Is VARS more intuitive and efficient than Sobol' indices?

R code

Arnald Puy

```r
# 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())
```

1 Figures

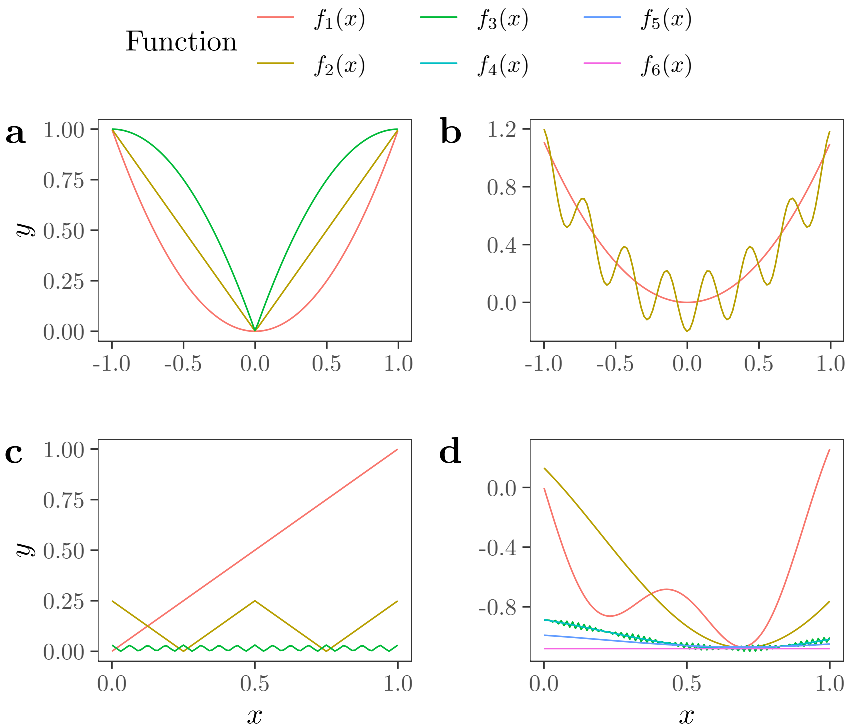
```r
# PRELIMINARY FUNCTIONS -------------------------------------------------------

# 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)
    }
  }
}

# Load the packages
loadPackages(c("tidyverse", "data.table", "cowplot"))

# 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))
}
```

2 Functions

```
# 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) /
)

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)
}
```

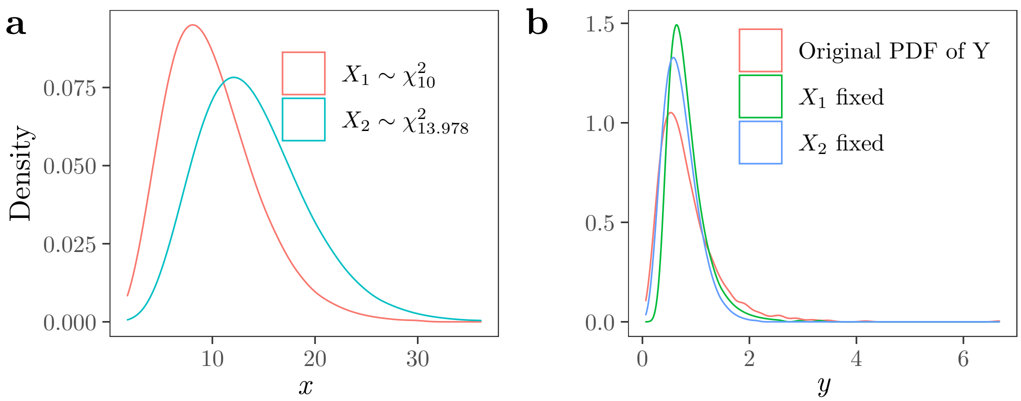
3 Plot the figures

```r
# 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) %>%
  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() %>%
```

```r
  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)
```



```r
# 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))
}

# 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
```

```r
  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)
}
```

```r
# 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)
```

```r
  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 Sample matrix

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

N <- 2 ^ 12 # Sample size of sample matrix
```

```r
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)

# 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
```

5 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)
}
```

```
# 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%
  {
```

```r
    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)
```

```r
# 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
```

```r
# 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
```

```r
# 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]
```

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

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

6 Uncertainty analysis

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

# Compute median and quantiles
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),
```

```r
             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`.
```

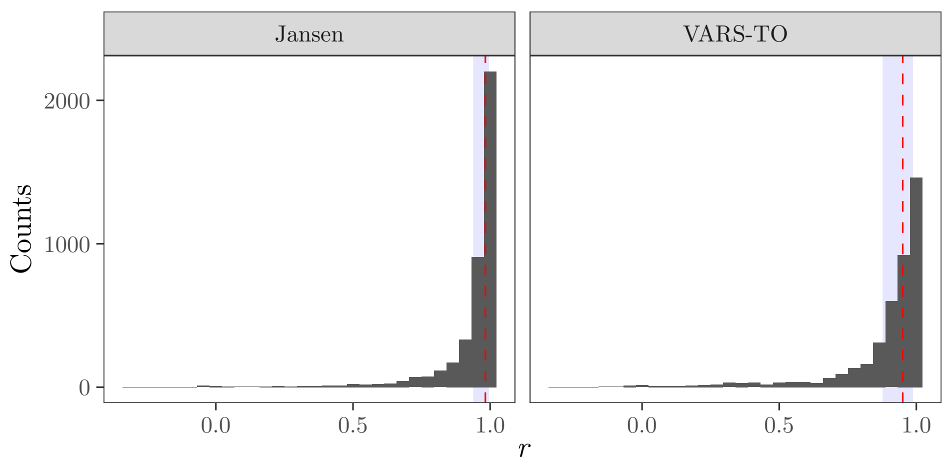


Figure 1: Empirical distribution of r for Jansen and VARS.

```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)),
              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
```

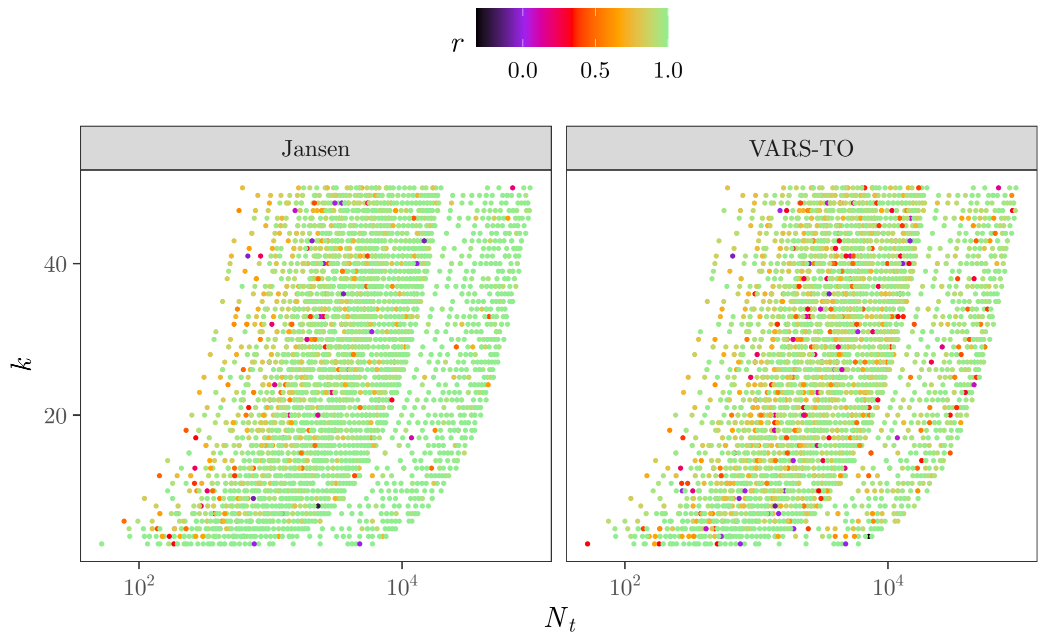
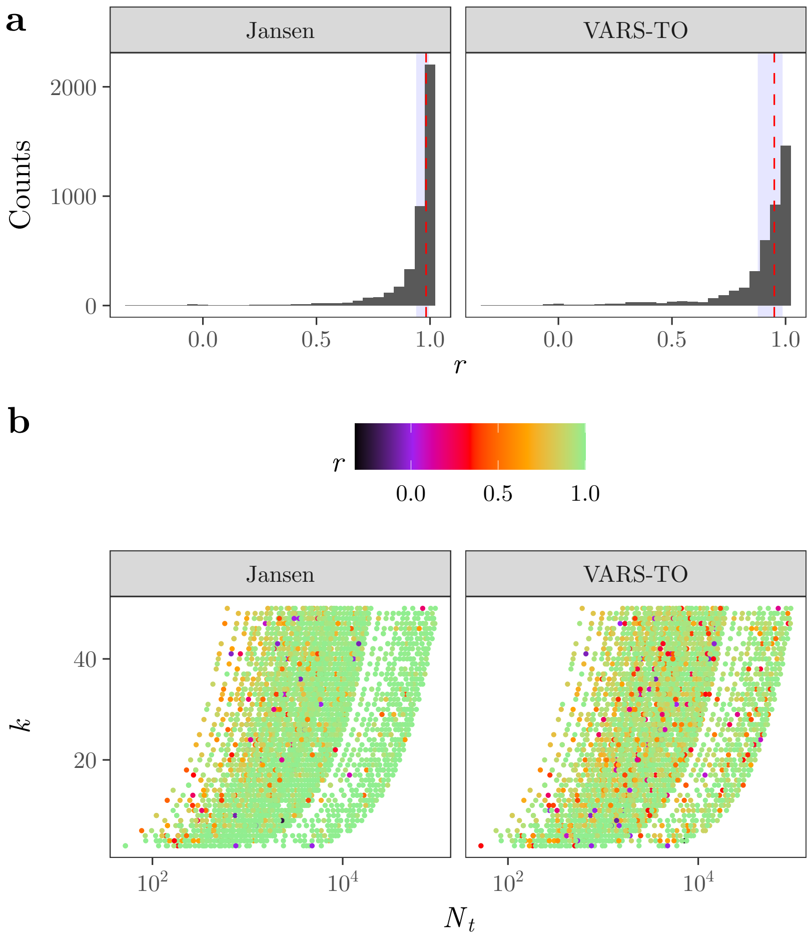


Figure 2: Scatterplots of the total number of model runs N_t against the function dimensionality k. The greener (darker) the colour, the better (worse) the performance.

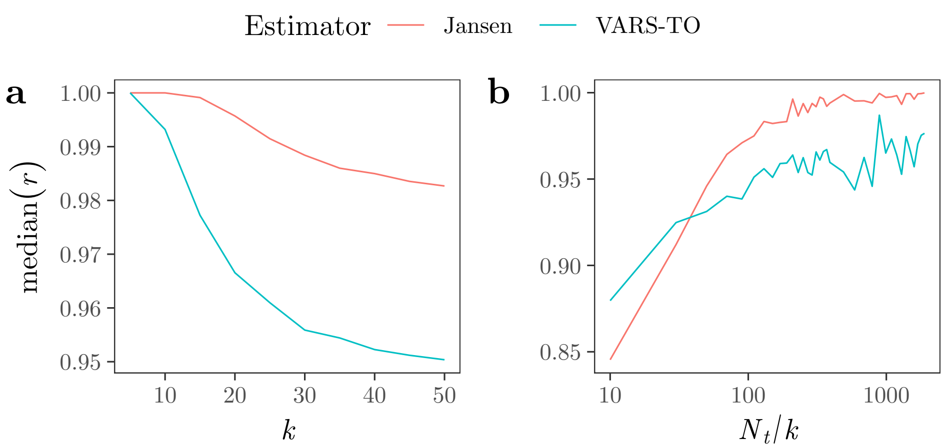
```
# MERGE PLOTS ---------------------------------------------------------------------

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))]
```

```r
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)
```



7 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),
                       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 = "",
```

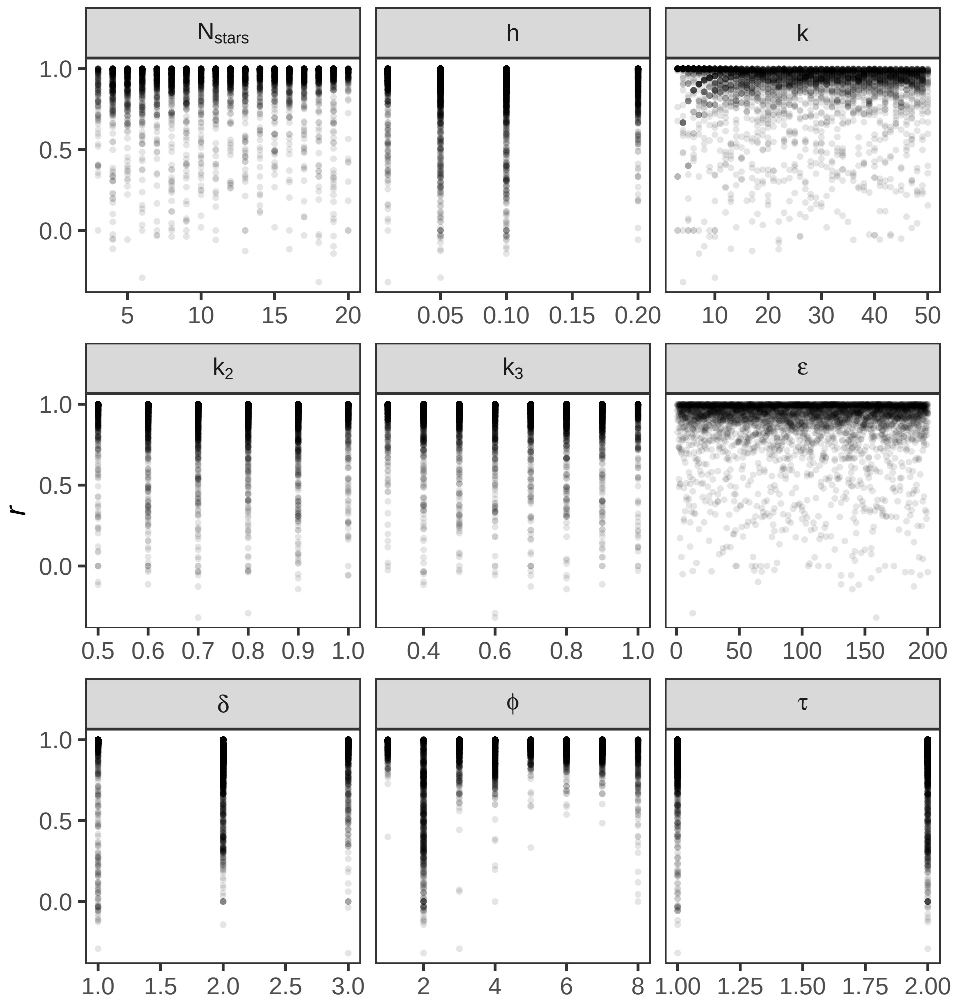


Figure 3: Scatterplots of model output r against the model inputs.

```r
       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")
```

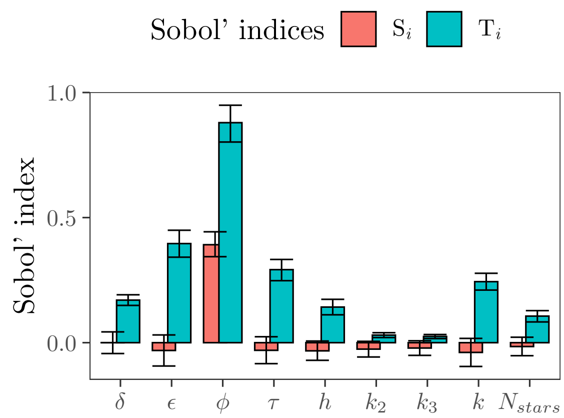


Figure 4: Sobol' indices.

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

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

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

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] checkpoint_0.4.9   Rfast_1.9.9        RcppZiggurat_0.1.5 Rcpp_1.0.5
##  [5] benchmarkme_1.0.4  logitnorm_0.8.37   cowplot_1.0.0      scales_1.1.1
##  [9] pcaPP_1.9-73       doParallel_1.0.15  iterators_1.0.12   foreach_1.5.0
## [13] data.table_1.12.8  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] fs_1.4.2              lubridate_1.7.9       httr_1.4.2
##  [4] tools_3.6.3           backports_1.1.8       R6_2.4.1
##  [7] DBI_1.1.0             colorspace_1.4-1      withr_2.2.0
## [10] tidyselect_1.1.0      curl_4.3              compiler_3.6.3
## [13] cli_2.0.2             rvest_0.3.6           xml2_1.3.2
## [16] labeling_0.3          mvtnorm_1.1-1         digest_0.6.25
## [19] rmarkdown_2.3         benchmarkmeData_1.0.4 pkgconfig_2.0.3
## [22] htmltools_0.5.0       bibtex_0.4.2.2        dbplyr_1.4.4
## [25] highr_0.8             rlang_0.4.7           readxl_1.3.1
## [28] rstudioapi_0.11       generics_0.0.2        farver_2.0.3
## [31] tikzDevice_0.12.3.1   jsonlite_1.7.0        magrittr_1.5
## [34] Matrix_1.2-18         munsell_0.5.0         fansi_0.4.1
## [37] lifecycle_0.2.0       stringi_1.4.6         yaml_2.2.1
## [40] gbRd_0.4-11           grid_3.6.3            blob_1.2.1
## [43] crayon_1.3.4          lattice_0.20-41       haven_2.3.1
## [46] hms_0.5.3             knitr_1.29            pillar_1.4.6
## [49] boot_1.3-25           randtoolbox_1.30.1    codetools_0.2-16
## [52] reprex_0.3.0          glue_1.4.1            evaluate_0.14
```

```
## [55] remotes_2.2.0         modelr_0.1.8          vctrs_0.3.2
## [58] png_0.1-7             Rdpack_1.0.0          cellranger_1.1.0
## [61] gtable_0.3.0          assertthat_0.2.1      xfun_0.16
## [64] broom_0.7.0           rngWELL_0.10-6        filehash_2.4-2
## [67] tinytex_0.25          ellipsis_0.3.1
```

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

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

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

```
## Num cores:
## [1] 8
```

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

```
## Num threads:
## [1] 8
```