_A - f0) ^ 2)
  Ti <- (1 / (2 * N) * Rfast::colsums((Y_A - Y_AB) ^ 2)) / VY
  output <- data.table(Ti)
  output[, `:=`(parameters = paste("X", 1:k, sep = ""))]
  return(output)
}

# DEFINE SAVAGE SCORES ---------------------------------------------------------
savage_scores <- function(x) {
  true.ranks <- rank(-x)
  p <- sort(1 / true.ranks)
  mat <- matrix(rep(p, length(p)), nrow = length(p), byrow = TRUE)
  mat[upper.tri(mat)] <- 0
  out <- sort(rowSums(mat), decreasing = TRUE)[true.ranks]
  return(out)
}

# DEFINE FUNCTION FOR RANDOM DISTRIBUTIONS -------------------------------------

sample_distributions <- list(
  "uniform" = function(x) x,
  "normal" = function(x) qnorm(x, 0.5, 0.2),
  "beta" = function(x) qbeta(x, 8, 2),
  "beta2" = function(x) qbeta(x, 2, 8),
  "beta3" = function(x) qbeta(x, 2, 0.5),
  "beta4" = function(x) qbeta(x, 0.5, 2),
  "logitnormal" = function(x) qlogitnorm(x, 0, 3.16)
  # Logit-normal, Bates too?
)

random_distributions <- function(X, phi) {
  names_ff <- names(sample_distributions)
  if(!phi == length(names_ff) + 1) {
    out <- apply(X, 2, function(x)
```

```
      sample_distributions[[names_ff[phi]]](x))
  } else {
    temp <- sample(names_ff, ncol(X), replace = TRUE)
    out <- sapply(seq_along(temp), function(x) sample_distributions[[temp[x]]](X[, x]))
  }
  return(out)
}
```

4 The simulations

4.1 The sample matrix

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

N <- 2 ^ 12 # Sample size of sample matrix
R <- 500 # Number of bootstrap replicas
n_cores <- ceiling(detectCores() * 0.5)
order <- "first"
params <- c("N.stars", "h", "k", "k_2", "k_3", "epsilon", "delta", "phi", "tau")
N.high <- 2 ^ 12 # Maximum sample size of the large sample matrix

# CREATE SAMPLE MATRIX -----------------------------------------------------------

mat <- sobol_matrices(N = N, params = params, order = order)

# TRANSFORM MATRIX ---------------------------------------------------------------

mat[, 1] <- round(qunif(mat[, 1], 3, 20), 0) # N.stars
mat[, 2] <- round(qunif(mat[, 2], 1, 4), 0) # h
mat[, 3] <- round(qunif(mat[, 3], 3, 50)) # k
mat[, 4] <- round(qunif(mat[, 4], 0.5, 1), 1) # k_2
mat[, 5] <- round(qunif(mat[, 5], 0.3, 1), 1) # k_3
mat[, 6] <- round(qunif(mat[, 6], 1, 200), 0) # epsilon
mat[, 7] <- round(qunif(mat[, 7], 1, 3), 0) # delta
mat[, 8] <- round(qunif(mat[, 8], 1, 8), 0) # phi
mat[, 9] <- floor(mat[, 9] * (2 - 1 + 1)) + 1 # tau

# DEFINE TOTAL NUMBER OF RUNS ----------------------------------------------------

# Correct h
mat[, "h"] <- ifelse(mat[, "h"] == 1, 0.01,
                     ifelse(mat[, "h"] == 2, 0.05,
                            ifelse(mat[, "h"] == 3, 0.1, 0.2)))

# For vars
Nt.vars <- round(apply(mat, 1, function(x)
  x["N.stars"] * (x["k"] * ((1 / x["h"]) - 1) + 1)), 0)
```

```r
# For jansen
N.jansen <- round(apply(cbind(mat, Nt.vars), 1, function(x)
  x["Nt.vars"] / (x["k"] + 1))) %>%
  ifelse(. == 1, 2, .) # Transform N = 1 to N = 2 for jansen

Nt.jansen <- apply(cbind(mat, Nt.vars, N.jansen), 1, function(x)
  x["N.jansen"] * (x["k"] + 1))

# FINAL MATRIX ------------------------------------------------------------------

mat <- cbind(mat, Nt.vars, N.jansen, Nt.jansen)

# Check min and max total number of runs
sapply(c(min, max), function(x) x(mat[, "Nt.vars"]))
```

```
## [1]    51 99020
```

```r
# SHOW SAMPLE MATRIX ------------------------------------------------------------

head(mat)
```

```
##      N.stars    h  k k_2 k_3 epsilon delta phi tau Nt.vars N.jansen Nt.jansen
## [1,]      12 0.05 26 0.8 0.6     100     2   4   2    5940      220      5940
## [2,]      16 0.05 38 0.6 0.8      51     2   3   1   11568      297     11583
## [3,]       7 0.10 15 0.9 0.5     150     2   6   2     952       60       960
## [4,]       9 0.05 32 0.6 0.9     175     1   5   1    5481      166      5478
## [5,]      18 0.20  9 0.8 0.6      76     2   2   2     666       67       670
## [6,]      14 0.01 21 0.7 0.4     125     3   7   1   29120     1324     29128
```

4.2 The model

```r
# DEFINE MODEL ------------------------------------------------------------------

model_ti <- function(N.stars, h, k, k_2, k_3, epsilon, delta, tau, phi, N.jansen, N.high) {
  if(tau == 1) {
    method <- "R"
  } else if(tau == 2) {
    method <- "QRN"
  }
  # Create sample matrices
  set.seed(epsilon)
  vars.matrix <- vars_matrices(star.centers = N.stars, params = paste("X", 1:k, sep = ""), h =
                               method = method)
  set.seed(epsilon)
  jansen.matrix <- sobol_matrices(matrices = c("A", "AB"), N = N.jansen,
                                  params = paste("X", 1:k, sep = ""))
  set.seed(epsilon)
  large.matrix <- sobol_matrices(matrices = c("A", "AB"), N = N.high,
```

```
                                  params = paste("X", 1:k, sep = ""),
                                  method = method)
# Compute metafunciton
set.seed(epsilon)
output <- sensobol::metafunction(data = random_distributions(X = rbind(jansen.matrix,
                                                                       vars.matrix,
                                                                       large.matrix),
                                                             phi = phi),
                                 k_2 = k_2, k_3 = k_3, epsilon = epsilon)
# Compute sobol' indices on a large sample size
full.ind <- jansen_ti(d = tail(output, nrow(large.matrix)),
                      N = N.high,
                      params = paste("X", 1:k, sep = ""))
full.ind[, sample.size:= "N"]
# Define indices of Y for VARS
lg.jansen <- 1:(N.jansen * (k + 1))
Nt.vars <- N.stars * (k * ((1 / h) - 1) + 1)
lg.vars <- (max(lg.jansen) + 1): (max(lg.jansen) + Nt.vars)
# Compute VARS
ind.vars <- vars_ti(output[lg.vars], star.centers = N.stars,
                    params = paste("X", 1:k, sep = ""), h = h) %>%
  .[, sample.size:= "n"]
full.vars <- rbind(ind.vars, full.ind)[, estimator:= "VARS-TO"]
# Compute Jansen
ind.jansen <- jansen_ti(d = output[lg.jansen], N = N.jansen,
                        params = paste("X", 1:k, sep = ""))
ind.jansen[, sample.size:= "n"]
full.jansen <- rbind(ind.jansen, full.ind)[, estimator:= "Jansen"]
out <- rbind(full.vars, full.jansen)
out.wide <- dcast(out, estimator + parameters ~ sample.size, value.var = "Ti")
# Replace NaN
for (i in seq_along(out.wide))
  set(out.wide, i=which(is.nan(out.wide[[i]])), j = i, value = 0)
# Replace Inf
for (i in seq_along(out.wide))
  set(out.wide, i=which(is.infinite(out.wide[[i]])), j = i, value = 0)
# Replcace Na
for (i in seq_along(out.wide))
  set(out.wide, i=which(is.na(out.wide[[i]])), j = i, value = 0)
# CHECK DELTA
if(delta == 1) { # Regular Pear
  final <- out.wide[, .(correlation = cor(N, n)), estimator]
} else if(delta == 2) { # kendall tau
  final <- out.wide[, .(correlation = pcaPP::cor.fk(N, n)), estimator]
} else { # Savage ranks
  final <- out.wide[, lapply(.SD, savage_scores), .SDcols = c("N", "n"), estimator][
    , .(correlation = cor(N, n)), estimator]
```

```
  }
  return(final)
}
```

4.3 Execution of the model

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

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

# Compute
Y.ti <- foreach(i=1:nrow(mat),
                .packages = c("sensobol", "data.table", "dplyr",
                              "pcaPP", "logitnorm")) %dopar%
  {
    model_ti(N.stars = mat[[i, "N.stars"]],
             h = mat[[i, "h"]],
             k = mat[[i, "k"]],
             k_2 = mat[[i, "k_2"]],
             k_3 = mat[[i, "k_3"]],
             epsilon = mat[[i, "epsilon"]],
             delta = mat[[i, "delta"]],
             phi = mat[[i, "phi"]],
             tau = mat[[i, "tau"]],
             N.jansen = mat[[i, "N.jansen"]],
             N.high = N.high)
  }

# Stop parallel cluster
stopCluster(cl)
```

4.4 Arrange the results

```
# ARRANGE OUTPUT -------------------------------------------------------------

out_cor <- rbindlist(Y.ti, idcol = "row")

mt.dt <- data.table(mat) %>%
  .[, row:= 1:.N]

full_output <- merge(mt.dt, out_cor) %>%
  .[, Nt:= ifelse(estimator == "VARS-TO", Nt.vars, Nt.jansen)]

# Show rows with NA or NaN
full_output[is.na(correlation), ]
```

```
##        row N.stars    h  k k_2 k_3 epsilon delta phi tau Nt.vars N.jansen
##   1:    42      20 0.05  5 0.7 0.9     166     2   2   2    1920      320
##   2:   369      13 0.10  6 1.0 0.7      72     3   2   2     715      102
##   3:  1087       3 0.10 10 0.5 0.5      67     2   2   2     273       25
##   4:  1386      20 0.05  5 0.6 0.7      60     3   2   2    1920      320
##   5:  1507       8 0.10  6 0.8 1.0     113     1   2   2     440       63
##  ---
## 157: 44333      18 0.10  3 0.5 0.6      27     2   2   2     504      126
## 158: 44621      17 0.10  7 0.6 0.9     165     1   2   2    1088      136
## 159: 44782      13 0.05  3 0.8 0.6     173     2   2   2     754      188
## 160: 44782      13 0.05  3 0.8 0.6     173     2   2   2     754      188
## 161: 44819       9 0.10 10 0.5 1.0      48     3   2   2     819       74
##      Nt.jansen estimator correlation   Nt
##   1:      1920   VARS-TO         NaN 1920
##   2:       714   VARS-TO          NA  715
##   3:       275   VARS-TO         NaN  273
##   4:      1920   VARS-TO          NA 1920
##   5:       441   VARS-TO          NA  440
##  ---
## 157:       504   VARS-TO         NaN  504
## 158:      1088   VARS-TO          NA 1088
## 159:       752    Jansen         NaN  752
## 160:       752   VARS-TO         NaN  754
## 161:       814   VARS-TO          NA  819
```

```
# Compute proportion of rows with Na or NaN
full_output[, sum(is.na(correlation)) / .N, estimator]
```

```
##    estimator           V1
## 1:    Jansen 0.0007324219
## 2:   VARS-TO 0.0028409091
```

```
# Substitute NA by 0
full_output <- full_output[, correlation:= ifelse(is.na(correlation) == TRUE, 0, correlation)]

A <- full_output[,.SD[1:N], estimator][, ratio:= Nt / k]
```

```
# EXPORT RESULTS ----------------------------------------------------------

fwrite(A, "A.csv")
fwrite(full_output, "full_output.csv")
```

5 Uncertainty analysis

```
# UNCERTAINTY ANALYSIS ----------------------------------------------------

# Compute median and quantiles
```

```r
dt_median <- A[, .(median = median(correlation),
                   low.ci = quantile(correlation, 0.25),
                   high.ci = quantile(correlation, 0.75)), estimator]

A[, .(median = median(correlation),
      low.ci = quantile(correlation, 0.25),
      high.ci = quantile(correlation, 0.75)), estimator][order(median)]
```

```
##    estimator    median    low.ci   high.ci
## 1:   VARS-TO 0.9503634 0.8740740 0.9905648
## 2:    Jansen 0.9826840 0.9354839 0.9985708
```

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

# Histograms
unc <- ggplot(A, aes(correlation)) +
  geom_rect(data = dt_median,
            aes(xmin = low.ci,
                xmax = high.ci,
                ymin = -Inf,
                ymax = Inf),
            fill = "blue",
            color = "white",
            alpha = 0.1,
            inherit.aes = FALSE) +
  geom_histogram() +
  geom_vline(data = dt_median, aes(xintercept = median),
             lty = 2,
             color = "red") +
  facet_wrap(~estimator,
             ncol = 4) +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  labs(x = expression(italic(r)),
       y = "Counts") +
  theme_AP()

unc
```

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

```r
# SCATTERPLOT OF MODEL RESULTS ------------------------------------------------

scat <- ggplot(A, aes(Nt, k, color = correlation)) +
  geom_point(size = 0.4) +
  scale_colour_gradientn(colours = c("black", "purple", "red", "orange", "lightgreen"),
                         name = expression(italic(r)),
                         breaks = c(0, 0.5, 1)) +
  scale_x_log10(breaks = scales::trans_breaks("log10", function(x) 10 ^ (2 * x)),
```

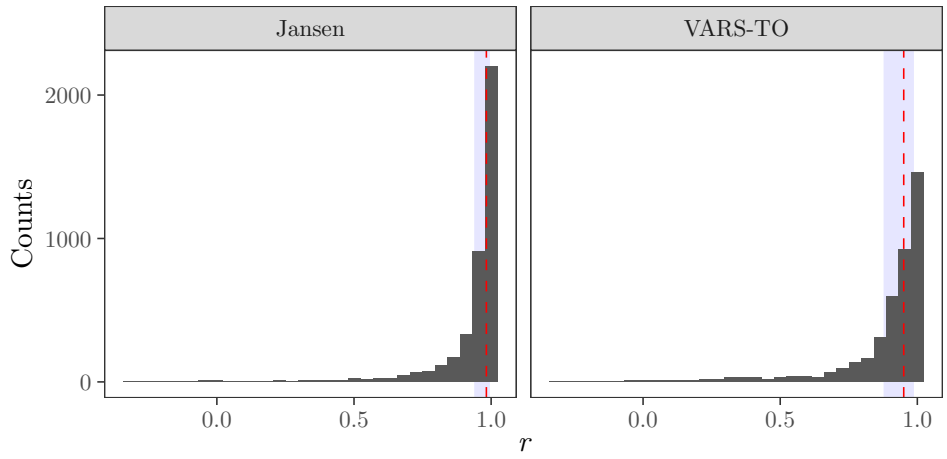


Figure 3: Empirical distribution of r for Jansen and VARS.

```
                labels = scales::trans_format("log10", scales::math_format(10^.x))) +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  labs(x = expression(italic(N[t])),
       y = expression(italic(k))) +
  facet_wrap(~estimator,
             ncol = 4) +
  theme_AP() +
  theme(legend.position = "top")

scat
```

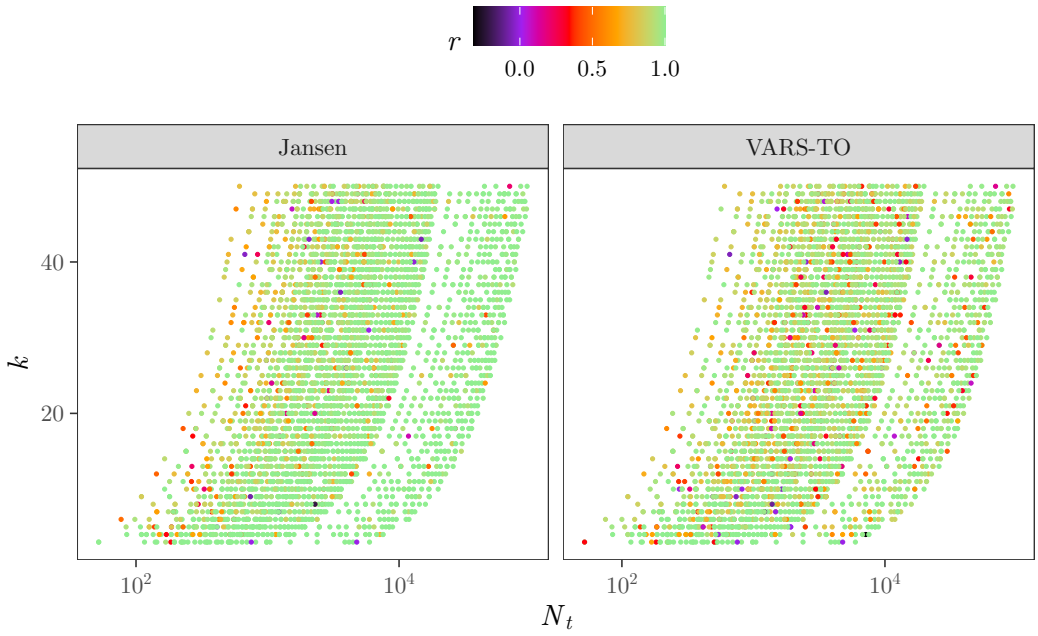
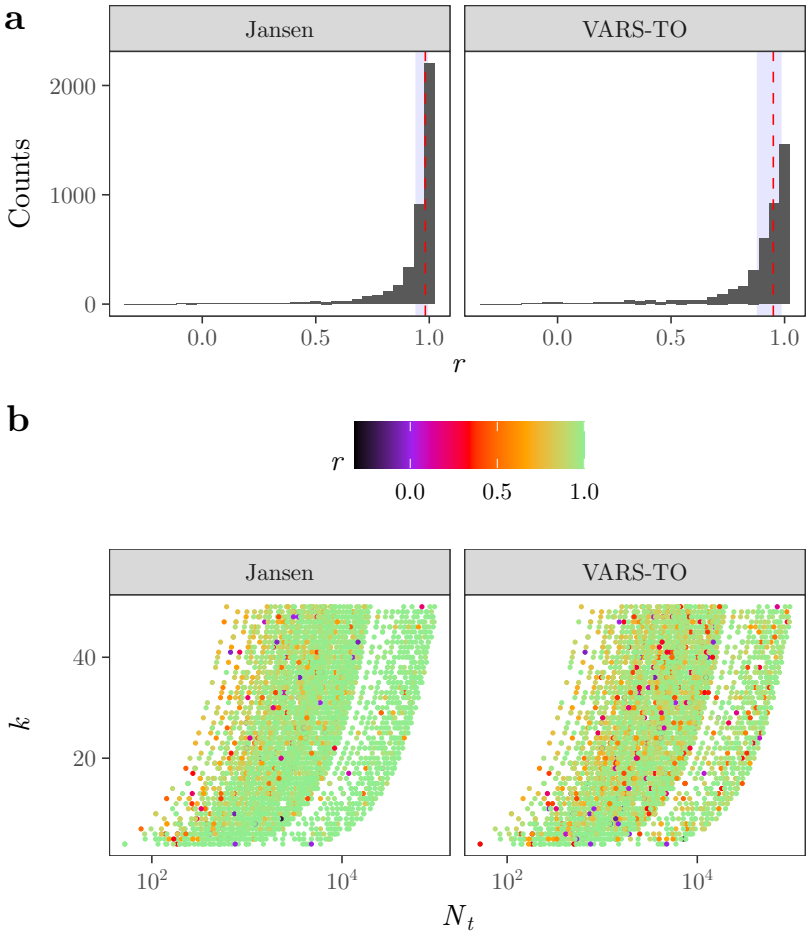


Figure 4: Scatterplots of the total number of model runs N_t against the function dimensionality k. The greener (darker) the colour, the better (worse) the performance.

```
# MERGE PLOTS ------------------------------------------------------------------

plot_grid(unc, scat, ncol = 1, labels = "auto", align = "hv",
          rel_heights = c(0.72, 1))
```

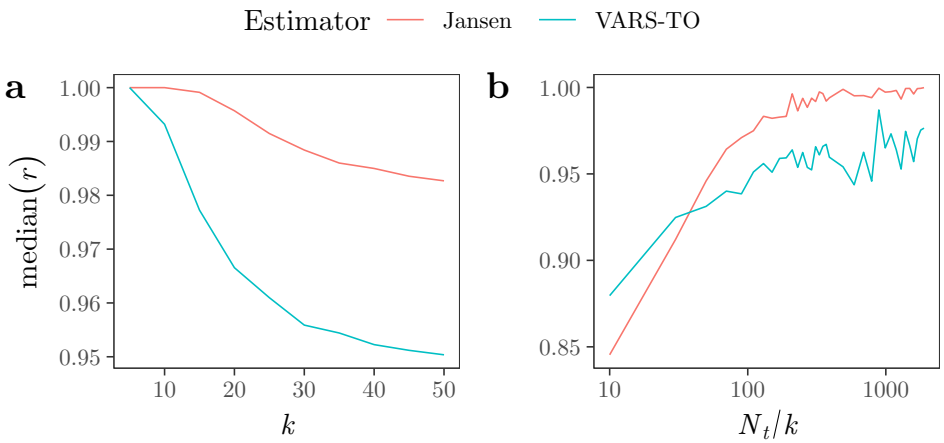
```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

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

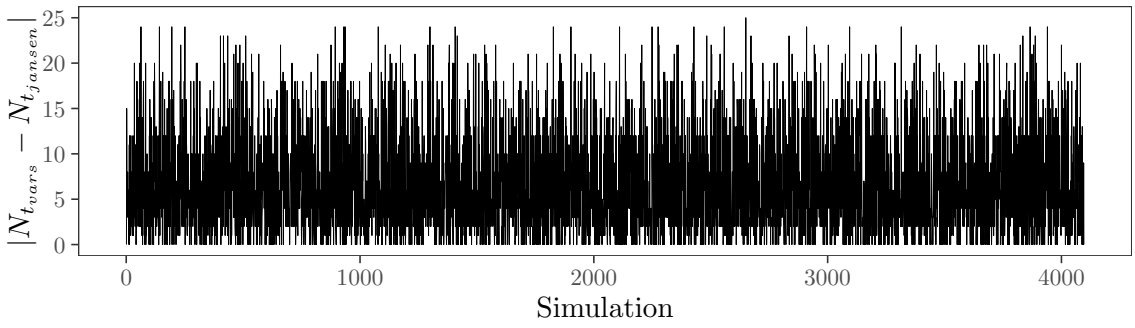



```
# PLOT R MEDIANS AS FUNCTION OF K AND NT/K -------------------------------------

vv <- seq(5, 50, 5)

dt <- lapply(vv, function(x) A[k <= x, median(correlation), estimator])

names(dt) <- vv

# Plot r as a function of k
a1 <- rbindlist(dt, idcol = "k") %>%
  .[, k:= as.numeric(k)] %>%
  ggplot(., aes(k, V1, color = estimator)) +
```

```
  scale_color_discrete(name = "Estimator") +
  labs(x = expression(italic(k)),
       y = expression(median(italic(r)))) +
  geom_line() +
  theme_AP() +
  theme(legend.position = "none")

# Median Nt/k
dt.tmp <- A[, .(min = min(ratio), max = max(ratio))]

v <-  seq(0, ceiling(dt.tmp$max), 20)
a <- c(v[1], rep(v[-c(1, length(v))], each = 2), v[length(v)])
indices <- matrix(a, ncol = 2, byrow = TRUE)

out <- list()
for(i in 1:nrow(indices)) {
  out[[i]] <- A[ratio > indices[i, 1] & ratio < indices[i, 2]]
}

names(out) <- Rfast::rowmeans(indices)

# Plot r as a function of Nt/k
a2 <- lapply(out, function(x) x[, median(correlation, na.rm = TRUE), estimator]) %>%
  rbindlist(., idcol = "N") %>%
  .[, N:= as.numeric(N)] %>%
  ggplot(., aes(N, V1, group = estimator, color = estimator)) +
  geom_line() +
  labs(x = expression(italic(N[t]/k)),
       y = "") +
  scale_color_discrete(name = "Estimator") +
  scale_x_log10() +
  theme_AP() +
  theme(legend.position = "none")

# Merge both plots
legend <- get_legend(a1 + theme(legend.position = "top"))
sides <- plot_grid(a1, a2, ncol = 2, rel_widths = c(1, 1), align = "hv",
                   labels = "auto")

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

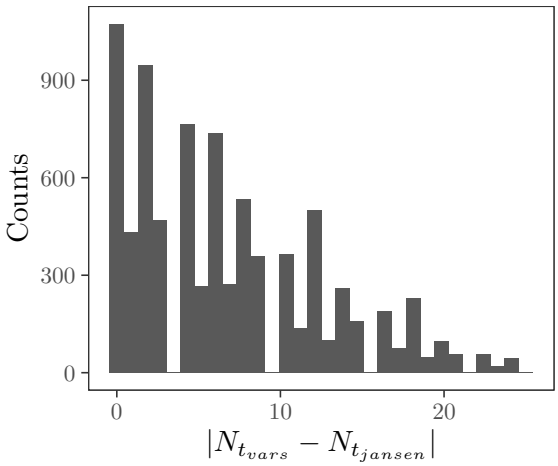



```
# CHECK HOW MUCH NT DIFFERS BETWEEN VARS AND JANSEN -----------------------------

A <- A[, diff:= abs(Nt.jansen - Nt.vars)]

# Plot
ggplot(A, aes(row, diff)) +
  geom_line(size = 0.02) +
  labs(x = "Simulation",
       y = "$ | N_{t_{vars}} - N_{t_{jansen}} | $") +
  theme_AP()
```




```
# CHECK HOW MUCH NT DIFFERS BETWEEN VARS AND JANSEN 2 ---------------------------

A %>%
  ggplot(., aes(diff)) +
  geom_histogram() +
  labs(y = "Counts",
       x = "$ | N_{t_{vars}} - N_{t_{jansen}} | $") +
  theme_AP()
```

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



6 Sensitivity analysis

```
# SCATTERPLOTS ------------------------------------------------------------------

params_notikz <- c("N[stars]", "h", "k", "k[2]", "k[3]",
                   "epsilon", "delta", "phi", "tau")

# Scatterplot of model inputs against output
A[estimator == "VARS-TO"] %>%
  setnames(., params, params_notikz) %>%
  melt(., measure.vars = params_notikz) %>%
  ggplot(., aes(value, correlation)) +
  geom_point(size = 0.5, alpha = 0.1) +
  facet_wrap(~variable,
             scales = "free_x",
             labeller = label_parsed) +
  labs(y = expression(italic(r)),
       x = "") +
  theme_AP()
```

```
# SOBOL' INDICES ----------------------------------------------------------------

params_tikz <- c("$N_{stars}$", "$h$", "$k$", "$k_2$", "$k_3$", "$\\epsilon$",
                 "$\\delta$", "$\\phi$", "$\\tau$")

 # Compute Sobol' indices except for the cluster Nt,k
indices <- full_output[, sobol_indices(Y = correlation,
                                       N = N,
                                       params = params_tikz,
                                       first = "jansen",
                                       boot = TRUE,
                                       R = R,
                                       order = order),
```

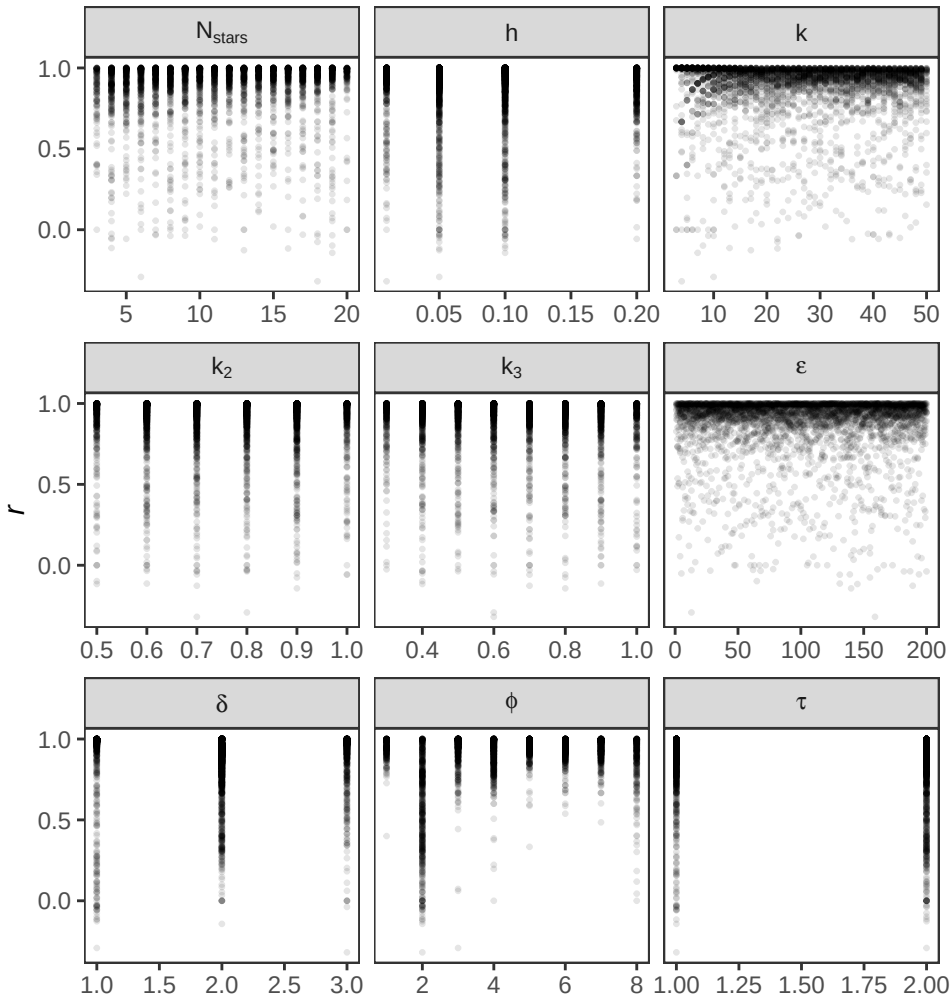


Figure 5: Scatterplots of model output r against the model inputs.

```
                          estimator]
```

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

indices[sensitivity == "Si" | sensitivity == "Ti"] %>%
  .[estimator == "VARS-TO"] %>%
  ggplot(., aes(parameters, original, fill = sensitivity)) +
  geom_bar(stat = "identity",
           position = position_dodge(0.6),
           color = "black") +
  geom_errorbar(aes(ymin = low.ci,
                    ymax = high.ci),
                position = position_dodge(0.6)) +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  labs(x = "",
       y = "Sobol' index") +
  scale_fill_discrete(name = "Sobol' indices",
                      labels = c(expression(S[italic(i)]),
                                 expression(T[italic(i)]))) +
  theme_AP() +
  theme(legend.position = "top")
```

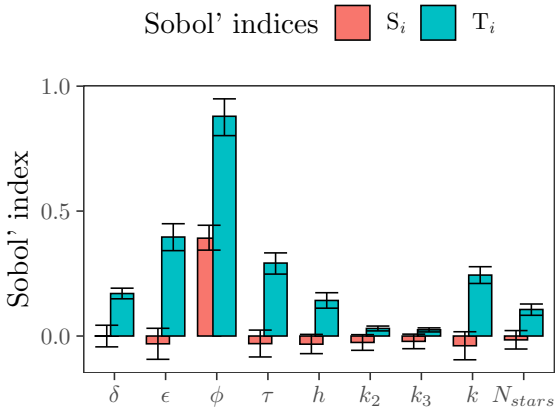


Figure 6: Sobol' indices.

```
# SUM OF FIRST-ORDER INDICES -----------------------------------------------

indices[sensitivity == "Si", sum(original)]
```

```
## [1] 0.5780782
```

7 References

8 Session information

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

sessionInfo()
```

```
## R version 3.6.3 (2020-02-29)
## Platform: x86_64-apple-darwin15.6.0 (64-bit)
## Running under: macOS Catalina 10.15.5
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/3.6/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/3.6/Resources/lib/libRlapack.dylib
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
## [1] parallel  stats     graphics  grDevices utils     datasets  methods
## [8] base
##
## other attached packages:
##  [1] data.table_1.12.8  checkpoint_0.4.9   Rfast_1.9.9        RcppZiggurat_0.1.5
##  [5] Rcpp_1.0.5         benchmarkme_1.0.4  logitnorm_0.8.37   cowplot_1.0.0
##  [9] scales_1.1.1       pcaPP_1.9-73       doParallel_1.0.15  iterators_1.0.12
## [13] foreach_1.5.0      sensobol_0.3       forcats_0.5.0      stringr_1.4.0
## [17] dplyr_1.0.0        purrr_0.3.4        readr_1.3.1        tidyr_1.1.0
## [21] tibble_3.0.3       ggplot2_3.3.2      tidyverse_1.3.0
##
## loaded via a namespace (and not attached):
##  [1] httr_1.4.2           jsonlite_1.7.0       modelr_0.1.8
##  [4] Rdpack_1.0.0         assertthat_0.2.1     blob_1.2.1
##  [7] cellranger_1.1.0     yaml_2.2.1           remotes_2.2.0
## [10] pillar_1.4.6         backports_1.1.8      lattice_0.20-41
## [13] glue_1.4.1           digest_0.6.25        rvest_0.3.6
## [16] colorspace_1.4-1     htmltools_0.5.0      Matrix_1.2-18
## [19] pkgconfig_2.0.3      bibtex_0.4.2.2       broom_0.7.0
## [22] haven_2.3.1          mvtnorm_1.1-1        generics_0.0.2
## [25] ellipsis_0.3.1       withr_2.2.0          cli_2.0.2
## [28] magrittr_1.5         crayon_1.3.4         readxl_1.3.1
## [31] evaluate_0.14        fs_1.4.2             fansi_0.4.1
## [34] xml2_1.3.2           tools_3.6.3          hms_0.5.3
## [37] gbRd_0.4-11          lifecycle_0.2.0      munsell_0.5.0
## [40] reprex_0.3.0         compiler_3.6.3       rlang_0.4.7
## [43] grid_3.6.3           rstudioapi_0.11      rmarkdown_2.3
## [46] gtable_0.3.0         codetools_0.2-16     DBI_1.1.0
## [49] curl_4.3             benchmarkmeData_1.0.4 R6_2.4.1
## [52] lubridate_1.7.9      knitr_1.29           stringi_1.4.6
```

```
## [55] vctrs_0.3.2           dbplyr_1.4.4          tidyselect_1.1.0
## [58] xfun_0.16
```

```
## Return the machine CPU
cat("Machine:     "); print(get_cpu()$model_name)
```

```
## Machine:
```

```
## [1] "Intel(R) Core(TM) i9-9900K CPU @ 3.60GHz"
```

```
## Return number of true cores
cat("Num cores:   "); print(detectCores(logical = FALSE))
```

```
## Num cores:
```

```
## [1] 8
```

```
## Return number of threads
cat("Num threads: "); print(detectCores(logical = FALSE))
```

```
## Num threads:
```

```
## [1] 8
```


Jansen, M. 1999. "Analysis of variance designs for model output." *Computer Physics Communications* 117 (1-2): 35–43. https://doi.org/10.1016/S0010-4655(98)00154-4.

Liu, Huibin, Wei Chen, and Agus Sudjianto. 2006. "Relative entropy based method for probabilistic sensitivity analysis in engineering design." *Journal of Mechanical Design, Transactions of the ASME* 128 (2): 326–36. https://doi.org/10.1115/1.2159025.

Razavi, Saman, and Hoshin V. Gupta. 2016. "A new framework for comprehensive, robust, and efficient global sensitivity analysis: 1. Theory." *Water Resources Research* 52 (1): 440–55. https://doi.org/10.1002/2015WR017559.

Savage, I. Richard. 1956. "Contributions to the theory of rank order statistics - the two sample case." *Annals of Mathematical StatisticsStatistics* 27: 590–615.

Sobol', Ilya. M. 1967. "On the distribution of points in a cube and the approximate evaluation of integrals." *USSR Computational Mathematics and Mathematical Physics* 7 (4): 86–112. https://doi.org/10.1016/0041-5553(67)90144-9.

———. 1976. "Uniformly distributed sequences with an additional uniform property." *USSR Computational Mathematics and Mathematical Physics* 16 (5): 236–42. https://doi.org/10.1016/0041-5553(76)90154-3.