

The battle of total-order sensitivity estimators

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```

# 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("Rcpp", "RcppArmadillo", "tidyverse", "parallel", "foreach",
              "doParallel", "Rfast", "data.table", "scales", "cowplot",
              "benchmarkme", "logitnorm", "sensobol", "ggrepel"))

# 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("2020-01-23",
           R.version ="3.6.1",
           checkpointLocation = getwd())

```

1 Functions

1.1 Savage scores

```
# 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)  
}
```

1.2 Sensitivity indices

```
# VARS FUNCTIONS -----  
  
vars_matrices <- function(star.centers, params, h) {  
  out <- center <- sections <- A <- B <- AB <- X <- out <- list()  
  mat <- randtoolbox::sobol(n = star.centers, dim = length(params))  
  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] # Remove zeroes  
    })  
    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))  
}  
  
# 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)
}

# Function to compute VARS-TI
vars_ti <- function(Y, star.centers, params, h) {
  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", ]
  }
  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])])
    }))
  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)
}

# COMPUTATION OF SOBOL' Ti INDICES -----
sobol_Ti <- function(d, N, params, total) {
  m <- matrix(d, nrow = N)
  k <- length(params)
  if(total == "jansen" | total == "homma" | total == "sobol" | total == "monod" |
    total == "glen") {
    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)
  }
}

```

```

# VY <- 1 / length(Y_A) * (sum(Y_A ^ 2) -
# (1 / N * sum(Y_A ^ 2))) ((Variance used by Becker))
}
if(total == "jansen") {
  Ti <- (1 / (2 * N) * Rfast::colsums((Y_A - Y_AB) ^ 2)) / VY
} else if(total == "homma") {
  Ti <- (VY - (1 / N) * Rfast::colsums(Y_A * Y_AB) + f0 ^ 2) / VY
} else if(total == "sobol") {
  Ti <- ((1 / N) * Rfast::colsums(Y_A * (Y_A - Y_AB))) / VY
} else if(total == "monod") {
  Ti <- 1 - (1 / N * Rfast::colsums(Y_A * Y_AB) -
    (1 / N * Rfast::colsums((Y_A + Y_AB) / 2)) ^ 2) /
    (1 / N * Rfast::colsums((Y_A ^ 2 + Y_AB ^ 2) / 2) -
      (1 / N * Rfast::colsums((Y_A + Y_AB) / 2)) ^ 2)
} else if(total == "glen") {
  Ti <- 1 - (1 / (N - 1) *
    Rfast::colsums(((Y_A - mean(Y_A)) * (Y_AB - Rfast::colmeans(Y_AB))) /
    sqrt(var(Y_A) * Rfast::colVars(Y_AB))))
}
if(total == "azzini" | total == "lamboni") {
  Y_A <- m[, 1]
  Y_B <- m[, 2]
  Y_AB <- m[, 3:(3 + k - 1)]
  Y_BA <- m[, (ncol(m) - k + 1):ncol(m)]
  f0 <- 1 / (2 * N) * sum(Y_A + Y_B)
  VY <- 1 / (2 * N - 1) * sum((Y_A - f0) ^ 2 + (Y_B - f0) ^ 2)
}
if(total == "azzini") {
  Ti <- 1 - abs(Rfast::colsums((Y_A - Y_BA) * (Y_B - Y_AB)) /
    (1 / 2 * Rfast::colsums((Y_A - Y_B) ^ 2 + (Y_AB - Y_BA) ^ 2)))
} else if(total == "lamboni") {
  Ti <- (1 / (4 * N) * colSums((Y_A - Y_AB) ^ 2 + (Y_B - Y_BA) ^ 2, na.rm = TRUE)) / VY
}
if(total == "owen") {
  Y_A <- m[, 1]
  Y_B <- m[, 2]
  Y_BA <- m[, 3:(3 + k - 1)]
  Y_CB <- m[, (ncol(m) - k + 1):ncol(m)]
  VY <- sapply(1:k, function(j)
    mean(Rfast::rowmeans(m[,c(1, 2, 2 + j, 2 + j + k)] ^ 2)) -
    mean(Rfast::rowmeans(m[,c(1, 2, 2 + j, 2 + j + k)])) ^ 2)
  Ti <- (VY - (1 / N * Rfast::colsums((Y_B - Y_CB) * (Y_BA - Y_A)))) / VY
}
output <- data.table(Ti)
output[, `:=` (parameters = paste("X", 1:k, sep = ""))]
return(output)
}

```

```

# CHECK THAT ALL TI ESTIMATORS WORK ----

# Settings
estimators <- c("jansen", "sobol", "homma", "azzini", "monod", "lamboni", "glen", "owen")
test_functions <- c("Ishigami", "Sobol'G", "Morris")
N <- 2 ^ 11

# Run model
ind <- Y <- mt <- list()
for(i in estimators) {
  for(j in test_functions) {
    if(i == "jansen" | i == "sobol" | i == "homma" | i == "monod" | i == "glen") {
      matrices <- c("A", "AB")
    } else if(i == "azzini" | i == "lamboni"){
      matrices <- c("A", "B", "AB", "BA")
    } else if(i == "owen") {
      matrices <- c("A", "B", "BA", "CB")
    }
    if(j == "Ishigami") {
      k <- 3
      modelRun <- sensobol::ishigami_Fun
    } else if(j == "Sobol'G") {
      k <- 8
      modelRun <- sensobol::sobol_Fun
    } else if(j == "Morris") {
      k <- 20
      modelRun <- sensitivity::morris.fun
    }
    mt[[i]][[j]] <- sobol_matrices(N = N, params = paste("X", 1:k, sep = ""), matrices = matrices)
    Y[[i]][[j]] <- modelRun(mt[[i]][[j]])
    ind[[i]][[j]] <- sobol_Ti(d = Y[[i]][[j]], params = paste("X", 1:k, sep = ""),
                                N = N, total = i)
  }
}

## Registered S3 method overwritten by 'sensitivity':
##   method     from
##   print.src  dplyr

# Run model for VARS
star.centers <- 200
h <- 0.2
vars.ind <- Y <- list()
for(j in test_functions) {
  if(j == "Ishigami") {
    k <- 3
    modelRun <- sensobol::ishigami_Fun
  } else if(j == "Sobol'G") {

```

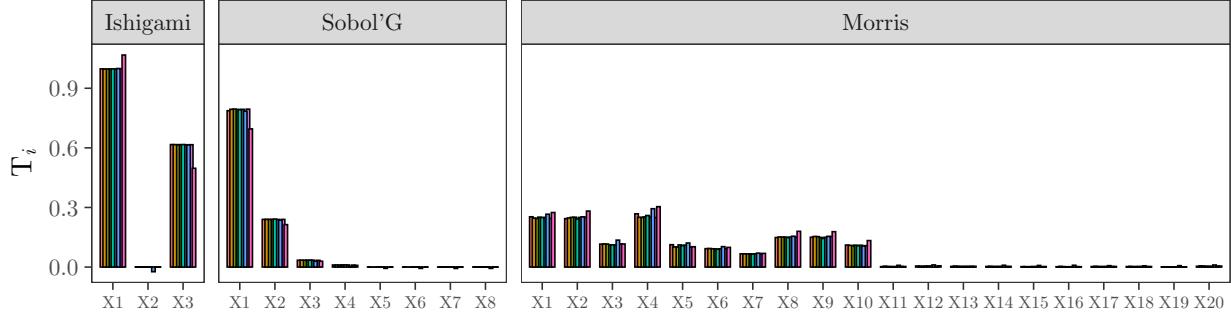
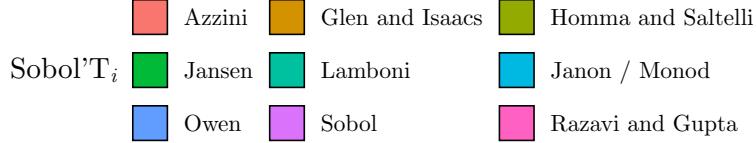
```

k <- 8
modelRun <- sensobol::sobol_Fun
} else if(j == "Morris") {
  k <- 20
  modelRun <- sensitivity::morris.fun
}
mt[[j]] <- vars_matrices(star.centers = star.centers,
                         params = paste("X", 1:k, sep = ""),
                         h = h)
Y[[j]] <- modelRun(mt[[j]])
vars.ind[[j]] <- vars_ti(Y = Y[[j]], star.centers = star.centers,
                         params = paste("X", 1:k, sep = ""), h = h)
}

vars.ind <- rbindlist(vars.ind, idcol = "Function")[
  , estimator:= "vars"] %>%
  setcolororder(., c("estimator", "Function", "Ti", "parameters"))

# PLOT SENSITIVITY INDICES -----
lapply(ind, function(x) rbindlist(x, idcol = "Function")) %>%
  rbindlist(., idcol = "estimator") %>%
  rbind(vars.ind) %>%
  .[, parameters:= factor(parameters, levels = paste("X", 1:20, sep = ""))] %>%
  .[, Function:= factor(Function, levels = test_functions)] %>%
  ggplot(., aes(parameters, Ti, fill = estimator)) +
  geom_bar(stat = "identity",
            position = position_dodge(0.7),
            color = "black") +
  scale_fill_discrete(name = expression(paste("Sobol' ", T[italic(i)])),
                      labels = c("Azzini", "Glen and Isaacs", "Homma and Saltelli",
                                "Jansen", "Lamboni", "Janon / Monod", "Owen",
                                "Sobol", "Razavi and Gupta")) +
  facet_grid(~Function,
            scales = "free_x",
            space = "free_x") +
  labs(x = "",
       y = expression(T[italic(i)])) +
  theme_AP() +
  theme(axis.text.x = element_text(size = 6.5),
        legend.position = "top") +
  guides(fill = guide_legend(nrow = 3,
                             byrow = TRUE))

```



2 The metafunction

```
# CREATE METAFUNCTION -----
function_list <- list(
  Linear = function(x) x,
  Quadratic = function(x) x ^ 2,
  Cubic = function(x) x ^ 3,
  Exponential = function(x) exp(1) ^ x / (exp(1) - 1),
  Periodic = function(x) sin(2 * pi * x) / 2,
  Discontinuous = function(x) ifelse(x > 0.5, 1, 0),
  Non.monotonic = function(x) 4 * (x - 0.5) ^ 2,
  Inverse = function(x) (10 - 1 / 1.1) ^ -1 * (x + 0.1) ^ -1,
  No.effect = function(x) x * 0,
  Trigonometric = function(x) cos(x)
)

# PLOT METAFUNCTION -----
a <- ggplot(data.frame(x = runif(100)), aes(x)) +
  map(1:length(function_list), function(nn) {
    stat_function(fun = function_list[[nn]],
                  geom = "line",
                  aes_(color = factor(names(function_list[nn])),
                       linetype = factor(names(function_list[nn]))))
  }) +
  labs(color= "Function", linetype = "Function",
       x = expression(italic(x)),
       y = expression(italic(y))) +
  theme_AP() +
  theme(legend.position = "right")

## Warning: `mapping` is not used by stat_function()
```

```

## Warning: `mapping` is not used by stat_function()

## Warning: `mapping` is not used by stat_function()
a

```

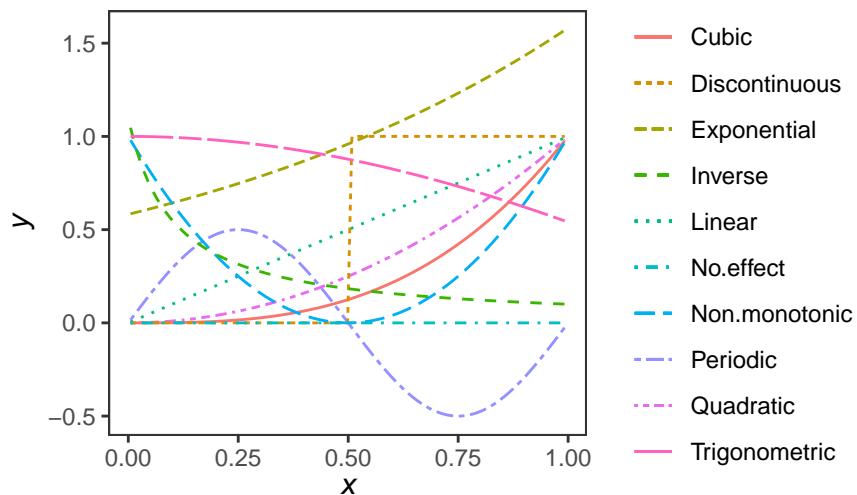


Figure 1: Functions used in the metafunction of Becker (2019).

```

# CREATE 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 <- 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)
}

# PLOT DISTRIBUTIONS -----
names_ff <- names(sample_distributions)
prove <- randtoolbox::sobol(n = 1000, dim = length(names_ff))

out <- data.table(sapply(seq_along(names_ff), function(x)
  sample_distributions[[names_ff[x]]])(prove[, x]))

b <- data.table::melt(out) %>%
  ggplot(., aes(value, group = variable, colour = variable)) +
  geom_density() +
  scale_color_discrete(labels = c("U(0, 1)",
                                    "N(0.5, 0.2)",
                                    "Beta(8, 2)",
                                    "Beta(2, 8)",
                                    "Beta(2, 0.5)",
                                    "Beta(0.5, 2)",
                                    "Logitnormal(0, 3.16)",
                                    name = ""))
  labs(x = expression(italic(x)),
       y = "Density") +
  theme_AP()

## Warning in melt.data.table(out): id.vars and measure.vars are internally
## guessed when both are 'NULL'. All non-numeric/integer/logical type columns are
## considered id.vars, which in this case are columns []. Consider providing at
## least one of 'id' or 'measure' vars in future.

b

# MERGE METAFUNCTION PLOT AND DISTRIBUTIONS PLOT -----
plot_grid(a, b, ncol = 1, labels = "auto", align = "hv")

```

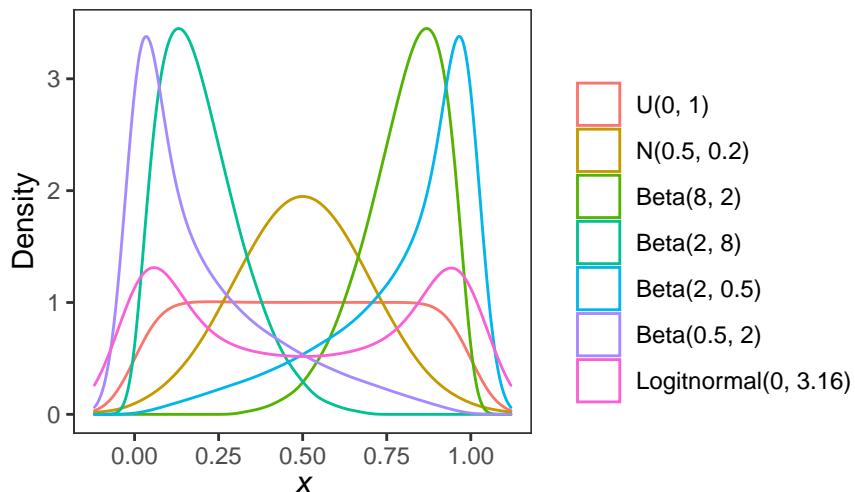
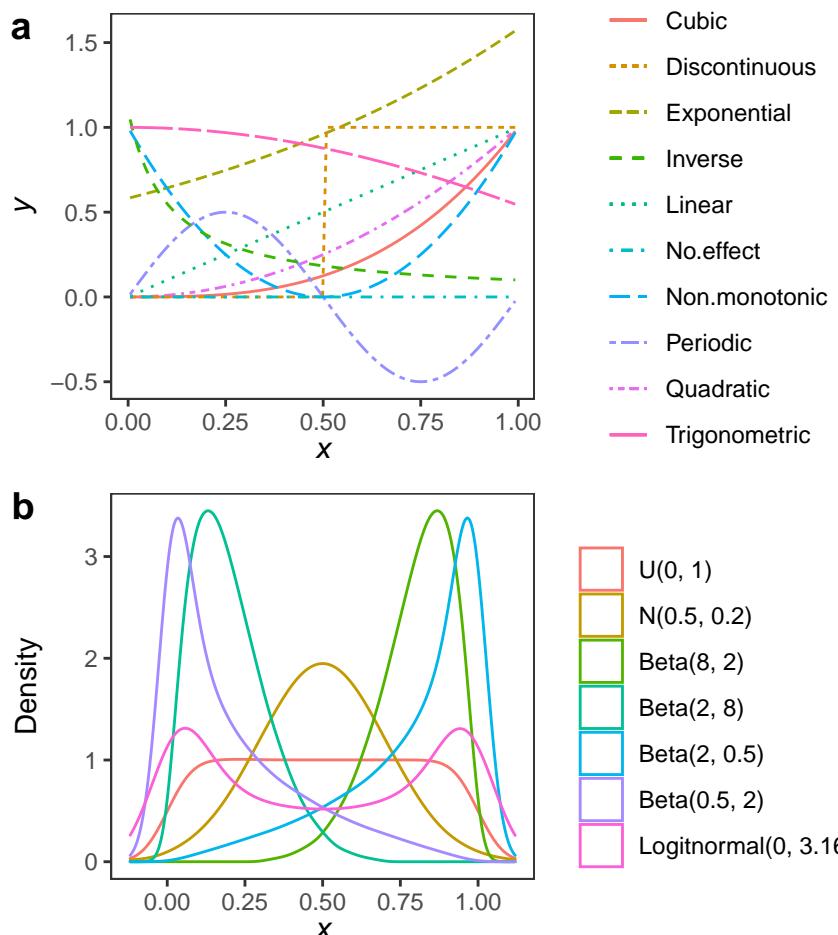


Figure 2: Distributions used in the metafunction of Becker (2019).



EXEMPLIFY THE METAFUNCTION WITH AN EXAMPLE -----

```

N <- 5000 # Sample size
R <- 100 # Number of bootstrap replications
k <- 55 # Number of model inputs

```

```

k_2 <- 0.5 # Fraction of active pairwise interactions
k_3 <- 0.3 # Fraction of active three-wise interactions
epsilon <- 5 # to reproduce the results
params <- paste("X", 1:k, sep = "")
A <- sobol_matrices(N = N, params = params)

# Compute
Y <- metafunction(data = A, k_2 = k_2, k_3 = k_3, epsilon = epsilon)
ind <- sobol_indices(Y = Y, N = N, params = params, R = R, boot = TRUE)

```

3 The model

3.1 Settings

```

# DEFINE SETTINGS -----
N <- 2 ^ 11 # Sample size of sample matrix
h <- 0.2 # step for VARS
R <- 500 # Number of bootstrap replicas
n_cores <- ceiling(detectCores() * 0.5)
order <- "second"
params <- c("k", "N_t", "k_2", "k_3", "epsilon", "phi", "delta")
N.high <- 2 ^ 11 # Maximum sample size of the large sample matrix

```

3.2 Sample matrix

```

# CREATE SAMPLE MATRIX -----
mat <- sobol_matrices(N = N, params = params, order = order)
mat[, 1] <- floor(qunif(mat[, 1], 3, 100)) # k
mat[, 2] <- floor(qunif(mat[, 2], 10, 1000)) # N_t
mat[, 3] <- round(qunif(mat[, 3], 0.3, 0.5), 2) # k_2
mat[, 4] <- round(qunif(mat[, 4], 0.1, 0.3), 2) # k_3
mat[, 5] <- floor(qunif(mat[, 5], 1, 200)) # Epsilon
mat[, 6] <- floor(mat[, 6] * (8 - 1 + 1)) + 1 # Phi
mat[, 7] <- floor(mat[, 7] * (3 - 1 + 1)) + 1 # Phi

colnames(mat) <- params

N.all <- apply(mat, 1, function(x) ceiling(x["N_t"] / (x["k"] + 1)))
N.azzini <- apply(mat, 1, function(x) ceiling(x["N_t"] / (2 * x["k"] + 2)))
N.vars <- apply(mat, 1, function(x) floor(x["N_t"] / ((x["k"] * ((1 / h) - 1) + 1))))
# N.vars <- apply(mat, 1, function(x) floor((x["N_t"] * h) / x["k"]))

tmp <- cbind(mat, N.all, N.azzini, N.vars)
sel <- c("N.all", "N.azzini", "N.vars")

```

```

mat <- as.matrix(data.table(tmp)[, (sel) := lapply(.SD, function(x)
  ifelse(x == 1 | x == 0, 2, x)), .SDcols = (sel)])

C.all <- apply(mat, 1, function(x) x["N.all"] * (x["k"] + 1))
C.azzini <- apply(mat, 1, function(x) x["N.azzini"] * (2 * x["k"] + 2))
C.vars <- apply(mat, 1, function(x) x["N.vars"] * (x["k"] * ((1 / h) - 1) + 1))

mat <- cbind(mat, C.all, C.azzini, C.vars)

```

3.3 Define the model

```

# DEFINE MODEL ----

model_Ti <- function(k, N.all, N.azzini, N.vars, h,
                      N.high, k_2, k_3, epsilon, phi, delta) {
  ind <- list()
  estimators <- c("jansen", "sobol", "homma", "monod", "azzini",
                  "lamboni", "glen", "owen", "vars")
  all.but.azzini <- sobol_matrices(N = N.all, params = paste("X", 1:k, sep = ""),
                                    matrices = c("A", "AB"))
  azzini <- sobol_matrices(N = N.azzini, params = paste("X", 1:k, sep = ""),
                           matrices = c("A", "B", "AB", "BA"))
  owen.matrix <- sobol_matrices(N = N.azzini, params = paste("X", 1:k, sep = ""),
                                 matrices = c("A", "B", "BA", "CB"))
  vars.matrix <- vars_matrices(star.centers = N.vars, params = paste("X", 1:k, sep = ""),
                                h = h)
  large.matrix <- sobol_matrices(N = N.high, params = paste("X", 1:k, sep = ""),
                                  matrices = c("A", "AB"))
  set.seed(epsilon)
  all.matrices <- random_distributions(X = rbind(all.but.azzini, azzini,
                                                   owen.matrix, vars.matrix,
                                                   large.matrix),
                                         phi = phi)
  output <- sensobol::metafunction(data = all.matrices,
                                    k_2 = k_2,
                                    k_3 = k_3,
                                    epsilon = epsilon)
  full.ind <- sobol_Ti(d = tail(output, nrow(large.matrix)),
                        N = N.high,
                        params = paste("X", 1:k, sep = ""),
                        total = "jansen")
  full.ind[, sample.size := "N"]

  # Define indices of Y for estimators
  Nt.all.but.azzini <- N.all * (k + 1)
  Nt.azzini.owen <- N.azzini * ((2 * k) + 2)

```

```

Nt.vars <- N.vars * (k * ((1 / h) - 1) + 1)
lg.all.but.azzini <- 1:Nt.all.but.azzini
lg.azzini <- (length(lg.all.but.azzini) + 1):(length(lg.all.but.azzini) + Nt.azzini.owen)
lg.owen <- (max(lg.azzini) + 1):(max(lg.azzini) + Nt.azzini.owen)
lg.vars <- (max(lg.owen) + 1):(max(lg.owen) + Nt.vars)

for(i in estimators) {
  if(i == "jansen" | i == "sobol" | i == "homma" | i == "monod" | i == "glen") {
    y <- output[lg.all.but.azzini]
    n <- N.all
  } else if(i == "azzini" | i == "lamboni") {
    y <- output[lg.azzini]
    n <- N.azzini
  } else if(i == "owen") {
    y <- output[lg.owen]
    n <- N.azzini
  } else if(i == "vars") {
    y <- output[lg.vars]
    star.centers <- N.vars
  }
  if(!i == "vars") {
    ind[[i]] <- sobol_Ti(d = y, N = n, params = paste("X", 1:k, sep = ""), total = i)
  }
  if(i == "vars") {
    ind[[i]] <- vars_ti(Y = y, star.centers = star.centers,
                           params = paste("X", 1:k, sep = ""), h = h)
  }
  ind[[i]][, sample.size:= "n"]
  ind[[i]] <- rbind(ind[[i]], full.ind)
}
# Arrange data
out <- rbindlist(ind, idcol = "estimator")
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)
# Replace 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)
}

```

3.4 Run 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", "pcaPP",
                               "logitnorm", "dplyr")) %dopar%
{
  model_Ti(k = mat[[i, "k"]],
            k_2 = mat[[i, "k_2"]],
            k_3 = mat[[i, "k_3"]],
            epsilon = mat[[i, "epsilon"]],
            phi = mat[[i, "phi"]],
            delta = mat[[i, "delta"]],
            N.all = mat[[i, "N.all"]],
            N.azzini = mat[[i, "N.azzini"]],
            N.vars = mat[[i, "N.vars"]],
            N.high = N.high,
            h = h)
}

# Stop parallel cluster
stopCluster(cl)

```

3.5 Arrange output

```

# 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 == "azzini" | estimator == "lamboni"

```

```

| estimator == "owen", N.azzini * (2 * k + 2),
ifelse(estimator == "vars", N.vars * (k * ((1 / h) -1) + 1), N.all * (k + 1))
[, estimator:= ifelse(estimator %in% "azzini", "Azzini and Rosati",
ifelse(estimator %in% "homma", "Homma and Saltelli",
ifelse(estimator %in% "monod", "Janon/Monod",
ifelse(estimator %in% "jansen", "Jansen",
ifelse(estimator %in% "glen", "Glen and Isaac",
ifelse(estimator %in% "lamboni", "Lamboni",
ifelse(estimator %in% "owen", "Owen",
ifelse(estimator %in% "vars"
"Sobol'"))))))]) %>%
[, ratio:= Nt / k]

# Define A matrix
A <- full_output[, .SD[1:N], estimator]

# EXPORT OUTPUT -----
fwrite(A, "A.csv")
fwrite(full_output, "full_output.csv")

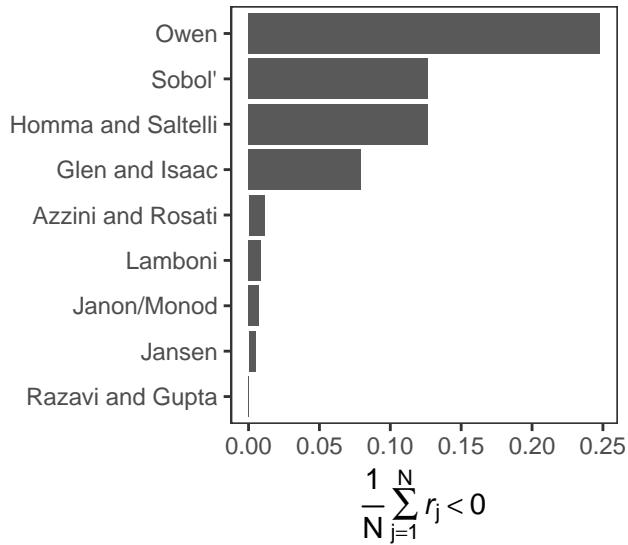
```

4 Uncertainty analysis

```

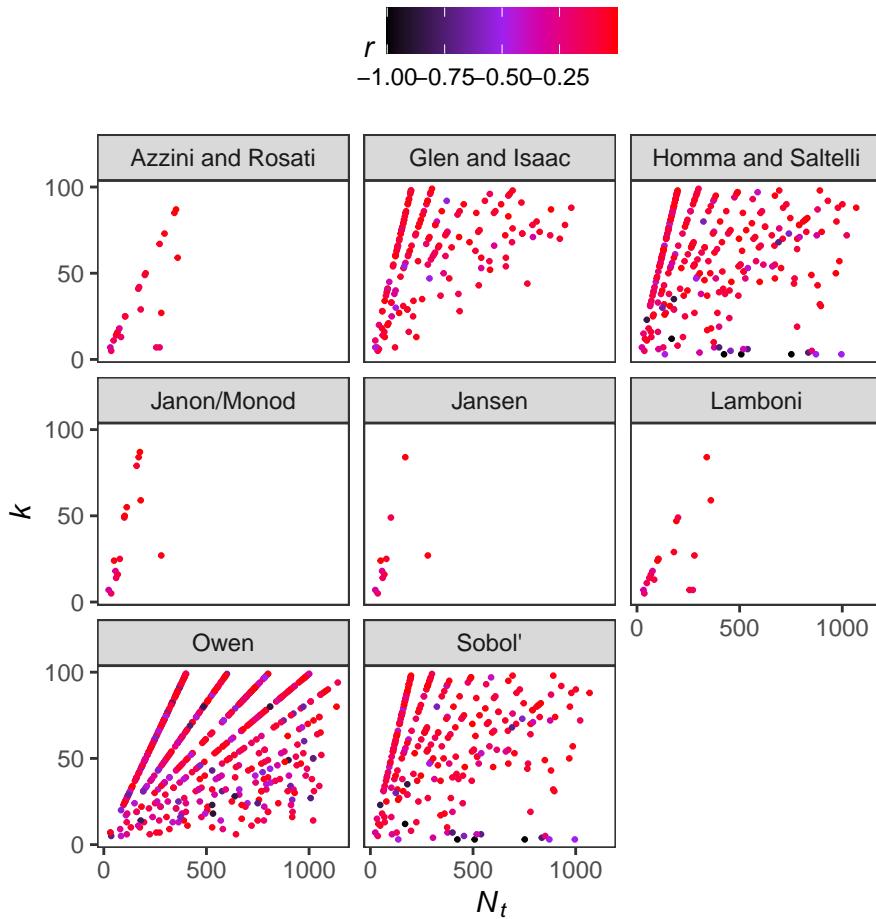
# PLOT PROPORTION OF NEGATIVE VALUES -----
A[, sum(correlation < 0)/ .N, estimator] %>%
ggplot(., aes(reorder(estimator, V1), V1)) +
geom_bar(stat = "identity") +
coord_flip() +
labs(y = expression(frac(1, N)^sum(italic(r)[j] < 0, j==1, N)),
x = "") +
theme_AP()

```



```
# MAP VALUES WITH NEGATIVE R -----
index.neg <- A[, .I[correlation < 0]]

A[index.neg] %>%
  ggplot(., aes(Nt, k, color = correlation)) +
  geom_point(size = 0.5) +
  scale_colour_gradientn(colours = c("black", "purple", "red"),
                         name = expression(italic(r))) +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  labs(x = expression(italic(N[t])),
       y = expression(italic(k))) +
  facet_wrap(~estimator) +
  theme_AP() +
  theme(legend.position = "top")
```



PLOT OUTPUT -----

```

# 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:          Owen 0.1952707 0.0000000 0.4828150
## 2:         Sobol' 0.3125050 0.1039631 0.5867431
## 3: Homma and Saltelli 0.3128686 0.1042273 0.5867431
## 4:     Glen and Isaac 0.3375124 0.1261882 0.6229799
## 5: Azzini and Rosati 0.6385908 0.4015177 0.8462274
## 6:        Lamboni 0.6652399 0.4407569 0.8695652
## 7: Janon/Monod 0.8000000 0.5916509 0.9318265
## 8:       Jansen 0.8071220 0.6040774 0.9386104
## 9: Razavi and Gupta 0.9336505 0.8512948 0.9798027

```

```

a <- 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 = 3) +
  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() +
  theme(axis.text.x = element_text(angle = 45, hjust = 1))

# Scatterplot
b <- ggplot(A, aes(Nt, k, color = correlation)) +
  geom_point(size = 0.1) +
  scale_colour_gradientn(colours = c("black", "purple", "red", "orange", "lightgreen"),
                         name = expression(italic(r))) +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  labs(x = expression(italic(N[t])),
       y = expression(italic(k))) +
  facet_wrap(~estimator,
             ncol = 3) +
  theme_AP() +
  theme(legend.position = "top")

# Ratio
c <- ggplot(A, aes(ratio, correlation)) +
  geom_point(alpha = 0.1, size = 0.2) +
  facet_wrap(~estimator,
             ncol = 3) +
  geom_smooth() +
  labs(x = expression(italic(N[t]/k)),
       y = expression(italic(r))) +
  scale_x_log10() +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +

```

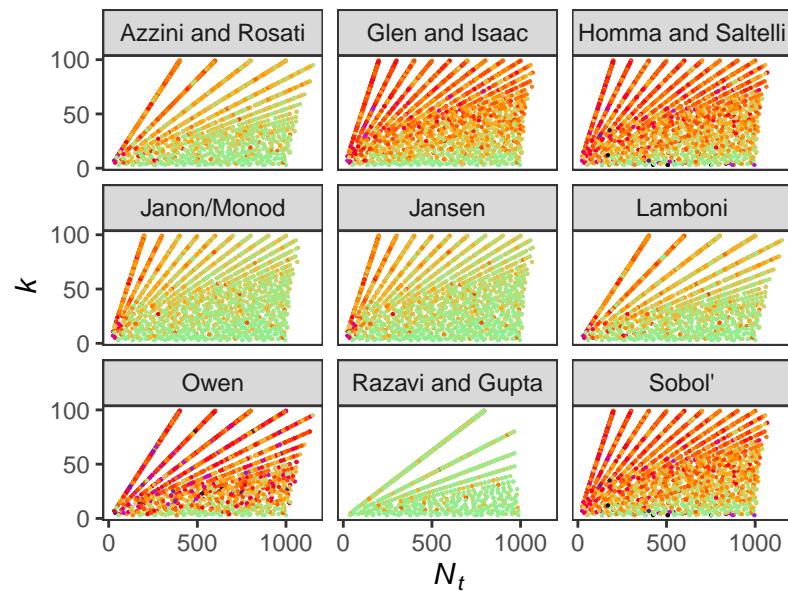
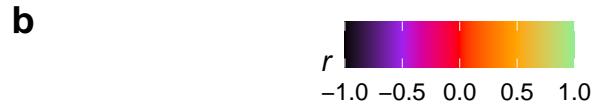
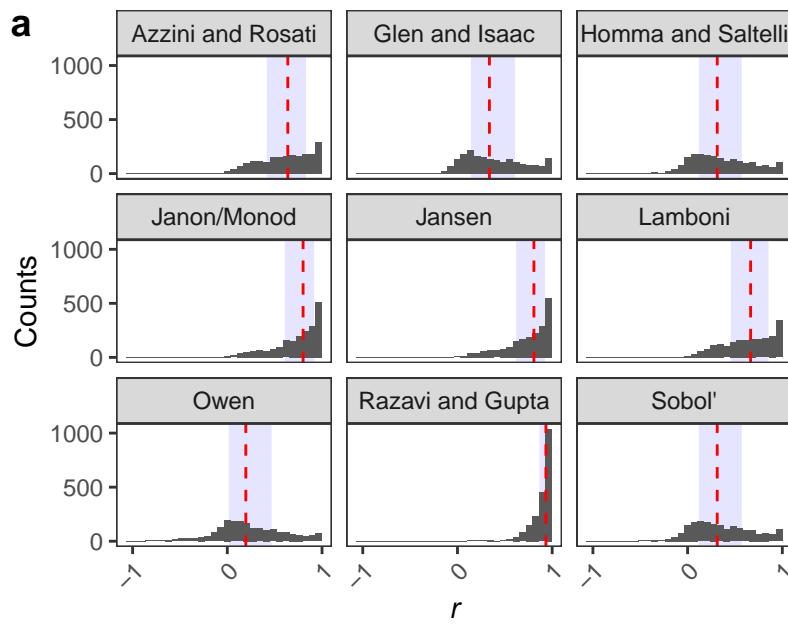
```

theme_AP()

# Merge plot
plot_grid(a, b, ncol = 1, labels = "auto", rel_heights = c(0.85, 1))

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

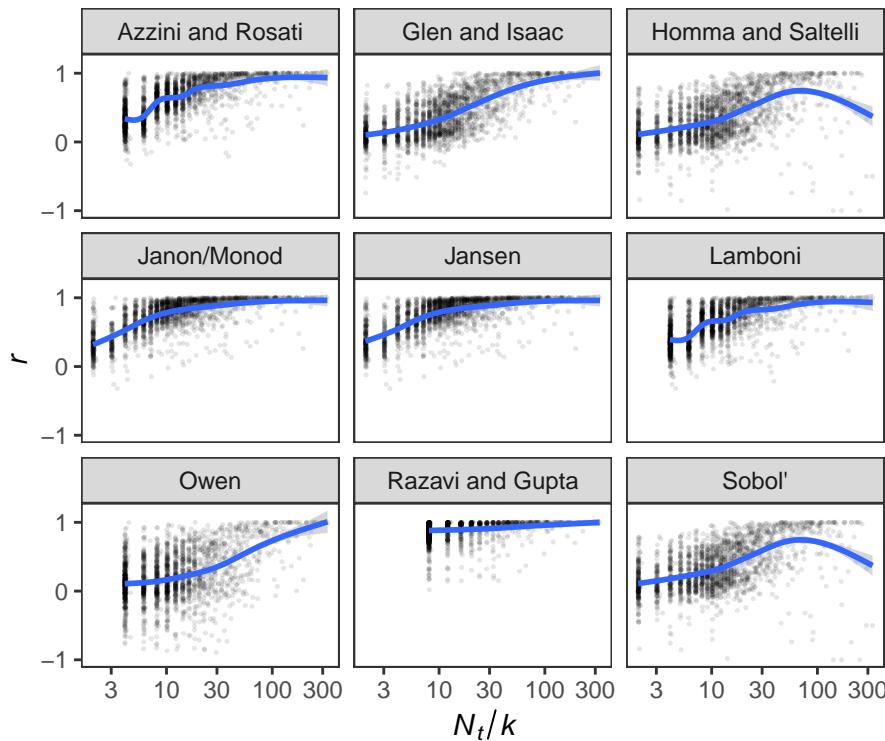
```



```
# DISPLAY THE RATIO NT/K FOR EACH SIMULATION AND ESTIMATOR -----
```

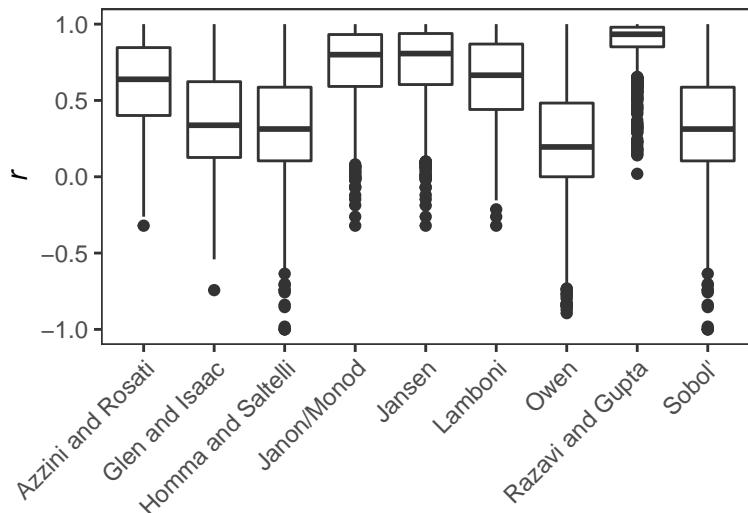
c

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```



PLOT BOXPLOT -----

```
ggplot(A, aes(estimator, correlation)) +
  geom_boxplot() +
  labs(x = "",
       y = expression(italic(r))) +
  theme_AP() +
  theme(axis.text.x = element_text(angle = 45, hjust = 1))
```



```

# PLOT MEDIANS ----

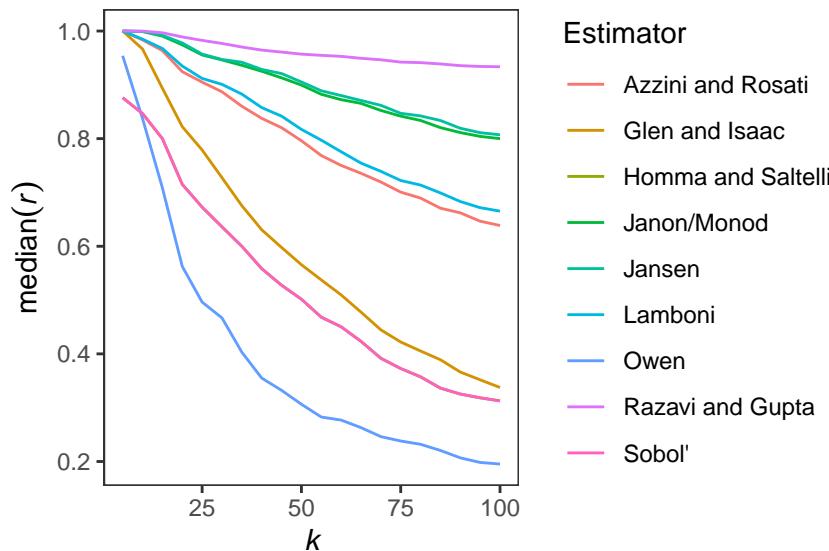
# Median k
vv <- seq(5, 100, 5)

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

names(dt) <- vv

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()

```



```

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

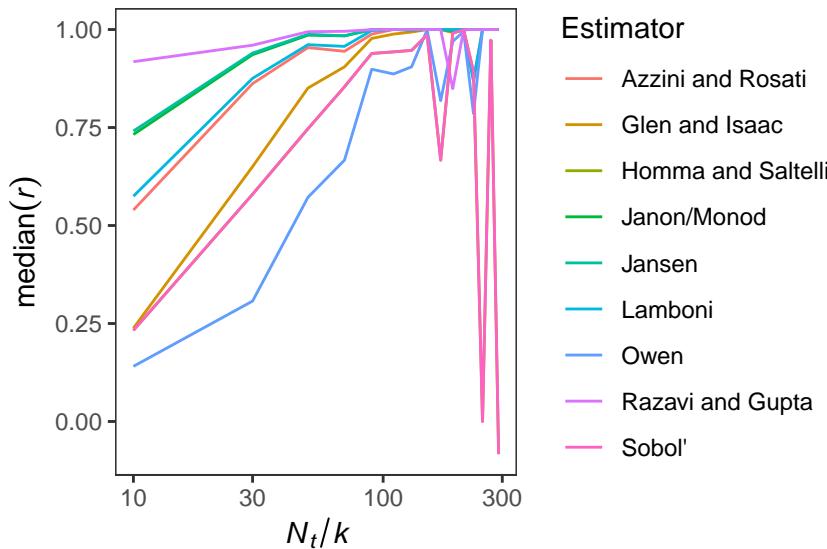
v <- seq(0, ceiling(dt.tmp$max), 20)
a <- c(v[1], rep(v[-c(1, length(v))], each = 2), v[length(v)])
indices <- matrix(a, ncol = 2 ,byrow = TRUE)

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

names(out) <- rowmeans(indices)

```

```
# Plot
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 = expression(median(italic(r)))) +
  scale_color_discrete(name = "Estimator") +
  scale_x_log10() +
  theme_AP()
```



5 Sensitivity analysis

5.1 Scatterplots

```
# SCATTERPLOTS OF MODEL OUTPUT AGAINST PARAMETERS -----
A <- setnames(A, c("N_t", "k_2", "k_3"), c("N[t]", "k[2]", "k[3]"))

scatter.dt <- melt(A, measure.vars = c("k", "N[t]", "k[2]", "k[3]",
                                         "epsilon", "phi", "delta")) %>%
  split(., .$estimator)

gg <- list()
for(i in names(scatter.dt)) {
  gg[[i]] <- ggplot(scatter.dt[[i]], aes(value, correlation)) +
    geom_point(alpha = 0.1, size = 0.3) +
    facet_wrap(~ variable,
               scales = "free_x",
```

```

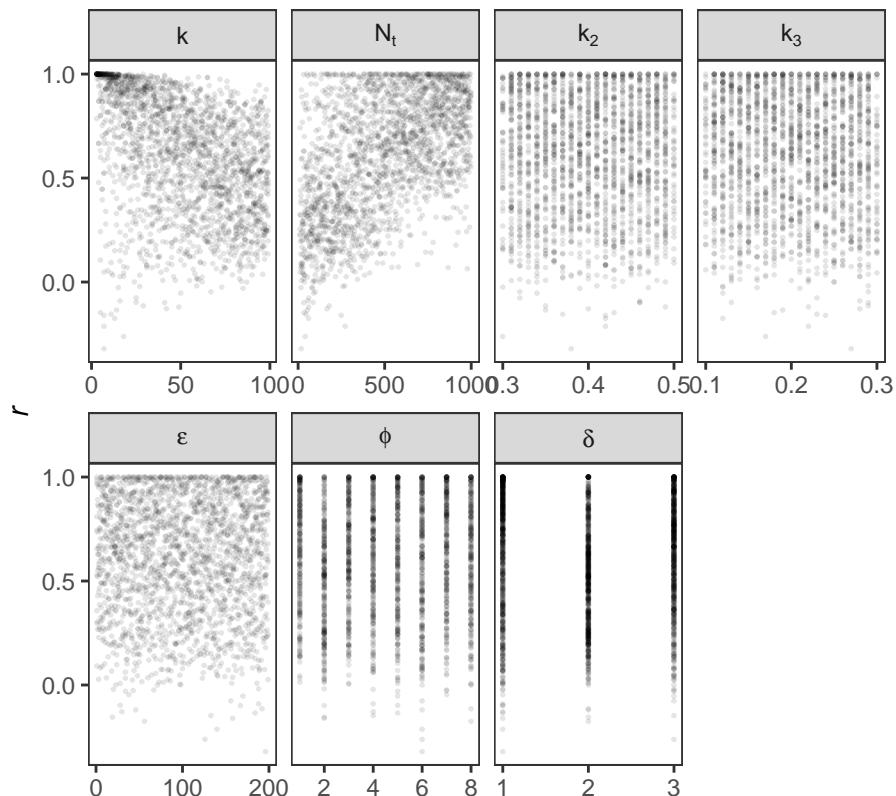
        labeller = label_parsed,
        ncol = 4) +
  scale_color_manual(values = c("#00BFC4", "#F8766D")) +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  theme_AP() +
  labs(x = "", y = expression(italic(r))) +
  theme() +
  ggtitle(names(scatter.dt[i]))
}

gg

```

\$`Azzini and Rosati`

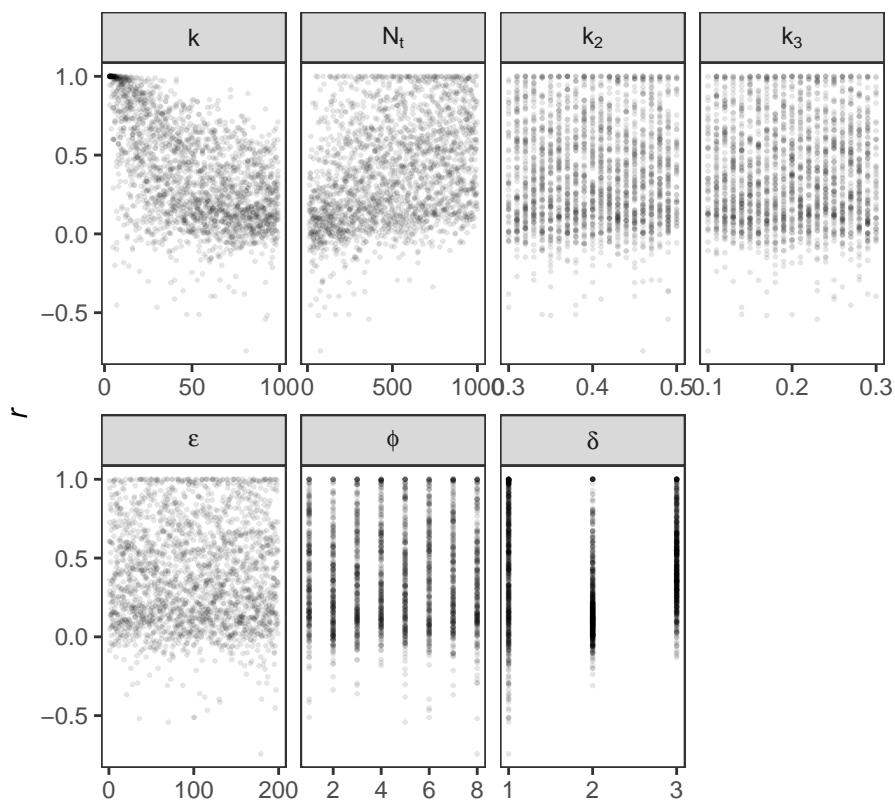
Azzini and Rosati



##

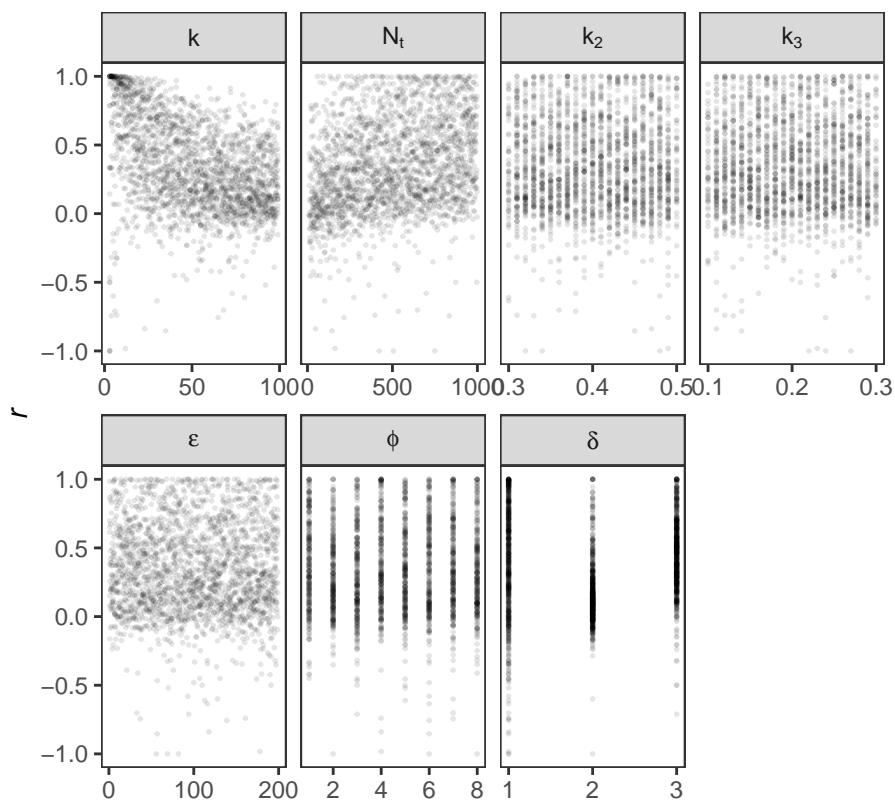
\$`Glen and Isaac`

Glen and Isaac



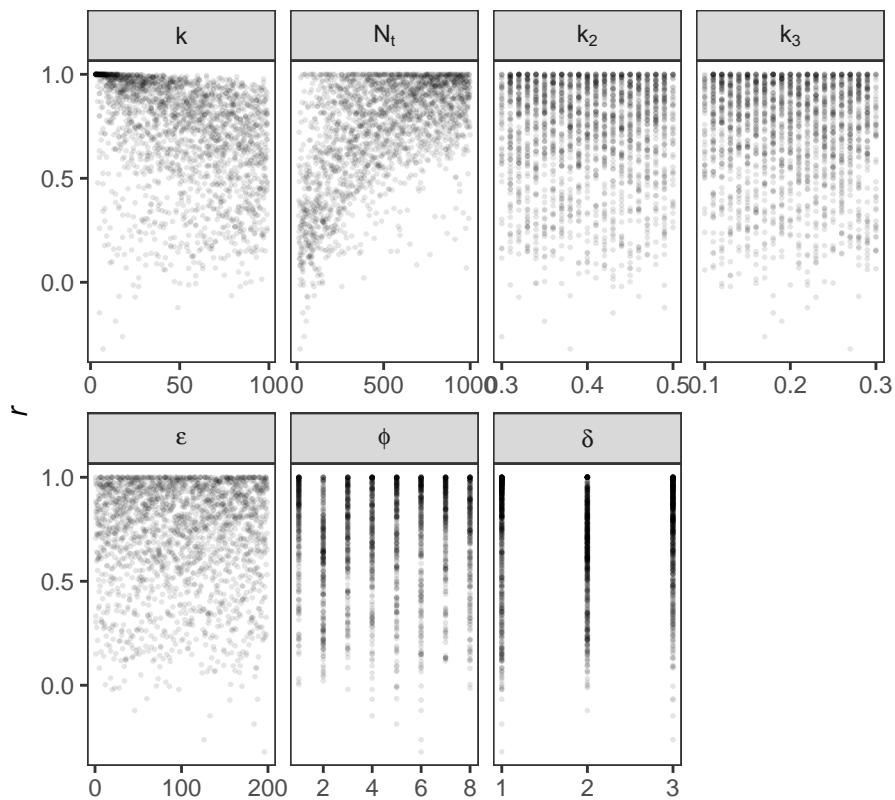
```
##  
## $`Homma and Saltelli`
```

Homma and Saltelli



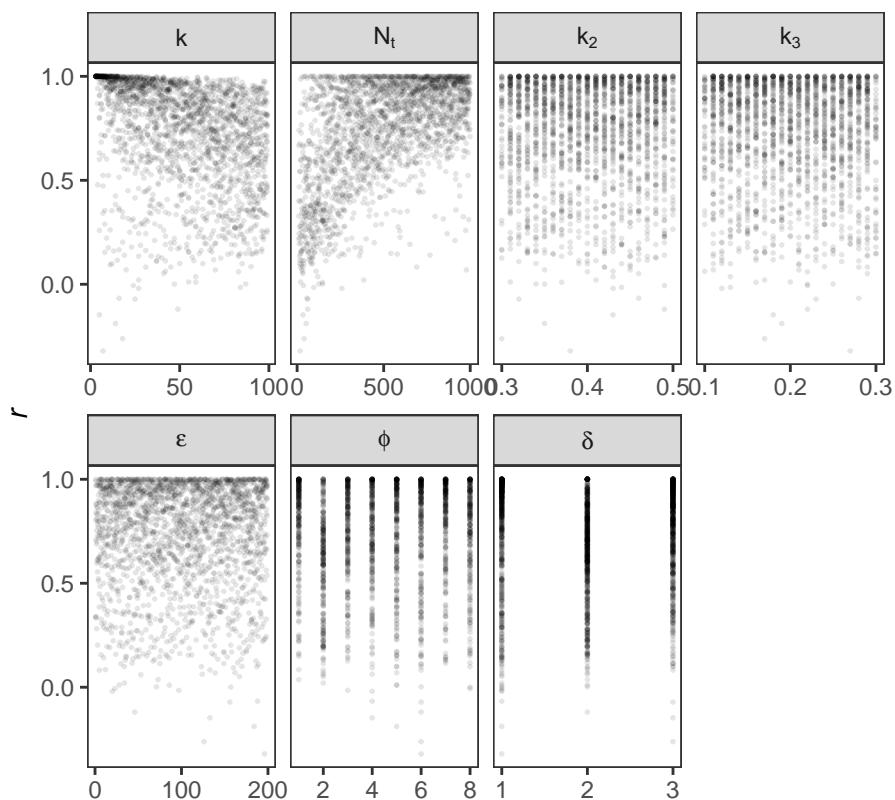
```
##  
## $`Janon/Monod`
```

Janon/Monod



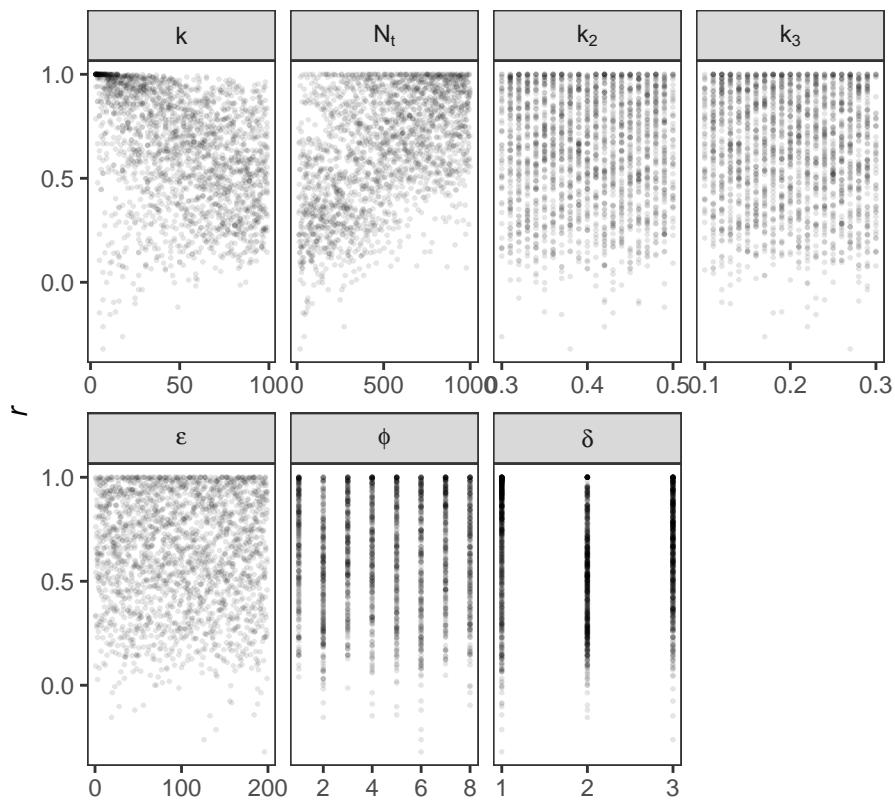
```
##  
## $Jansen
```

Jansen



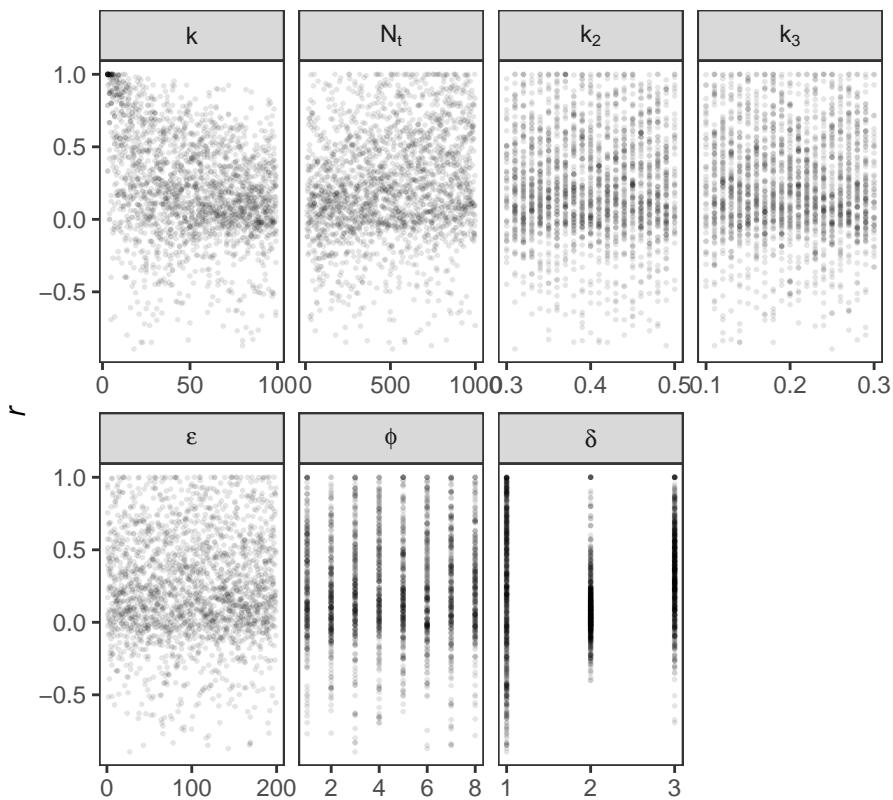
```
##  
## $Lamboni
```

Lamboni



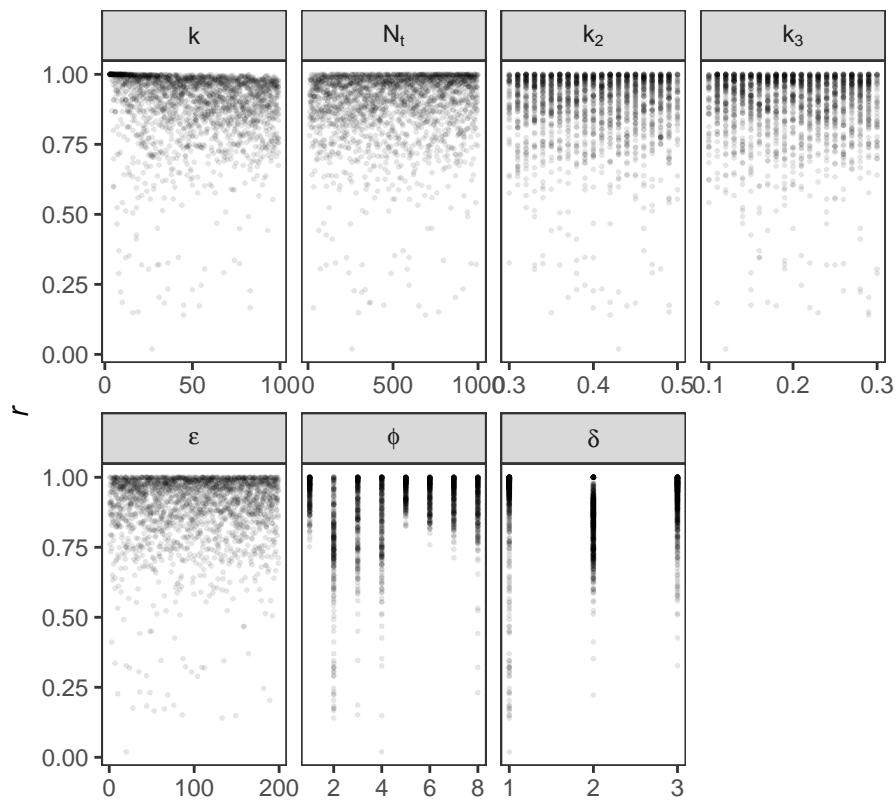
```
##  
## $Owen
```

Owen

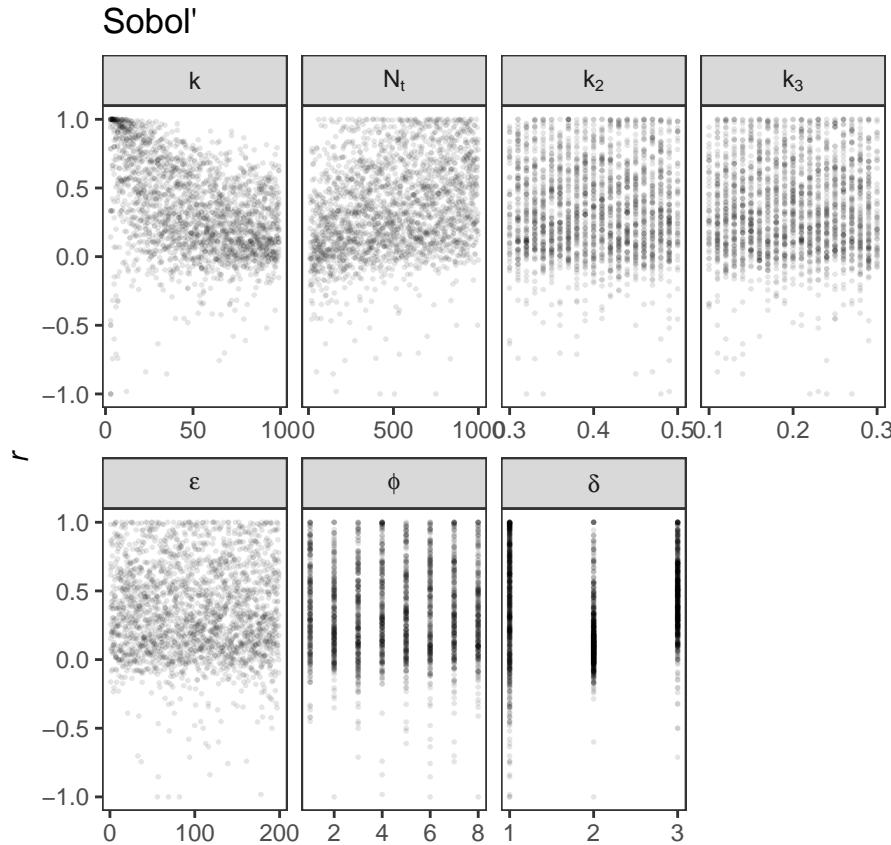


```
##  
## $`Razavi and Gupta`
```

Razavi and Gupta



```
##  
## $`Sobol`
```



5.2 Sobol' indices

```
# SENSITIVITY ANALYSIS -----
```

```
# Show rows with NA
```

```
full_output[is.na(correlation), ]
```

##	row	k	N_t	k_2	k_3	epsilon	phi	delta	N.all	N.azzini	N.vars	C.all	
## 1:	4164	9	33	0.46	0.29		167	2	1	4	2	2	40
## 2:	8032	7	27	0.46	0.22		37	3	3	4	2	2	32
## 3:	8032	7	27	0.46	0.22		37	3	3	4	2	2	32
## 4:	8032	7	27	0.46	0.22		37	3	3	4	2	2	32
## 5:	16063	5	725	0.44	0.27		152	4	3	121	61	34	726
## 6:	20056	16	87	0.39	0.22		119	4	2	6	3	2	102
## 7:	20056	16	87	0.39	0.22		119	4	2	6	3	2	102
## 8:	20056	16	87	0.39	0.22		119	4	2	6	3	2	102
## 9:	20548	9	33	0.45	0.29		167	2	1	4	2	2	40
## 10:	22596	9	33	0.46	0.26		167	2	1	4	2	2	40
## 11:	28740	9	33	0.46	0.29		167	2	1	4	2	2	40
## 12:	32608	7	27	0.34	0.22		37	3	3	4	2	2	32
## 13:	32608	7	27	0.34	0.22		37	3	3	4	2	2	32
## 14:	32608	7	27	0.34	0.22		37	3	3	4	2	2	32
## 15:	34656	7	27	0.46	0.15		37	3	3	4	2	2	32

```

## 16: 34656 7 27 0.46 0.15      37 3 3 4 2 2 32
## 17: 34656 7 27 0.46 0.15      37 3 3 4 2 2 32
## 18: 36592 9 53 0.39 0.15     169 5 3 6 3 2 60
## 19: 36592 9 53 0.39 0.15     169 5 3 6 3 2 60
## 20: 36592 9 53 0.39 0.15     169 5 3 6 3 2 60
## 21: 36704 7 27 0.46 0.22     34 3 3 4 2 2 32
## 22: 38591 5 896 0.44 0.27    152 4 3 150 75 42 900
## 23: 40800 7 27 0.46 0.22     37 3 1 4 2 2 32
## 24: 40800 7 27 0.46 0.22     37 3 1 4 2 2 32
## 25: 40800 7 27 0.46 0.22     37 3 1 4 2 2 32
## 26: 46783 5 725 0.31 0.27    152 4 3 121 61 34 726
## 27: 52927 5 725 0.44 0.26    152 4 3 121 61 34 726
## 28: 55840 7 26 0.45 0.24     70 8 3 4 2 2 32
## 29: 61119 5 725 0.44 0.27    152 4 2 121 61 34 726
##       row k N_t k_2 k_3 epsilon phi delta N.all N.azzini N.vars C.all
##       C.azzini C.vars           estimator correlation Nt      ratio
## 1:        40 74          Owen          NA 40 4.444444
## 2:        32 58 Azzini and Rosati    NA 32 4.571429
## 3:        32 58          Lamboni     NA 32 4.571429
## 4:        32 58          Owen        NA 32 4.571429
## 5:       732 714 Razavi and Gupta   NA 714 142.800000
## 6:       102 130 Azzini and Rosati  NaN 102 6.375000
## 7:       102 130          Lamboni   NaN 102 6.375000
## 8:       102 130          Owen      NaN 102 6.375000
## 9:        40 74          Owen        NA 40 4.444444
## 10:       40 74          Owen        NA 40 4.444444
## 11:       40 74          Owen        NA 40 4.444444
## 12:       32 58 Azzini and Rosati  NA 32 4.571429
## 13:       32 58          Lamboni   NA 32 4.571429
## 14:       32 58          Owen      NA 32 4.571429
## 15:       32 58 Azzini and Rosati  NA 32 4.571429
## 16:       32 58          Lamboni   NA 32 4.571429
## 17:       32 58          Owen      NA 32 4.571429
## 18:       60 74 Azzini and Rosati  NA 60 6.666667
## 19:       60 74          Lamboni   NA 60 6.666667
## 20:       60 74          Owen      NA 60 6.666667
## 21:       32 58          Owen      NA 32 4.571429
## 22:      900 882 Razavi and Gupta  NA 882 176.400000
## 23:       32 58 Azzini and Rosati  NA 32 4.571429
## 24:       32 58          Lamboni   NA 32 4.571429
## 25:       32 58          Owen      NA 32 4.571429
## 26:      732 714 Razavi and Gupta  NA 714 142.800000
## 27:      732 714 Razavi and Gupta  NA 714 142.800000
## 28:       32 58          Owen      NA 32 4.571429
## 29:      732 714 Razavi and Gupta  NaN 714 142.800000
##       C.azzini C.vars           estimator correlation Nt      ratio

```

```

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


# New vector of parameters to plot better
params.new <- c("k", "N[t]", "k[2]", "k[3]", "epsilon", "phi", "delta")

# Compute Sobol' indices
indices <- full_output[, sobol_indices(Y = correlation,
                                         N = N,
                                         params = params.new,
                                         first = "jansen",
                                         R = R,
                                         boot = TRUE,
                                         order = order),
                           estimator]

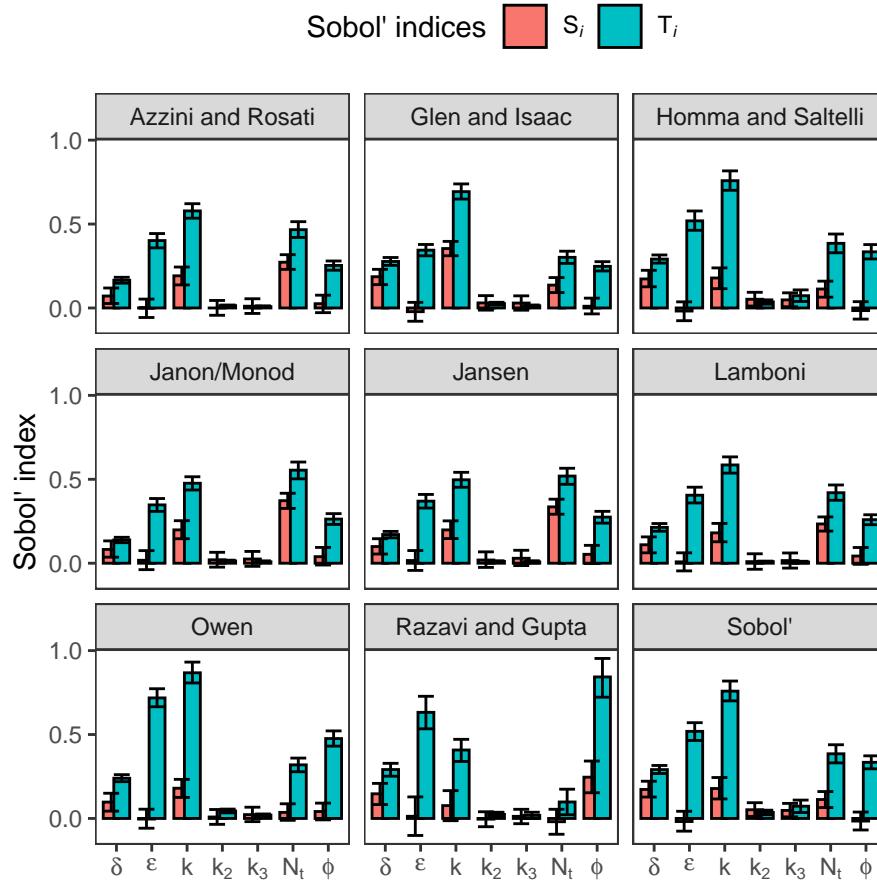
# Compute Sobol' indices for dummy parameter
indicesD <- full_output[, sobol_dummy(Y = correlation,
                                         N = N,
                                         params = params.new,
                                         boot = TRUE,
                                         R = R),
                           estimator]

# Export
fwrite(indices, "indices.csv")

# PLOT SOBOL' INDICES -----
# Reorder the levels of the parameters
ggplot(indices[sensitivity == "Si" |
               sensitivity == "Ti"], 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_x_discrete(labels = ggplot2:::parse_safe) +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  facet_wrap(~estimator,
             ncol = 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")
```



SUM OF FIRST-ORDER INDICES -----

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

```
##           estimator      V1
## 1: Azzini and Rosati 0.5722286
## 2:     Glen and Isaac 0.7243739
## 3: Homma and Saltelli 0.5307930
## 4:         Jansen 0.7510287
## 5:     Lamboni 0.6007199
## 6: Janon/Monod 0.7552958
## 7:       Owen 0.3834172
## 8:     Sobol' 0.5298899
## 9: Razavi and Gupta 0.4709970
```

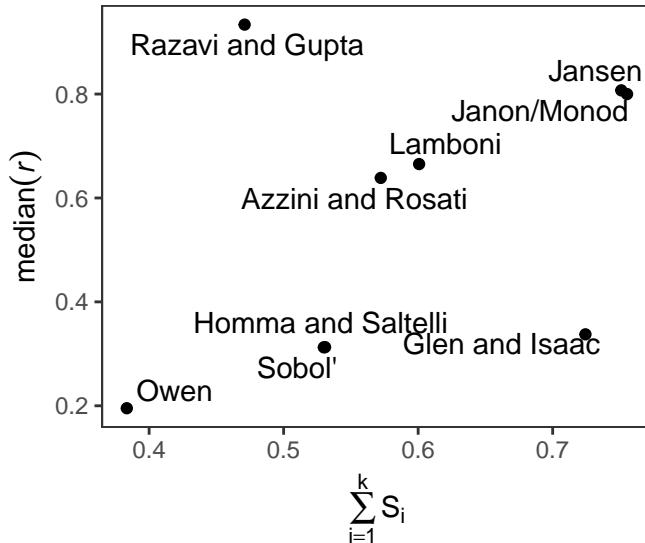
Plot

```
merge(indices[sensitivity == "Si", sum(original), estimator],
      dt_median, by = "estimator") %>%
  ggplot(., aes(V1, median)) +
  geom_point()
```

```

  labs(x = expression(sum(S[i], i==1, k)),
       y = expression(median(italic(r)))) +
  geom_text_repel(aes(label = estimator)) +
  theme_AP()

```

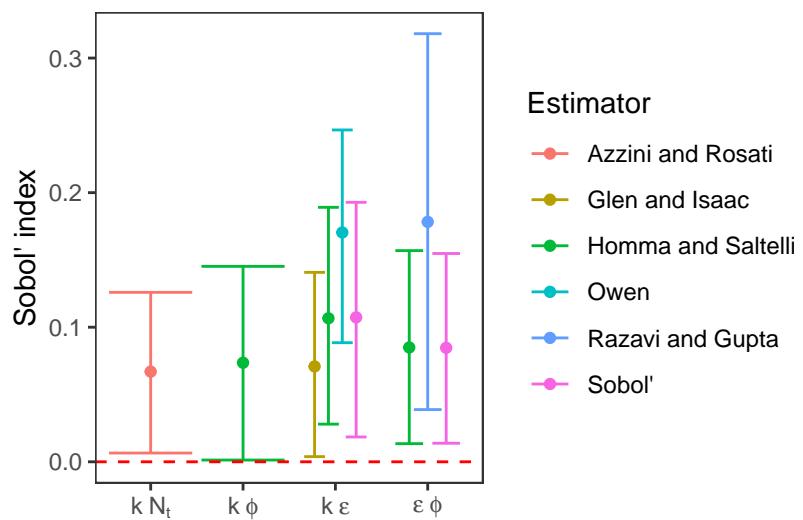


PLOT SECOND-ORDER EFFECTS -----

```

indices[sensitivity == "Sij"] %>%
  .[low.ci > 0] %>%
  .[, parameters := gsub(parameters,
                         pattern = ".",
                         replacement = "~",
                         fixed = TRUE)] %>%
  ggplot(., aes(reorder(parameters, original), original, color = estimator)) +
  geom_point(position = position_dodge(0.6)) +
  geom_errorbar(aes(ymax = high.ci, ymin = low.ci),
                position = position_dodge(0.6)) +
  geom_hline(yintercept = 0,
             lty = 2,
             color = "red") +
  scale_x_discrete(labels = ggplot2:::parse_safe) +
  scale_color_discrete(name = "Estimator") +
  labs(x = "",
       y = "Sobol' index") +
  theme_AP()

```



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

```
fwrite(dt_median, "dt_median.csv")
```

6 Session information

```
# SESSION INFORMATION -----
sessionInfo()

## R version 3.6.1 (2019-07-05)
## Platform: x86_64-apple-darwin15.6.0 (64-bit)
## Running under: macOS Catalina 10.15.4
##
## 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] pcaPP_1.9-73           checkpoint_0.4.8
##  [3] ggrepel_0.8.2          sensobol_0.3
##  [5] logitnorm_0.8.37       benchmarkme_1.0.3
##  [7] cowplot_1.0.0          scales_1.1.0
##  [9] data.table_1.12.8      Rfast_1.9.9
## [11] RcppZiggurat_0.1.5     doParallel_1.0.15
## [13] iterators_1.0.12       foreach_1.4.8
## [15]forcats_0.4.0          stringr_1.4.0
## [17] dplyr_0.8.3            purrr_0.3.3
## [19] readr_1.3.1            tidyverse_1.3.0
## [21] tibble_2.1.3           ggplot2_3.3.0
## [23] tidyverse_1.3.0         RcppArmadillo_0.9.850.1.0
## [25] Rcpp_1.0.4
##
## loaded via a namespace (and not attached):
##  [1] httr_1.4.1              jsonlite_1.6            modelr_0.1.5
##  [4] Rdpack_0.11-1           assertthat_0.2.1        cellranger_1.1.0
##  [7] yaml_2.2.0               remotes_2.1.1           pillar_1.4.3
## [10] backports_1.1.5         lattice_0.20-38         glue_1.3.2
## [13] digest_0.6.25           rvest_0.3.5             colorspace_1.4-1
## [16] htmltools_0.4.0          Matrix_1.2-18           pkgconfig_2.0.3
## [19] bibtex_0.4.2.2          broom_0.5.3             haven_2.2.0
## [22] mvtnorm_1.0-12          farver_2.0.3            generics_0.0.2
## [25] withr_2.1.2             cli_2.0.2               magrittr_1.5
## [28] crayon_1.3.4            readxl_1.3.1            evaluate_0.14
## [31] fs_1.3.1                fansi_0.4.1             nlme_3.1-143
```

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## [34] xml2_1.2.2           tools_3.6.1          hms_0.5.3
## [37] gbRd_0.4-11          lifecycle_0.2.0    munsell_0.5.0
## [40] reprex_0.3.0          compiler_3.6.1     rlang_0.4.5
## [43] grid_3.6.1            rstudioapi_0.11   labeling_0.3
## [46] rmarkdown_2.1           gtable_0.3.0       codetools_0.2-16
## [49] DBI_1.1.0              curl_4.3           benchmarkmeData_1.0.3
## [52] R6_2.4.1                lubridate_1.7.4   knitr_1.27
## [55] stringi_1.4.6          vctrs_0.2.4       dbplyr_1.4.2
## [58] tidyselect_0.2.5        xfun_0.12

## 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 = TRUE))

## Num threads:
## [1] 16

## Return the machine RAM
cat("RAM:         "); print (get_ram()); cat("\n")

## RAM:
## 34.4 GB

```

References

Becker, William. 2019. “Sensitivity analysis on a shoestring : screening model inputs at low sample size.”