The battle of total-order sensitivity estimators

R code

Arnald Puy

Contents

```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("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("2021-02-05",
           R.version ="4.0.3",
           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 VARS-TO

```
# VARS FUNCTIONS ---------------------------------------------------------------

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 if(method == "LHS") {
    mat <- lhs::randomLHS(star.centers, length(params))
  } 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] # 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)
}

# VARS-TO algorithm
vars_ti <- function(Y, star.centers, params, h, method = "one.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)
}
```

1.3 Sobol' total-order indices

```
# COMPUTATION OF SOBOL' Ti INDICES -----------------------------------------------

# SOBOL MATRICES ------------

scrambled_sobol <- function(matrices, A, B, C, order, cluster) {
  first <- 1:ncol(A)
  N <- nrow(A)
  if(order == "first") {
    loop <- first
  } else if(order == "second") {
    second <- c(first, utils::combn(1:ncol(A), 2, simplify = FALSE))
    loop <- second
  } else if(order == "third") {
    second <- c(first, utils::combn(1:ncol(A), 2, simplify = FALSE))
    third <- c(second, utils::combn(1:ncol(A), 3, simplify = FALSE))
    loop <- third
  } else {
    stop("order should be either first, second or third")
  }
  if(is.null(cluster) == FALSE) {
    loop <- cluster
  }
  AB.mat <- "AB" %in% matrices
  BA.mat <- "BA" %in% matrices
  CB.mat <- "CB" %in% matrices
  if(AB.mat == TRUE) {
    X <- rbind(A, B)
    for(i in loop) {
      AB <- A
      AB[, i] <- B[, i]
      X <- rbind(X, AB)
    }
    AB <- X[(2 * N + 1):nrow(X), ]
  } else if(AB.mat == FALSE) {
    AB <- NULL
  }
  if(BA.mat == TRUE) {
    W <- rbind(A, B)
```

```
    for(i in loop) {
      BA <- B
      BA[, i] <- A[, i]
      W <- rbind(W, BA)
    }
    BA <- W[(2 * N + 1) : nrow(W), ]
  } else if(BA.mat == FALSE) {
    BA <- NULL
  }
  if(CB.mat == TRUE) {
    Z <- rbind(A, B)
    for(i in loop) {
      CB <- C
      CB[, i] <- B[, i]
      Z <- rbind(Z, CB)
    }
    CB <- Z[(2 * N + 1) : nrow(Z), ]
  } else if(CB.mat == FALSE) {
    CB <- NULL
  }
  final <- rbind(AB, BA, CB)
  return(final)
}


sobol_matrices <- function(matrices = c("A", "B", "AB"),
                           N, params, order = "first",
                           method = "QRN", cluster = NULL) {
  k <- length(params)
  n.matrices <- ifelse(any(stringr::str_detect(matrices, "C")) == FALSE, 2, 3)
  if(method == "QRN") {
    df <- randtoolbox::sobol(n = N, dim = k * n.matrices, scrambling = 1)
  } else if(method == "R") {
    df <- replicate(k * n.matrices, stats::runif(N))
  } else if(method == "LHS") {
    df <- lhs::randomLHS(N, n.matrices * k)
  } else {
    stop("method should be either QRN, R or LHS")
  }
  A <- df[, 1:k]
  B <- df[, (k + 1) : (k * 2)]
  if(n.matrices == 3) {
    C <- df[, ((k * 2) + 1):(k * 3)]
  } else {
    C <- NULL
  }
  out <- scrambled_sobol(matrices = matrices,
```

```
                          A = A, B = B, C = C,
                          order = order, cluster = cluster)
  A.mat <- "A" %in% matrices
  B.mat <- "B" %in% matrices
  C.mat <- "C" %in% matrices
  if(A.mat == FALSE) {
    A <- NULL
  }
  if(B.mat == FALSE) {
    B <- NULL
  }
  if(C.mat == FALSE) {
    C <- NULL
  }
  final <- rbind(A, B, C, out)
  colnames(final) <- params
  return(final)
}

# COMPUTATION OF SOBOL' TOTAL-ORDER INDICES

sobol_Ti <- function(d, N, params, total) {
  m <- matrix(d, nrow = N)
  k <- length(params)
  if(total == "jansen" | total == "homma" | 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 == "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 == "saltelli") {
```

```
    Y_A <- m[, 1]
    Y_B <- m[, 2]
    Y_BA <- m[, -c(1, 2)]
    f02 <- (1 / N * sum(Y_A)) ^ 2
    VY <- 1 / N * sum(Y_A ^ 2) - f02
    Ti <- 1 - ((1 / N * Rfast::colsums(Y_B * Y_BA - f02)) / VY)
  }
  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 <- Rfast::colsums((Y_B - Y_BA) ^ 2 + (Y_A - Y_AB) ^ 2) /
      Rfast::colsums((Y_A - Y_B) ^ 2 + (Y_BA - Y_AB) ^ 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)
}
```

1.4 Prove that estimators work as expected

```
# CHECK THAT ALL TI ESTIMATORS WORK ------------------------------------------------

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

# Run model
ind <- Y <- mt <- list()
```

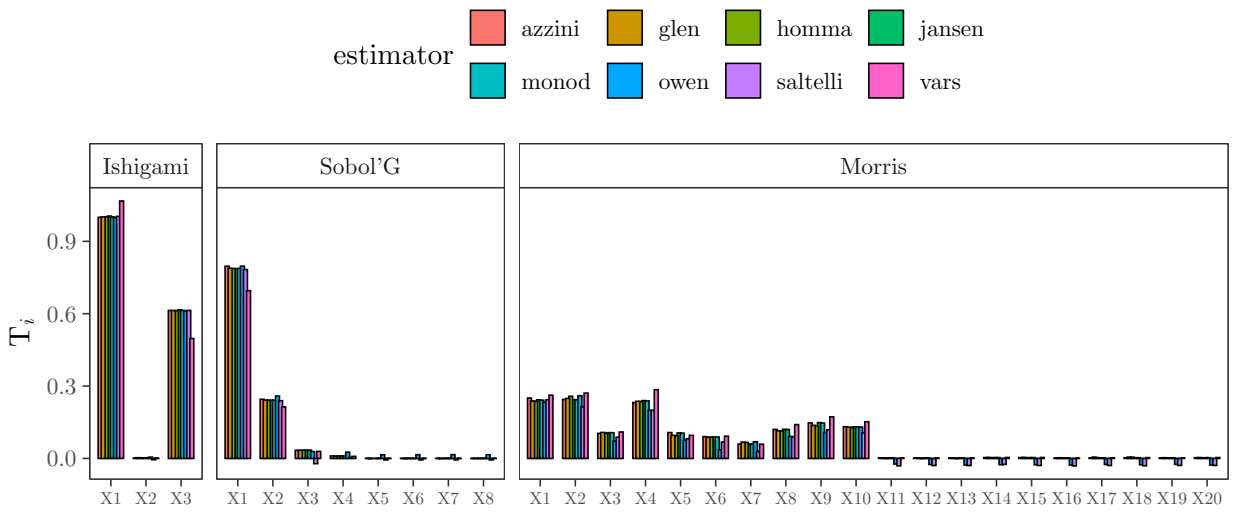
```r
for(i in estimators) {
  for(j in test_functions) {
    if(i == "jansen" | i == "homma" | i == "monod" | i == "glen") {
      matrices <- c("A", "AB")
    } else if(i == "azzini"){
      matrices <- c("A", "B", "AB", "BA")
    } else if(i == "owen") {
      matrices <- c("A", "B", "BA", "CB")
    } else if(i == "saltelli") {
      matrices <- c("A", "B", "BA")
    }
    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 = matri
    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
```

```r
# 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,
```

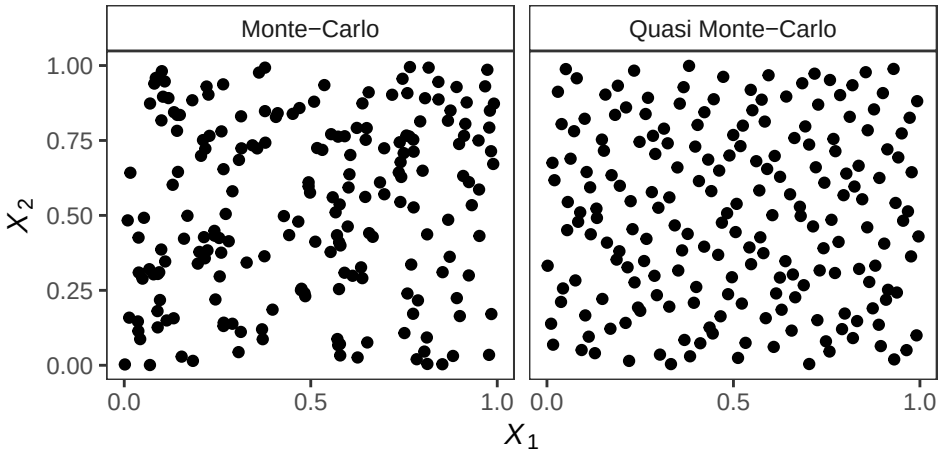
```
                              params = paste("X", 1:k, sep = ""),
                              h = h)
  Y[[j]] <- modelRun(mt[[j]])
  vars.ind[[j]] <- vars_ti(Y = Y[[j]], star.centers = star.centers,
                              params = paste("X", 1:k, sep = ""), h = h)
}

vars.ind <- rbindlist(vars.ind, idcol = "Function")[
  , estimator:= "vars"] %>%
  setcolorder(., 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") +
  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",
        strip.background = element_rect(fill = "white")) +
  guides(fill = guide_legend(nrow = 2,
                             byrow = TRUE))
```



1.5 Differences between random and quasi-random sequences

```
# PLOT THE SAMPLING METHODS AVAILABLE ----------------------------------------

method <- c("R", "QRN")
matrices <- "A"
N <- 200
set.seed(666) # For the random sampling
params <- paste("X", 1:2, sep = "")
A <- lapply(method, function(x)
  sobol_matrices(N = N, params = params,
                 matrices = matrices, method = x))

names(A) <- method
lapply(A, data.table) %>%
  rbindlist(., idcol = "method") %>%
  .[, method:= ifelse(method == "R", "Monte-Carlo", "Quasi Monte-Carlo")] %>%
  .[, method:= factor(method, levels = c("Monte-Carlo", "Quasi Monte-Carlo"))] %>%
  ggplot(., aes(X1, X2)) +
  geom_point() +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  labs(x = expression(italic(X)[1]),
       y = expression(italic(X)[2])) +
  facet_wrap(~method, ncol = 3) +
  theme_AP() +
  theme(strip.background = element_rect(fill = "white"))
```



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]))))
  }) +
  labs(color= "Function", linetype = "Function",
       x = expression(italic(x)),
       y = expression(italic(y))) +
  scale_color_discrete(labels = c(expression(f[1](x) == x ^ 3),
                                  expression(paste(f[2](x) == 1, " if ", x>1/2, ", otherwise "
                                  expression(f[3](x) == (e ^ x - 1) / (e - 1)),
                                  expression(f[4](x) == (10 - 1 / 1.1) ^ -1 * (x + 0.1) ^ - 1)
                                  expression(f[5](x) == x),
                                  expression(f[6](x) == 0),
                                  expression(f[7](x) == 4~~(x - 0.5) ^ 2),
                                  expression(f[8](x) == sin(2~~pi~~x) / 2),
                                  expression(f[9](x) == x ^ 2),
                                  expression(f[10](x) == cos(x)))) +
  theme_AP() +
  theme(legend.text.align = 0)

a
```

```
# CREATE FUNCTION FOR RANDOM DISTRIBUTIONS -------------------------------------

# Density function
sample_distributions_PDF <- list(
  "uniform" = function(x) dunif(x, 0, 1),
  "normal" = function(x) dnorm(x, 0.5, 0.15),
  "beta" = function(x) dbeta(x, 8, 2),
  "beta2" = function(x) dbeta(x, 2, 8),
  "beta3" = function(x) dbeta(x, 2, 0.8),
  "beta4" = function(x) dbeta(x, 0.8, 2),
  "logitnormal" = function(x) dlogitnorm(x, 0, 3.16)
  # Logit-normal, Bates too?
```

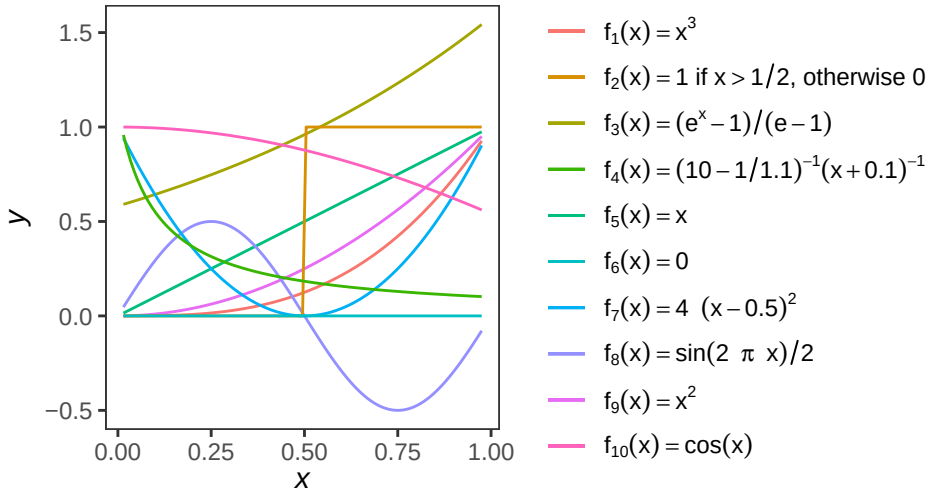


Figure 1: Functions used in the metafunction of Becker (2020).

```
)

# Quantile function
sample_distributions <- list(
  "uniform" = function(x) x,
  "normal" = function(x) qnorm(x, 0.5, 0.15),
  "beta" = function(x) qbeta(x, 8, 2),
  "beta2" = function(x) qbeta(x, 2, 8),
  "beta3" = function(x) qbeta(x, 2, 0.8),
  "beta4" = function(x) qbeta(x, 0.8, 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)
x <- seq(0, 1, .001)

out <- matrix(rep(x, length(names_ff)), ncol = length(names_ff))
```

```
dt <- data.table(sapply(seq_along(names_ff), function(x)
  sample_distributions_PDF[[names_ff[x]]](out[, x])))

dt <- setnames(dt, paste("V", 1:length(names_ff), sep = ""), names_ff) %>%
  .[, x:= x] %>%
  melt(., measure.vars = names_ff)

b <- ggplot(dt, aes(x = x, y = value, group = variable)) +
  geom_line(aes(color = variable)) +
  scale_color_discrete(labels = c("U(0, 1)",
                                  expression(N[T](0.5, 0.15, 0, 1)),
                                  "Beta(8, 2)",
                                  "Beta(2, 8)",
                                  "Beta(2, 0.8)",
                                  "Beta(0.8, 2)",
                                  "Logitnormal(0, 3.16)"),
                       name = "Distribution") +
  labs(x = expression(italic(x)),
       y = "PDF") +
  theme_AP() +
  theme(legend.text.align = 0)

b
```

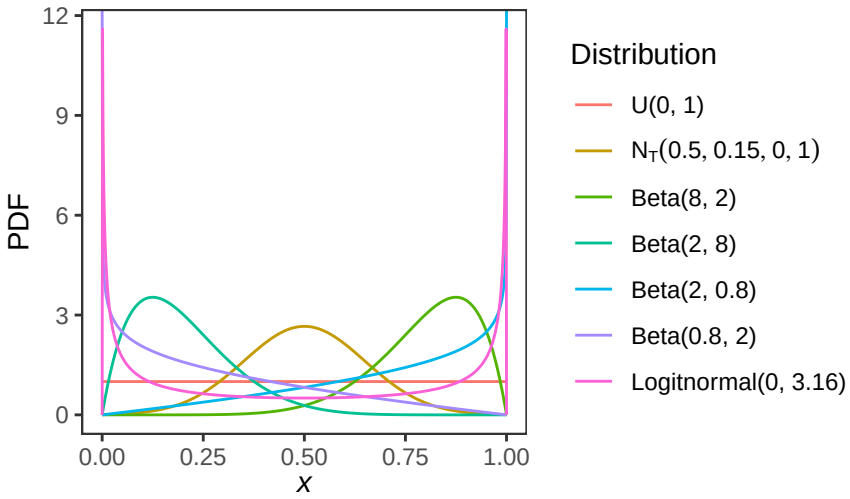
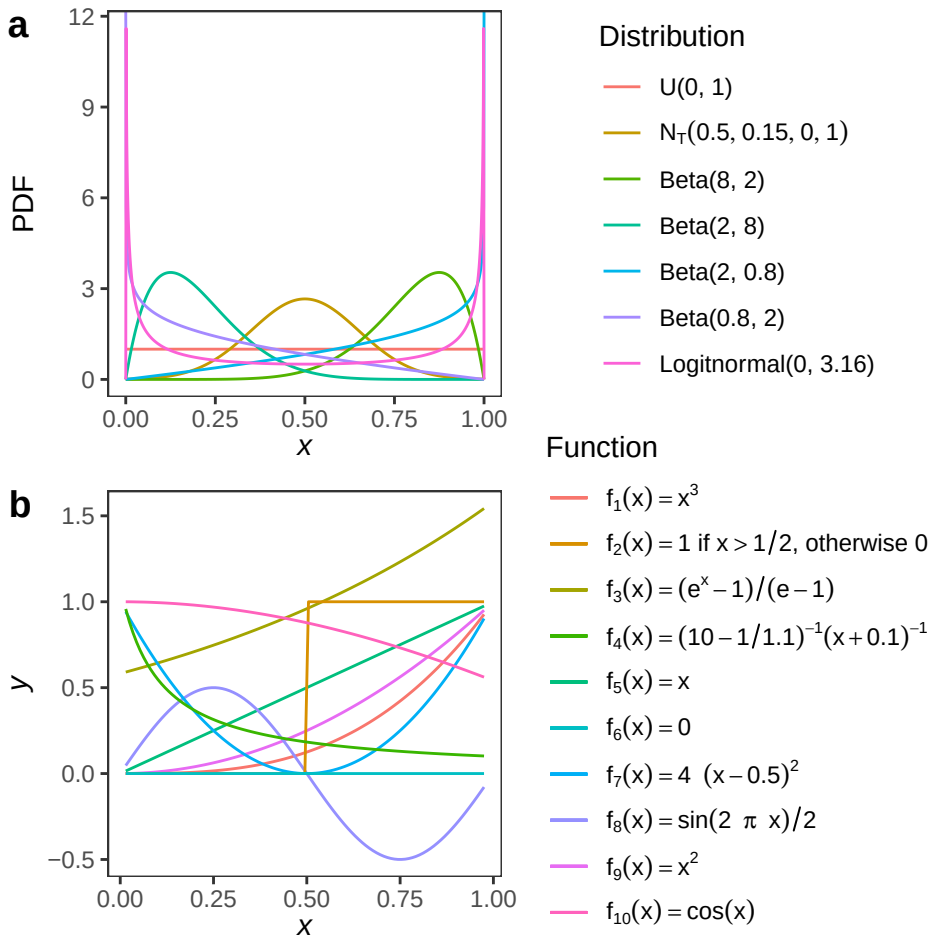


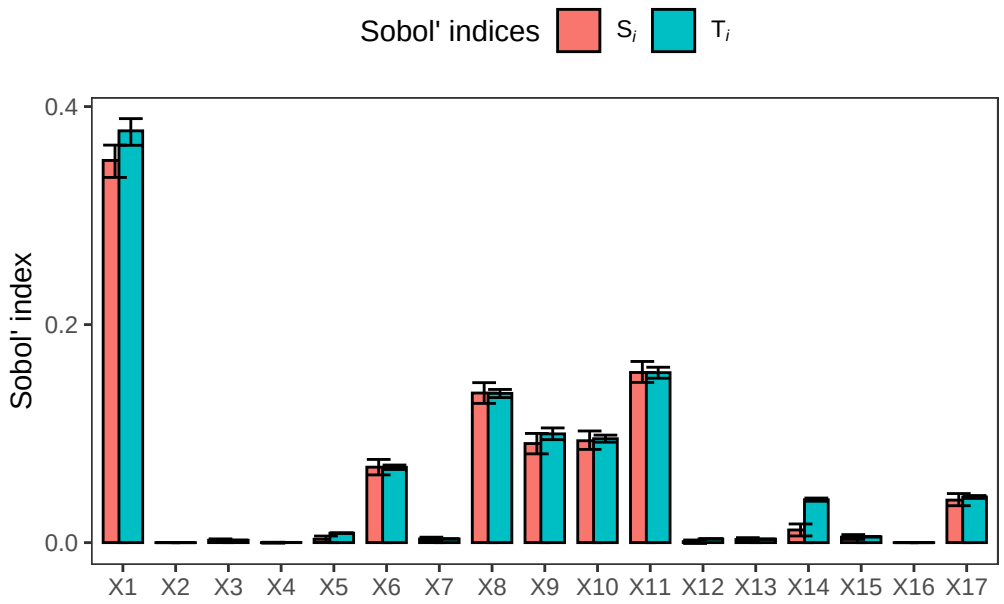
Figure 2: Distributions used in the metafunction of Becker (2020).

```
# MERGE METAFUNCTION PLOT AND DISTRIBUTIONS PLOT ---------------------------------

plot_grid(b, a, ncol = 1, labels = "auto", align = "hv")
```




```
# EXEMPLIFY THE METAFUNCTION WITH AN EXAMPLE ----------------------------------------

N <- 10^4 # Sample size
R <- 10^2 # Number of bootstrap replications
k <- 17 # Number of model inputs
k_2 <- 0.5 # Fraction of active pairwise interactions
k_3 <- 0.2 # Fraction of active three-wise interactions
epsilon <- 666  # to reproduce the results
params <- paste("X", 1:k, sep = "")
A <- sobol_matrices(N = N, params = params)

# Compute
Y <- sensobol::metafunction(data = A, k_2 = k_2, k_3 = k_3, epsilon = epsilon)
indices <- data.table(sensobol::sobol_indices(Y = Y, N = N, params = params, boot = TRUE, R = R
  .[, parameters:= factor(parameters, levels = paste("X", 1:k, sep = ""))]

ggplot(indices, 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)) +
  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")
```



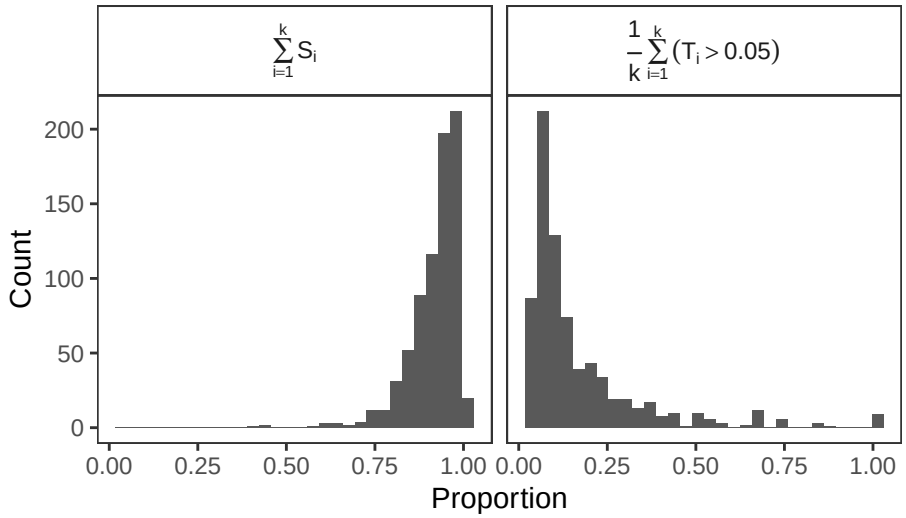

```
# FUNCTIONS TO COMPUTE SUM OF SI AND PROPORTION OF SI > 0.05 FOR METAFUNCTION -----

# Function to replicate in parallel
RepParallel <- function(n, expr, simplify = "array",...) {
  answer <-
    mclapply(integer(n), eval.parent(substitute(function(...) expr)),...)
  if (!identical(simplify, FALSE) && length(answer))
    return(simplify2array(answer, higher = (simplify == "array")))
  else return(answer)
}

# Function to replicate
try_metafunction <- function(x) {
  k <- sample(x)[1]
  params <- paste("X", 1:k, sep = "")
  N <- 500
  A <- sobol_matrices(N = N, params = params)
  Y <- sensobol::metafunction(A)
```

```
  ind <- sobol_indices(Y = Y, N = N, params = params)
  out1 <- ind[sensitivity == "Si", sum(original)]
  out2 <- ind[sensitivity == "Ti", sum(original > 0.05)/.N]
  output <- c(out1, out2)
  return(output)
}
```

```
# COMPUTE SUM OF SI AND PROPORTION OF SI > 0.05 FOR METAFUNCTION --------------------

n <- 10^3
out <- do.call(rbind, RepParallel(n, try_metafunction(3:100), simplify = FALSE))
dt.out <- data.table(out)
```

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

dt.out[V1 < 1 & V1 > 0] %>%
  setnames(., c("V1", "V2"),
           c("sum(S[i], i==1, k)",
             "frac(1,k)~sum((T[i]>0.05), i == 1, k)")) %>%
  melt(., measure.vars = c("sum(S[i], i==1, k)",
                           "frac(1,k)~sum((T[i]>0.05), i == 1, k)")) %>%
  ggplot(., aes(value)) +
  geom_histogram() +
  facet_wrap(~variable,
             labeller = label_parsed) +
  labs(x = "Proportion", y = "Count") +
  theme_AP() +
  theme(strip.background = element_rect(fill = "white"))
```

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



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 <- "first"
params <- c("k_2", "k_3", "epsilon", "phi", "delta", "tau")
N.high <- 2 ^ 11 # Maximum sample size of the large sample matrix
```

3.2 Sample matrix

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

# Create sample matrix
mat <- sensobol::sobol_matrices(N = N, params = c(params, "N_t", "k"), order = order)
Nt.k.rows <- which(rep(c("A", "B", params, "N_t", "k"), each = N) %in% c("N_t", "k"))
mat <- mat[-Nt.k.rows, ] # Exclude AB matrices for Nt and k

# Create A and B matrices to create the clusters
A <- mat[1:N, ]
B <- mat[(N + 1):(2 * N), ]

# Matrix with clusters (Nt,k), (k_2, k_3, epsilon, phi), (delta, tau)
AB <- AB2 <- AB3 <- A
AB[, c("N_t", "k")] <- B[, c("N_t", "k")] # (Nt,k)
AB2[, c("k_2", "k_3", "epsilon", "phi")] <-  B[, c("k_2", "k_3", "epsilon", "phi")] # Model un
AB3[, c("delta", "tau")] <- B[, c("delta", "tau")] # Manageable uncertainties

# Final matrices
mat <- rbind(mat, AB, AB2, AB3)

# TRANSFORM MATRIX --------

mat[, 1] <- round(qunif(mat[, 1], 0.3, 0.5), 2) # k_2
mat[, 2] <- round(qunif(mat[, 2], 0.1, 0.3), 2) # k_3
mat[, 3] <- floor(qunif(mat[, 3], 1, 200)) # Epsilon
mat[, 4] <- floor(mat[, 4] * (8 - 1 + 1)) + 1 # Phi
mat[, 5] <- floor(mat[, 5] * (2 - 1 + 1)) + 1 # Delta
mat[, 6] <- floor(mat[, 6] * (2 - 1 + 1)) + 1 # Tau
mat[, 7] <- floor(qunif(mat[, 7], 10, 1000)) # Nt
mat[, 8] <- floor(qunif(mat[, 8], 3, 100)) # k
```

```r
# Define the base sample matrix
N.all <- apply(mat, 1, function(x) ceiling(x["N_t"] / (x["k"] + 1)))
N.saltelli <- apply(mat, 1, function(x) ceiling(x["N_t"] / (x["k"] + 2)))
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))))

tmp <- data.table(cbind(mat, N.all, N.azzini, N.vars))

# Now constrain N as a function of vars
tmp <- tmp[, N.all:= ifelse(N.vars == 1 | N.vars == 0, ceiling(2 * (4 * k + 1) / (k + 1)), N.al
tmp <-  tmp[, N.saltelli:= ifelse(N.vars == 1 | N.vars == 0, ceiling(2 * (4 * k + 1) / (k + 2))
tmp <- tmp[, N.azzini:= ifelse(N.vars == 1 | N.vars == 0, ceiling(2 * (4 * k + 1) / (2 * k + 2
tmp <- tmp[, N.vars:= ifelse(N.vars == 1 | N.vars == 0, 2, N.vars)]

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

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

# CREATE MATRICES FOR RANKS AND MAE

mat.ranks <- mat # Define matrix for ranks
rows.delta <- which(rep(c("A", "B", params), each = N) %in% "delta") # Rows for delta
rows.nt.k <- (nrow(mat) - N + 1):nrow(mat) # Rows for cluster Nt_k
mat.mae <- mat[-c(rows.delta, rows.nt.k)] # Define matrix for mae
```

```r
# EXPORT SAMPLE MATRIX ------------------------------------------------------
fwrite(mat, "mat.csv")
```

3.3 Define the model

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

model_Ti <- function(k, N.all, N.azzini, N.saltelli, N.vars, h,
                     N.high, k_2, k_3, epsilon, phi, delta, tau,
                     ranks = TRUE) {
  ind <- list()
  estimators <- c("jansen", "homma", "monod", "azzini", "glen", "owen", "vars", "saltelli")
  if(tau == 1) {
    method <- "R"
  } else if(tau == 2) {
    method <- "QRN"
  }
  set.seed(epsilon)
  all.but.azzini <- sobol_matrices(N = N.all, params = paste("X", 1:k, sep = ""),
```

```
                                    matrices = c("A", "AB"), method = method)
set.seed(epsilon)
saltelli <- sobol_matrices(N = N.saltelli, params = paste("X", 1:k, sep = ""),
                           matrices = c("A", "B", "BA"), method = method)
set.seed(epsilon)
azzini <- sobol_matrices(N = N.azzini, params = paste("X", 1:k, sep = ""),
                         matrices = c("A", "B", "AB", "BA"), method = method)
set.seed(epsilon)
owen.matrix <- sobol_matrices(N = N.azzini, params = paste("X", 1:k, sep = ""),
                              matrices = c("A", "B", "BA", "CB"), method = method)
set.seed(epsilon)
vars.matrix <- vars_matrices(star.centers = N.vars, params = paste("X", 1:k, sep = ""),
                             h = h, method = method)
set.seed(epsilon)
large.matrix <- sobol_matrices(N = N.high, params = paste("X", 1:k, sep = ""),
                               matrices = c("A", "AB"), method = method)
set.seed(epsilon)
all.matrices <- random_distributions(X = rbind(all.but.azzini,
                                               azzini,
                                               owen.matrix,
                                               vars.matrix,
                                               saltelli,
                                               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)
Nt.saltelli <- N.saltelli * (k + 2)
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)
lg.saltelli <- (max(lg.vars) + 1):(max(lg.vars) + Nt.saltelli)
```

```
  for(i in estimators) {
    if(i == "jansen" | i == "homma" | i == "monod" | i == "glen") {
      y <- output[lg.all.but.azzini]
      n <- N.all
    } else if(i == "saltelli") {
      y <- output[lg.saltelli]
      n <- N.saltelli
    } else if(i == "azzini") {
      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)
  # Replcace Na
  for (i in seq_along(out.wide))
    set(out.wide, i=which(is.na(out.wide[[i]])), j = i, value = 0)

  # COMPUTE RANKS
  if(ranks == TRUE) {
    if(delta == 1) { # kendall tau
      final <- out.wide[, .(value = pcaPP::cor.fk(N, n)), estimator]
    } else { # Savage ranks
      final <- out.wide[, lapply(.SD, savage_scores), .SDcols = c("N", "n"), estimator][
```

```
        , .(value = cor(N, n)), estimator]
    }

    # COMPUTE MAE
  } else if(ranks == FALSE) {
    final <- out.wide[, .(value = mean(abs(N - n))), estimator]
  }
  return(final)
}
```

3.4 Run the model

```
# DEFINE THE PARALLEL COMPUTING ------------------------------------------------

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

```
# RUN MODEL FOR RANKS ----------------------------------------------------------

# Compute for ranks
Y.ranks <- foreach(i=1:nrow(mat.ranks),
                   .packages = c("sensobol", "data.table", "pcaPP",
                                 "logitnorm", "dplyr")) %dopar%
  {
    model_Ti(k = mat.ranks[[i, "k"]],
             k_2 = mat.ranks[[i, "k_2"]],
             k_3 = mat.ranks[[i, "k_3"]],
             epsilon = mat.ranks[[i, "epsilon"]],
             phi = mat.ranks[[i, "phi"]],
             delta = mat.ranks[[i, "delta"]],
             tau = mat.ranks[[i, "tau"]],
             N.all = mat.ranks[[i, "N.all"]],
             N.azzini = mat.ranks[[i, "N.azzini"]],
             N.saltelli = mat.ranks[[i, "N.saltelli"]],
             N.vars = mat.ranks[[i, "N.vars"]],
             N.high = N.high,
             h = h,
             ranks = TRUE)
  }
```

```
# RUN MODEL FOR MAE ------------------------------------------------------------

# Compute for MAE
Y.mae <- foreach(i=1:nrow(mat.mae),
                   .packages = c("sensobol", "data.table", "pcaPP",
                                 "logitnorm", "dplyr")) %dopar%
  {
```

```
    model_Ti(k = mat.mae[[i, "k"]],
             k_2 = mat.mae[[i, "k_2"]],
             k_3 = mat.mae[[i, "k_3"]],
             epsilon = mat.mae[[i, "epsilon"]],
             phi = mat.mae[[i, "phi"]],
             delta = mat.mae[[i, "delta"]],
             tau = mat.mae[[i, "tau"]],
             N.all = mat.mae[[i, "N.all"]],
             N.azzini = mat.mae[[i, "N.azzini"]],
             N.saltelli = mat.mae[[i, "N.saltelli"]],
             N.vars = mat.mae[[i, "N.vars"]],
             N.high = N.high,
             h = h,
             ranks = FALSE)
  }
```

```
# STOP PARALLEL COMPUTING ------------------------------------------------------

stopCluster(cl)
```

3.5 Arrange output

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

out.ranks <- rbindlist(Y.ranks, idcol = "row")[, type:= "r"]
out.mae <- rbindlist(Y.mae, idcol = "row")[, type:= "MAE"]

full.output <- rbind(merge(mat.ranks[, row:= 1:.N], out.ranks),
                     merge(mat.mae[, row:= 1:.N], out.mae)) %>%
  .[, Nt:= ifelse(estimator == "azzini" | estimator == "owen", N.azzini * (2 * k + 2),
                  ifelse(estimator == "vars", N.vars * (k * ((1 / h) -1) + 1),
                         ifelse(estimator == "saltelli", N.saltelli * (k + 2), 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 Isaacs",
                                                     ifelse(estimator %in% "owen", "pseudo-Owe
                                                            ifelse(estimator %in% "saltelli",

# Define A matrices
A.ranks <- full.output[type == "r",.SD[1:N], estimator][, ratio:= Nt / k]
A.mae <- full.output[type == "MAE",.SD[1:N], estimator][, ratio:= Nt / k]
A.both <- rbind(A.ranks, A.mae)

# Define matrix for total variance
VY.dt <- full.output[row %in% c(1:N)][
```

```
  , .(VY = 1 / N * sum((value - ((1 / N) * sum(value))) ^ 2)),
  estimator]
```

```
# EXPORT OUTPUT ------------------------------------------------------------------

fwrite(full.output, "full.output.csv")
fwrite(A.ranks, "A.ranks.csv")
fwrite(A.mae, "A.mae.csv")
```

4 Uncertainty analysis

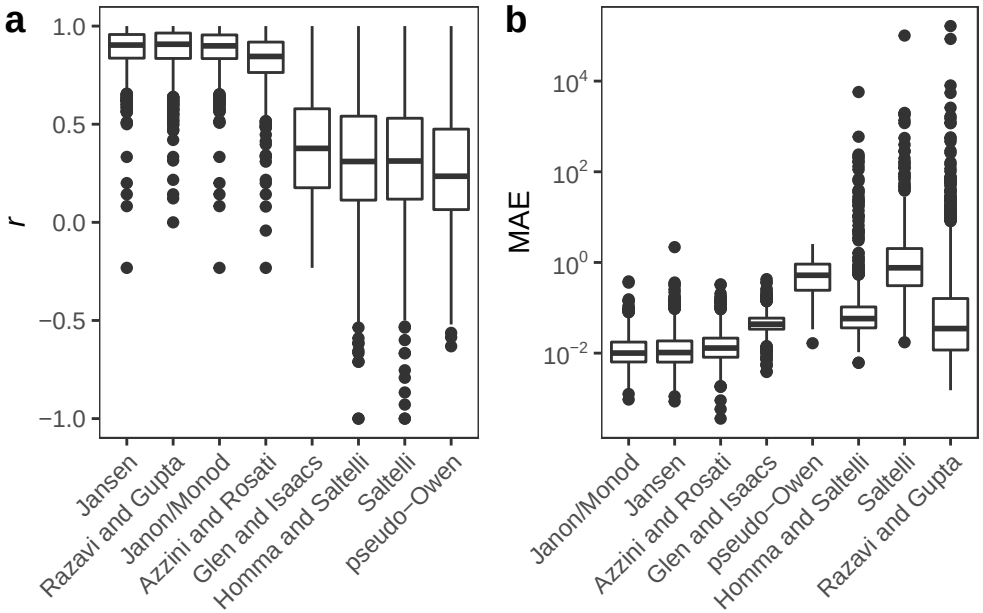
4.1 Boxplots

```
# QUANTILES ----------------------------------------------------------------------

tmp <- A.both[, .(median = median(value),
                  v.low.co = quantile(value, 0.025),
                  low.ci = quantile(value, 0.25),
                  high.ci = quantile(value, 0.75),
                  v.high.ci = quantile(value, 0.975)), .(estimator, type)]

tmp[tmp[, do.call(order, .SD), .SDcols = c("type", "median")]]
```

```
##              estimator type     median     v.low.co      low.ci    high.ci
##  1:        Janon/Monod  MAE 0.01004761  0.003319945 0.006388092 0.01754499
##  2:             Jansen  MAE 0.01031266  0.003355846 0.006335840 0.01859782
##  3:  Azzini and Rosati  MAE 0.01295522  0.004452327 0.008123290 0.02143318
##  4:   Razavi and Gupta  MAE 0.03480095  0.003706873 0.011714348 0.16019528
##  5:    Glen and Isaacs  MAE 0.04350877  0.019484431 0.033749134 0.05920599
##  6: Homma and Saltelli  MAE 0.05778854  0.019501235 0.036073114 0.10447928
##  7:        pseudo-Owen  MAE 0.52212030  0.072787352 0.243572464 0.91950509
##  8:           Saltelli  MAE 0.76276603  0.053651085 0.307395459 2.02673511
##  9:        pseudo-Owen    r 0.23493101 -0.200000000 0.064951715 0.47490203
## 10: Homma and Saltelli    r 0.31006634 -0.117014702 0.113120636 0.54092139
## 11:           Saltelli    r 0.31249111 -0.136020104 0.118126877 0.53034034
## 12:    Glen and Isaacs    r 0.37681104 -0.014843481 0.176284001 0.57857354
## 13:  Azzini and Rosati    r 0.84522052  0.591437851 0.763476795 0.91851852
## 14:        Janon/Monod    r 0.89914630  0.671730560 0.834336880 0.95490787
## 15:             Jansen    r 0.90325312  0.673011739 0.836494387 0.95701282
## 16:   Razavi and Gupta    r 0.90739346  0.639853935 0.835005530 0.96448563
##       v.high.ci
##  1:  0.05513422
##  2:  0.07563105
##  3:  0.06693832
##  4: 15.09093976
##  5:  0.12025340
##  6:  0.55294638
```

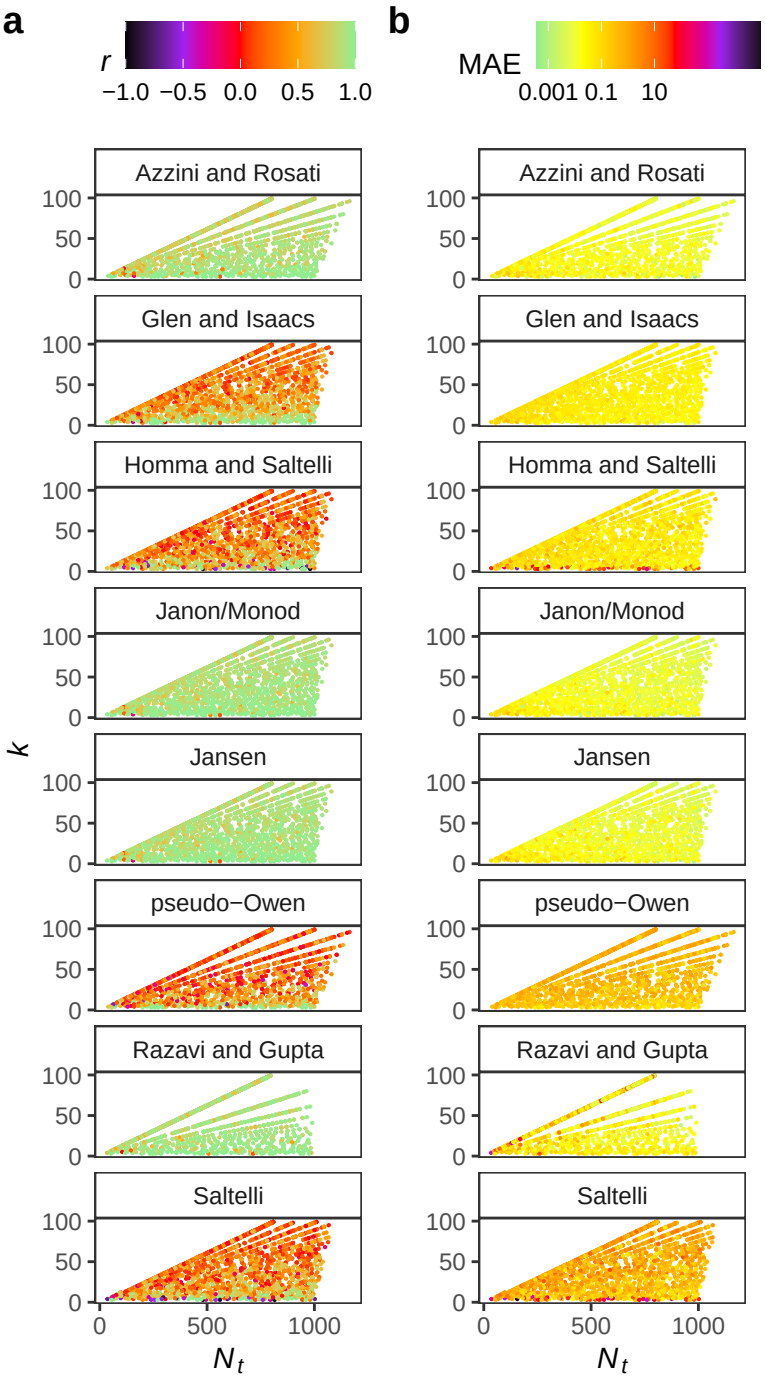
```
##  7:  1.88420331
##  8: 16.08920143
##  9:  0.89412248
## 10:  0.92840515
## 11:  0.92341341
## 12:  0.97179194
## 13:  1.00000000
## 14:  1.00000000
## 15:  1.00000000
## 16:  1.00000000
```

```r
# PLOT BOXPLOT ------------------------------------------------------------------

a <- ggplot(A.ranks, aes(x = reorder(estimator, -value), value)) +
  geom_boxplot() +
  labs(x = "",
       y = expression(italic(r))) +
  theme_AP() +
  theme(axis.text.x = element_text(angle = 45, hjust = 1))

b <- ggplot(A.mae, aes(x = reorder(estimator, value), value)) +
  geom_boxplot() +
  labs(x = "",
       y = "MAE") +
  scale_y_log10(breaks = scales::trans_breaks("log10", function(x) 10^x),
                labels = scales::trans_format("log10", scales::math_format(10^.x))) +
  theme_AP() +
  theme(axis.text.x = element_text(angle = 45, hjust = 1))

plot_grid(a, b, ncol = 2, labels = "auto")
```



4.2 Scatterplots

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

a <- ggplot(A.ranks, aes(Nt, k, color = value)) +
  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 = 1) +
  theme_AP() +
  theme(legend.position = "top",
        strip.background = element_rect(fill = "white"))

b <- ggplot(A.mae, aes(Nt, k, color = value)) +
  geom_point(size = 0.1) +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  scale_colour_gradientn(colours = c("lightgreen", "yellow", "orange", "red", "purple", "black
                         name = "MAE",
                         trans = "log",
                         breaks = c(0.001, 0.1, 10),
                         labels = c(0.001, 0.1, 10)) +
  labs(x = expression(italic(N[t])),
       y = "") +
  facet_wrap(~estimator,
             ncol = 1) +
  theme_AP() +
  theme(legend.position = "top",
        strip.background = element_rect(fill = "white"))

plot_grid(a, b, ncol = 2, labels = "auto")
```

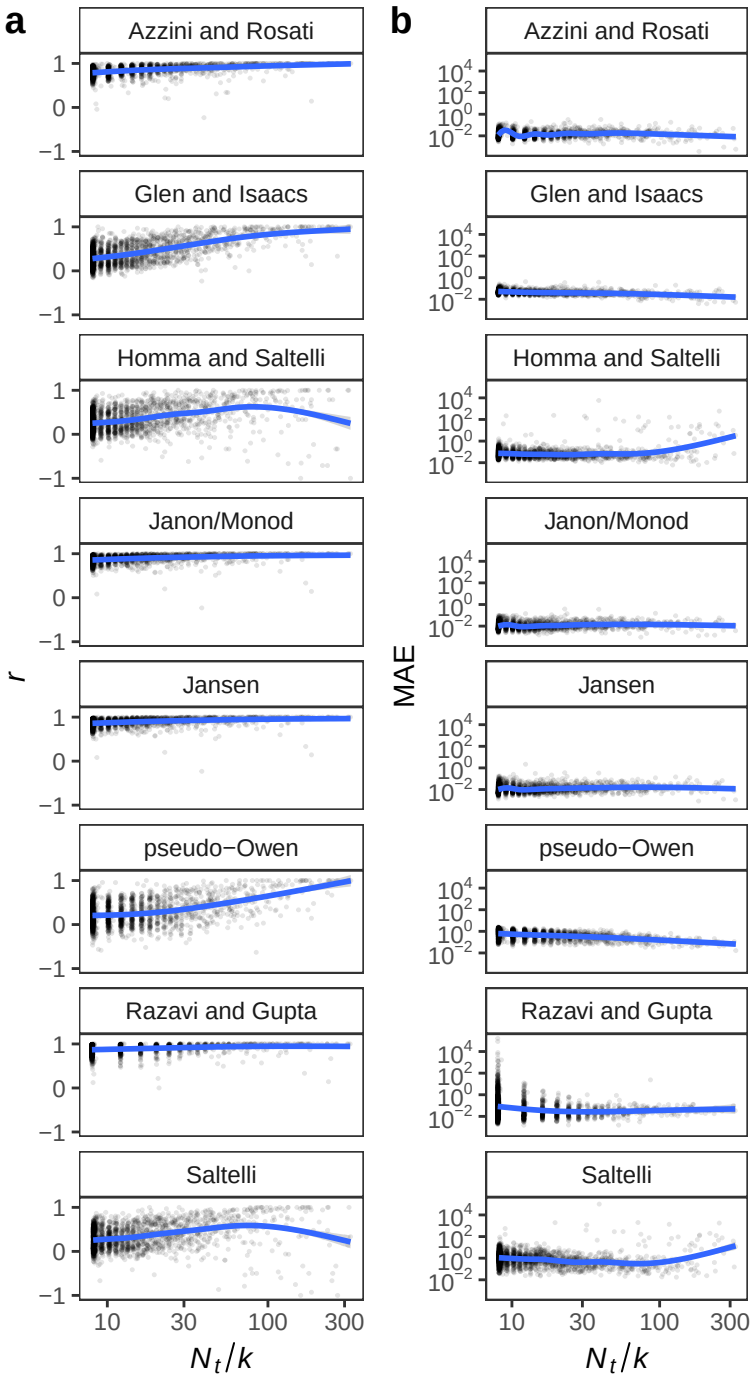


4.3 Scatterplots with ratios

```
# PLOT SCATTERPLOTS WITH RATIOS ------------------------------------------------

a <- A.ranks[, ratio:= Nt / k] %>%
  ggplot(., aes(ratio, value)) +
  geom_point(alpha = 0.1, size = 0.2) +
  facet_wrap(~estimator,
```

```
            ncol = 1) +
  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() +
  theme(strip.background = element_rect(fill = "white"))


b <- A.mae[, ratio:= Nt / k] %>%
  ggplot(., aes(ratio, value)) +
  geom_point(alpha = 0.1, size = 0.2) +
  facet_wrap(~estimator,
             ncol = 1) +
  geom_smooth() +
  labs(x = expression(italic(N[t]/k)),
       y = "MAE") +
  scale_x_log10() +
  scale_y_log10(breaks = scales::trans_breaks("log10", function(x) 10^x),
                labels = scales::trans_format("log10", scales::math_format(10^.x))) +
  theme_AP() +
  theme(strip.background = element_rect(fill = "white"))

plot_grid(a, b, ncol = 2, labels = "auto")
```

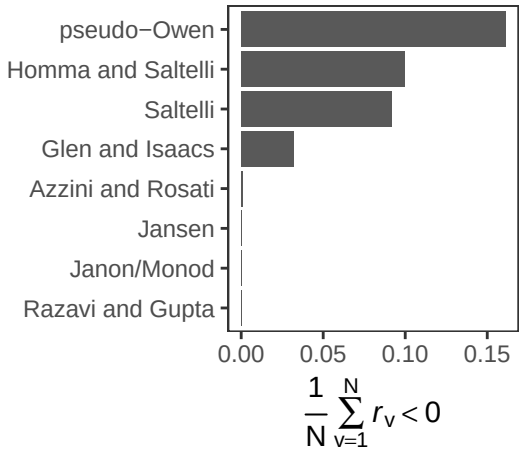
```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```



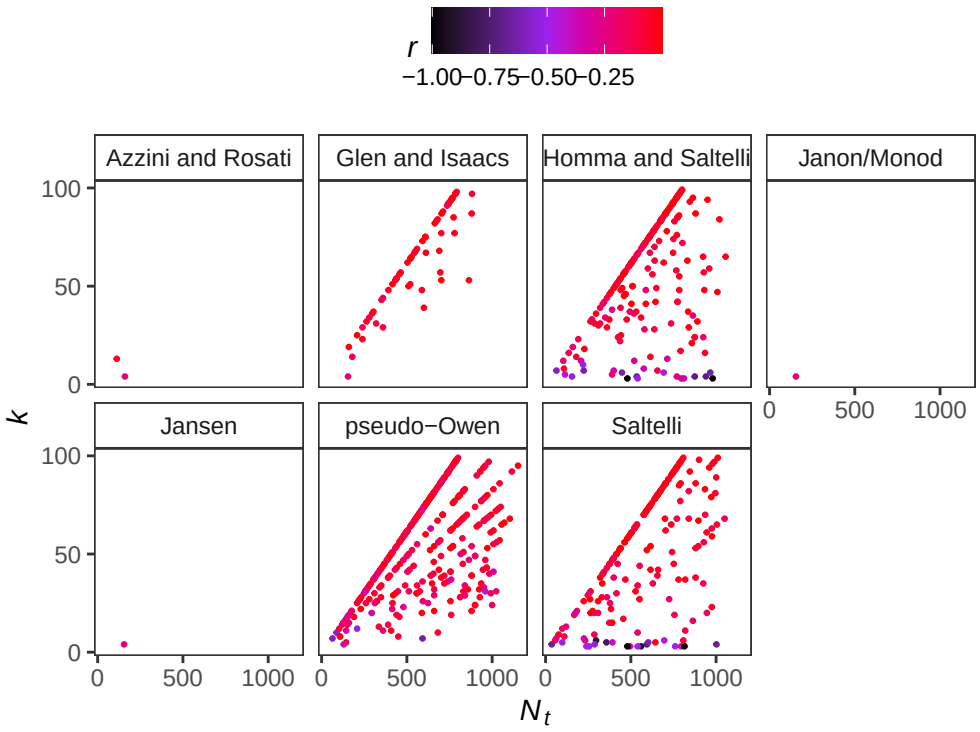
4.4 Negative r values

```
# PLOT PROPORTION OF NEGATIVE R ------------------------------------------------

A.ranks[, sum(value < 0)/ .N, estimator] %>%
  ggplot(., aes(reorder(estimator, V1), V1)) +
  geom_bar(stat = "identity") +
  coord_flip() +
```

```
  labs(y = expression(frac(1, N)~sum(italic(r)[v] < 0, v==1, N)),
       x = "") +
  theme_AP()
```




```
# MAP VALUES WITH NEGATIVE R ------------------------------------------------------

index.neg <- A.ranks[, .I[value < 0]]

A.ranks[index.neg] %>%
  ggplot(., aes(Nt, k, color = value)) +
  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,
             ncol = 4) +
  theme_AP() +
  theme(legend.position = "top",
        strip.background = element_rect(fill = "white"))
```



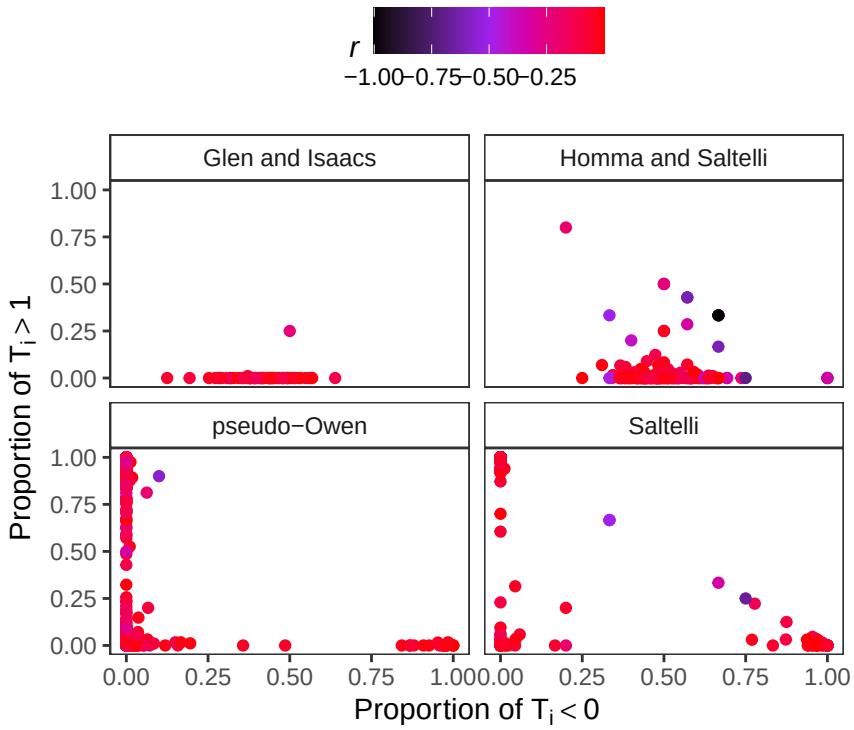

```
# MODEL TO RETRIEVE SIMULATIONS THAT YIELDED R < 0 ---------------------------------

model_Ti2 <- function(k, N.all, N.azzini, N.saltelli, N.vars, h,
                      N.high, k_2, k_3, epsilon, phi, delta, tau) {
  ind <- list()
  estimators <- c("jansen", "homma", "monod", "azzini", "glen", "owen", "vars", "saltelli")
  if(tau == 1) {
    method <- "R"
  } else if(tau == 2) {
    method <- "QRN"
  }
  set.seed(epsilon)
  all.but.azzini <- sobol_matrices(N = N.all, params = paste("X", 1:k, sep = ""),
                                   matrices = c("A", "AB"), method = method)
  set.seed(epsilon)
  saltelli <- sobol_matrices(N = N.saltelli, params = paste("X", 1:k, sep = ""),
                             matrices = c("A", "B", "BA"), method = method)
  set.seed(epsilon)
  azzini <- sobol_matrices(N = N.azzini, params = paste("X", 1:k, sep = ""),
                           matrices = c("A", "B", "AB", "BA"), method = method)
  set.seed(epsilon)
  owen.matrix <- sobol_matrices(N = N.azzini, params = paste("X", 1:k, sep = ""),
                                matrices = c("A", "B", "BA", "CB"), method = method)
  set.seed(epsilon)
  vars.matrix <- vars_matrices(star.centers = N.vars, params = paste("X", 1:k, sep = ""),
                               h = h, method = method)
  set.seed(epsilon)
```

```
large.matrix <- sobol_matrices(N = N.high, params = paste("X", 1:k, sep = ""),
                               matrices = c("A", "AB"), method = method)
set.seed(epsilon)
all.matrices <- random_distributions(X = rbind(all.but.azzini,
                                               azzini,
                                               owen.matrix,
                                               vars.matrix,
                                               saltelli,
                                               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)
Nt.saltelli <- N.saltelli * (k + 2)
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)
lg.saltelli <- (max(lg.vars) + 1):(max(lg.vars) + Nt.saltelli)

for(i in estimators) {
  if(i == "jansen" | i == "homma" | i == "monod" | i == "glen") {
    y <- output[lg.all.but.azzini]
    n <- N.all
  } else if(i == "saltelli") {
    y <- output[lg.saltelli]
    n <- N.saltelli
  } else if(i == "azzini") {
    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")
  return(out.wide)
}

A.ranks <- A.ranks[, ID:= .I]
rowsToExtract <- A.ranks[value < 0  & estimator %in% c("Saltelli", "pseudo-Owen", "Homma and Sa
                                     "Glen and Isaacs")][, ID]

prove <- A.ranks[ID %in% rowsToExtract]

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

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

# Compute
Y.ti2 <- foreach(i=1:nrow(prove),
                 .packages = c("sensobol", "data.table", "pcaPP",
                               "logitnorm", "dplyr")) %dopar%
  {
    model_Ti2(k = prove[[i, "k"]],
              k_2 = prove[[i, "k_2"]],
              k_3 = prove[[i, "k_3"]],
              epsilon = prove[[i, "epsilon"]],
              phi = prove[[i, "phi"]],
              delta = prove[[i, "delta"]],
              tau = prove[[i, "tau"]],
              N.all = prove[[i, "N.all"]],
              N.azzini = prove[[i, "N.azzini"]],
              N.saltelli = prove[[i, "N.saltelli"]],
              N.vars = prove[[i, "N.vars"]],
              N.high = N.high,
              h = h)
```

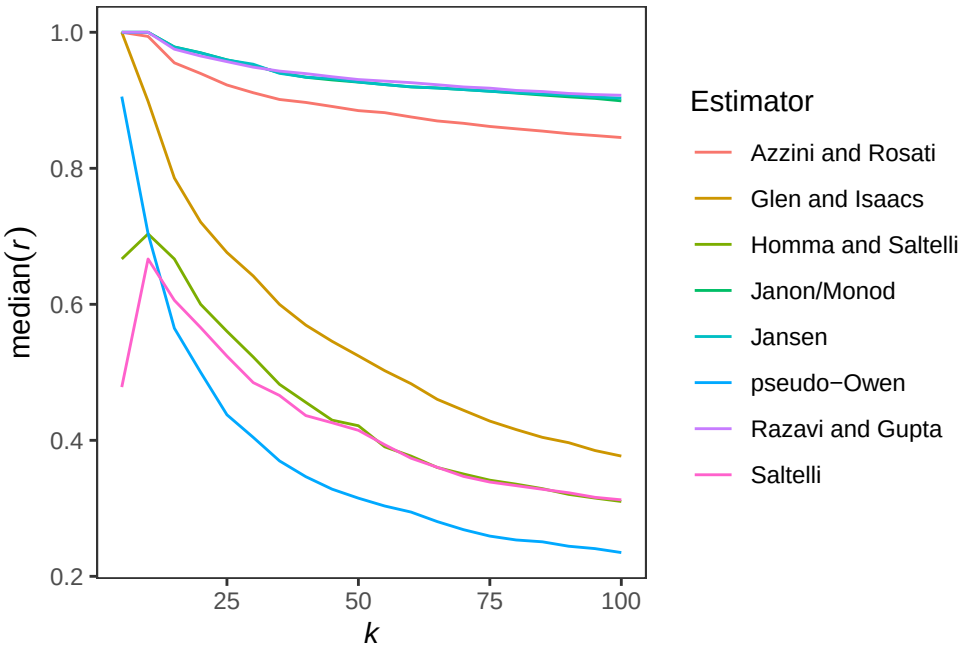
```
  }

# Stop parallel cluster
stopCluster(cl)
```

```
# PLOT DISTRIBUTION OF R<0 AND R>1 ------------------------------------------------

# Arrange output
names(Y.ti2) <- rowsToExtract

out.neg <- rbindlist(Y.ti2, idcol = "ID") %>%
  .[, ID:= as.numeric(ID)]

out.dt <- out.neg[, 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
                                                                   ifelse(estimator %in% "owen"
                                                                          ifelse(estimator %in%




dd <- out.dt[, .(prop.negative = sum(n < 0) / .N,
                 prop.above.one = sum(n > 1) / .N), .(estimator, ID)]

merge(dd, prove, by = c("ID", "estimator")) %>%
  ggplot(., aes(prop.negative, prop.above.one, color = value)) +
  geom_point() +
  scale_colour_gradientn(colours = c("black", "purple", "red"),
                         name = expression(italic(r))) +
  labs(y = expression(paste("Proportion of ", T[i] > 1)),
       x = expression(paste("Proportion of ", T[i] < 0))) +
  facet_wrap(~estimator) +
  theme_AP() +
  theme(legend.position = "top",
        strip.background = element_rect(fill = "white"))
```



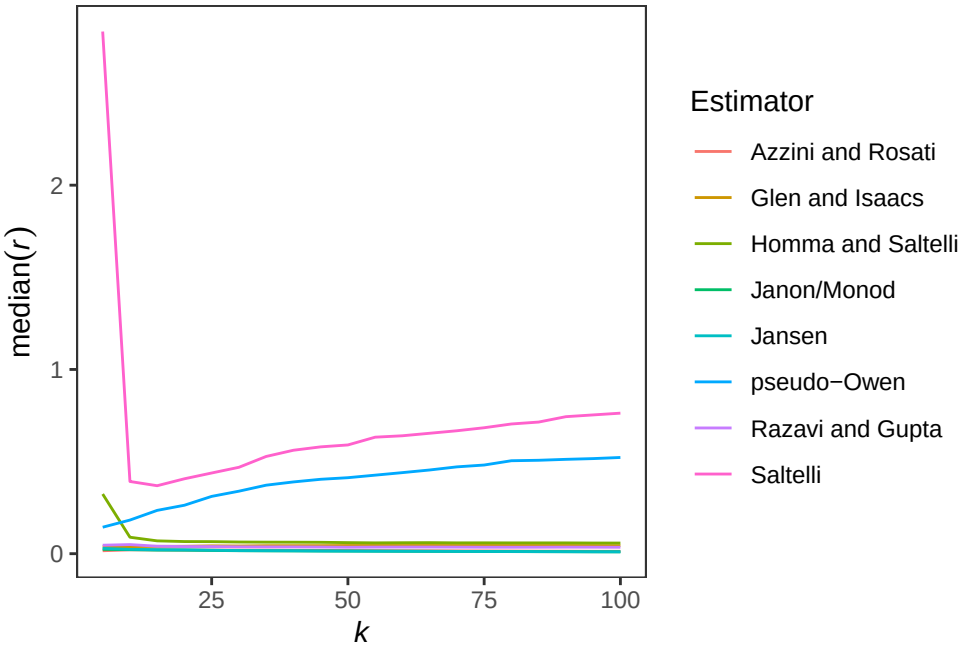
4.5 Plot medians

```
# PLOT MEDIANS ------------------------------------------------------------------

# FOR RANKS-----------
vv <- seq(5, 100, 5)
dt <- lapply(vv, function(x) A.ranks[k <= x, median(value), 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() +
  theme(strip.background = element_rect(fill = "white"))
```



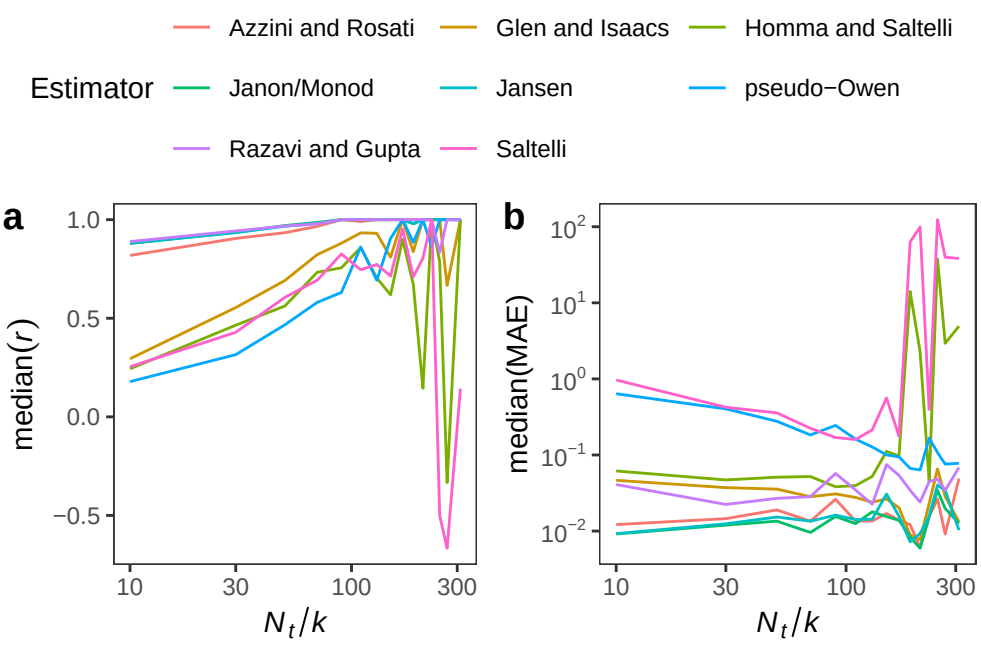

```
# Median Nt/k
dt.tmp <- A.ranks[, .(min = min(ratio), max = max(ratio))]

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

names(out.ranks) <- rowmeans(indices)

# Plot
median.ranks <- lapply(out.ranks, function(x) x[, median(value, na.rm = TRUE), estimator]) %>%
  rbindlist(., idcol = "N") %>%
  .[, N:= as.numeric(N)] %>%
  .[, type:= "r"]

# FOR MAE-----------
dt <- lapply(vv, function(x) A.mae[k <= x, median(value), 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.mae[, .(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.mae <- list()
for(i in 1:nrow(indices)) {
  out.mae[[i]] <- A.mae[ratio > indices[i, 1] & ratio < indices[i, 2]]
}

names(out.mae) <- rowmeans(indices)

# Plot
median.mae <- lapply(out.mae, function(x) x[, median(value, na.rm = TRUE), estimator]) %>%
  rbindlist(., idcol = "N") %>%
  .[, N:= as.numeric(N)] %>%
  .[, type:= "MAE"]

# PLOT ALL

a <- ggplot(median.ranks, aes(N, V1, group = estimator, color = estimator)) +
  geom_line() +
  labs(x = expression(italic(N[t]/k)),
```

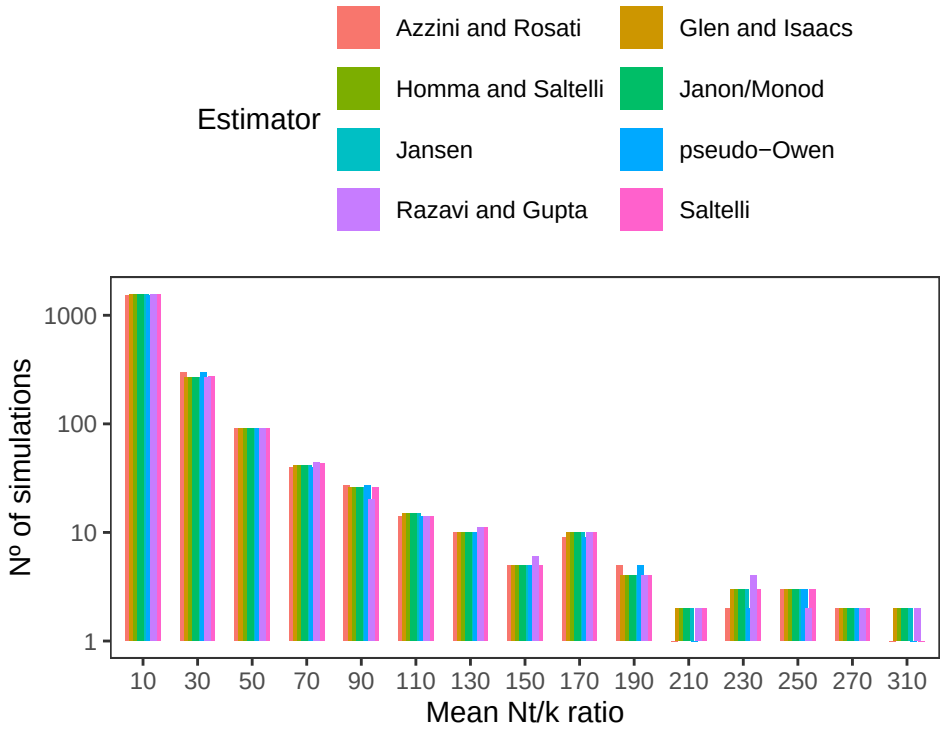
```
       y = expression(median(italic(r)))) +
  scale_color_discrete(name = "Estimator") +
  scale_x_log10() +
  theme_AP() +
  theme(legend.position = "none")


b <- ggplot(median.mae, aes(N, V1, group = estimator, color = estimator)) +
  geom_line() +
  labs(x = expression(italic(N[t]/k)),
       y = "median(MAE)") +
  scale_color_discrete(name = "Estimator") +
  scale_x_log10() +
  scale_y_log10(breaks = scales::trans_breaks("log10", function(x) 10^x),
                labels = scales::trans_format("log10", scales::math_format(10^.x))) +
  theme_AP() +
  theme(legend.position = "none")

legend <- get_legend(a + theme(legend.position = "top") +
                       guides(color = guide_legend(nrow = 3, byrow = TRUE)))
bottom <- plot_grid(a, b, ncol = 2, labels = "auto")
plot_grid(legend, bottom, ncol = 1, rel_heights = c(0.3, 0.7))
```



4.6 Number of simulations per mean Nt/k ratio

```
# PLOT MEAN NT/K RATIO AS A FUNCTION OF Nº SIMULATIONS ----------------------------

rbindlist(out.ranks, idcol = "samples")[, .N, .(estimator, samples)] %>%
  .[, samples:= factor(samples, levels = rowmeans(indices))] %>%
```

```
  ggplot(., aes(samples, N, fill = estimator)) +
  scale_y_log10() +
  scale_fill_discrete(name = "Estimator") +
  labs(x = "Mean Nt/k ratio",
       y = "Nº of simulations") +
  geom_bar(stat = "identity",
           position = position_dodge(0.6)) +
  theme_AP() +
  theme(legend.position = "top") +
  guides(fill = guide_legend(nrow = 4, byrow = TRUE))
```



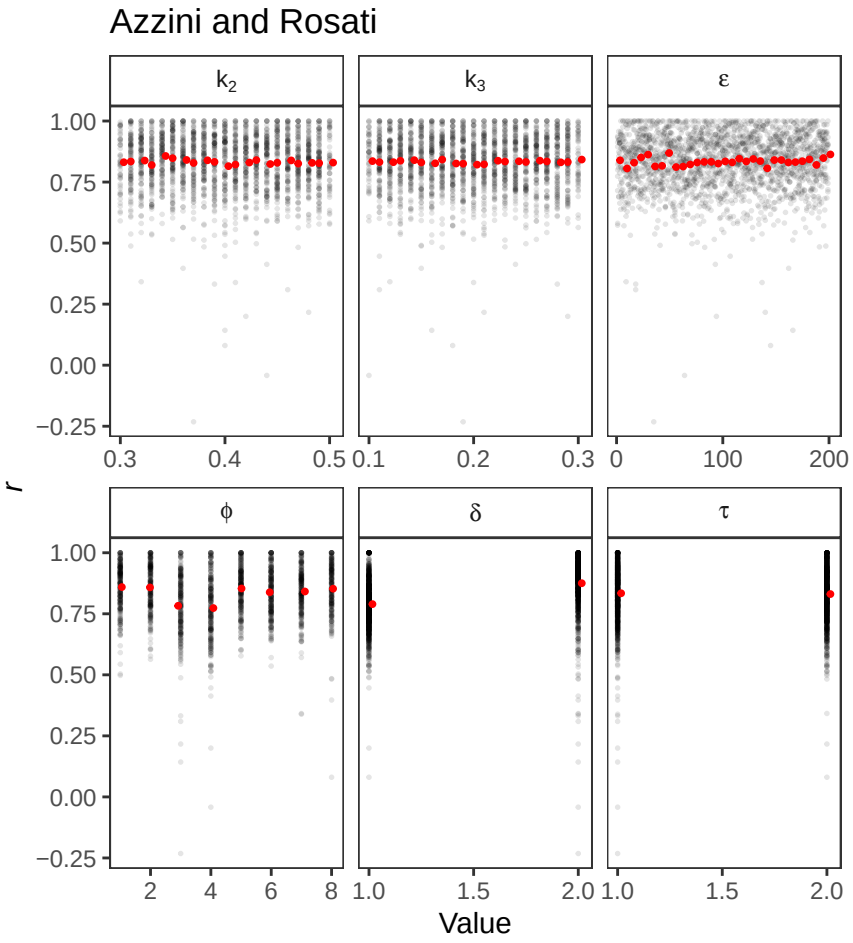
5 Sensitivity analysis

5.1 Scatterplots

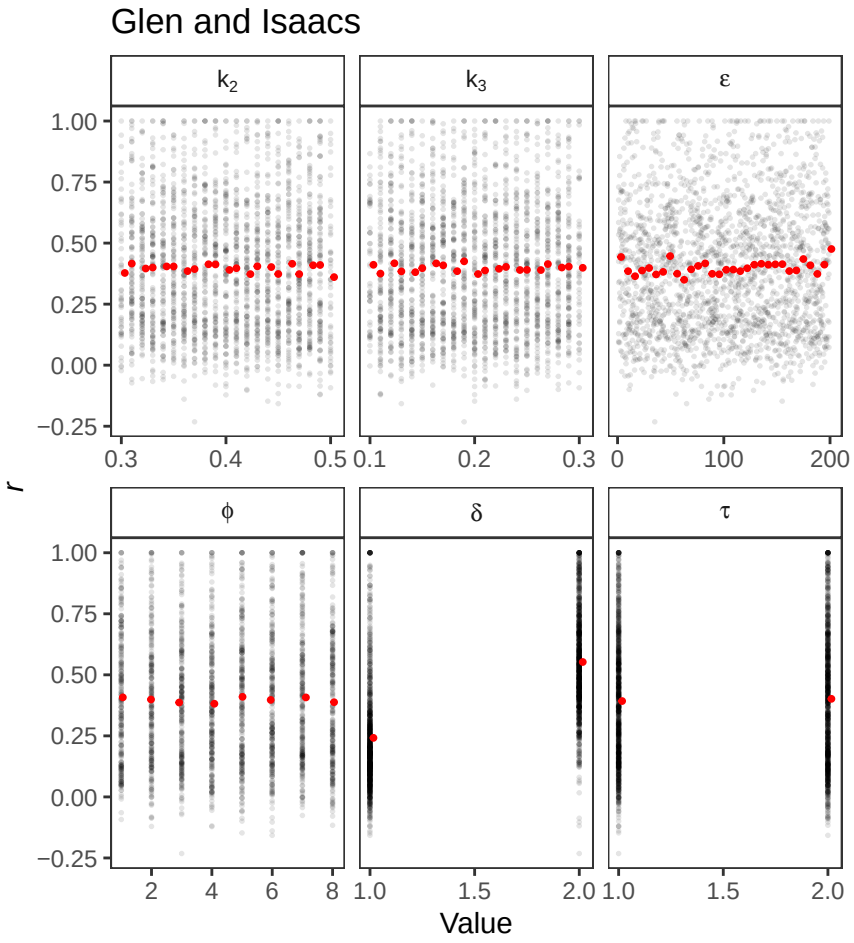
```
# SCATTERPLOTS OF MODEL OUTPUT AGAINST PARAMETERS ----------------------------------

A.ranks <- setnames(A.ranks, c("N_t", "k_2", "k_3"), c("N[t]", "k[2]", "k[3]"))
A.mae <- setnames(A.mae, c("N_t", "k_2", "k_3"), c("N[t]", "k[2]", "k[3]"))

scatter.ranks <- melt(A.ranks, measure.vars = c("k[2]", "k[3]", "epsilon", "phi", "delta", "tau
                      value.name = "value.parameters") %>%
  split(., .$estimator)

scatter.mae <- melt(A.mae, measure.vars = c("k[2]", "k[3]", "epsilon", "phi", "delta", "tau"),
                    value.name = "value.parameters") %>%
```

```
  split(., .$estimator)

gg.ranks <- list()
for(i in names(scatter.ranks)) {
  gg.ranks[[i]] <- ggplot(scatter.ranks[[i]], aes(value.parameters, value)) +
    geom_point(alpha = 0.1, size = 0.3) +
    facet_wrap(~ variable,
               scales = "free_x",
               labeller = label_parsed,
               ncol = 3) +
    scale_color_manual(values = c("#00BFC4", "#F8766D")) +
    scale_x_continuous(breaks = pretty_breaks(n = 3)) +
    stat_summary_bin(fun = "mean", geom = "point",
                     colour = "red", size = 0.7) +
    theme_AP() +
    labs(x = "Value", y = expression(italic(r))) +
    theme(strip.background = element_rect(fill = "white")) +
    ggtitle(names(scatter.ranks[i]))
}

gg.mae <- list()
for(i in names(scatter.mae)) {
  gg.mae[[i]] <- ggplot(scatter.mae[[i]], aes(value.parameters, value)) +
    geom_point(alpha = 0.1, size = 0.3) +
    facet_wrap(~ variable,
               scales = "free_x",
               labeller = label_parsed,
               ncol = 3) +
    scale_color_manual(values = c("#00BFC4", "#F8766D")) +
    scale_x_continuous(breaks = pretty_breaks(n = 3)) +
    stat_summary_bin(fun = "mean", geom = "point",
                     colour = "red", size = 0.7) +
    theme_AP() +
    scale_y_log10() +
    labs(x = "Value", y = "MAE") +
    theme(strip.background = element_rect(fill = "white")) +
    ggtitle(names(scatter.mae[i]))
}

gg.ranks
```

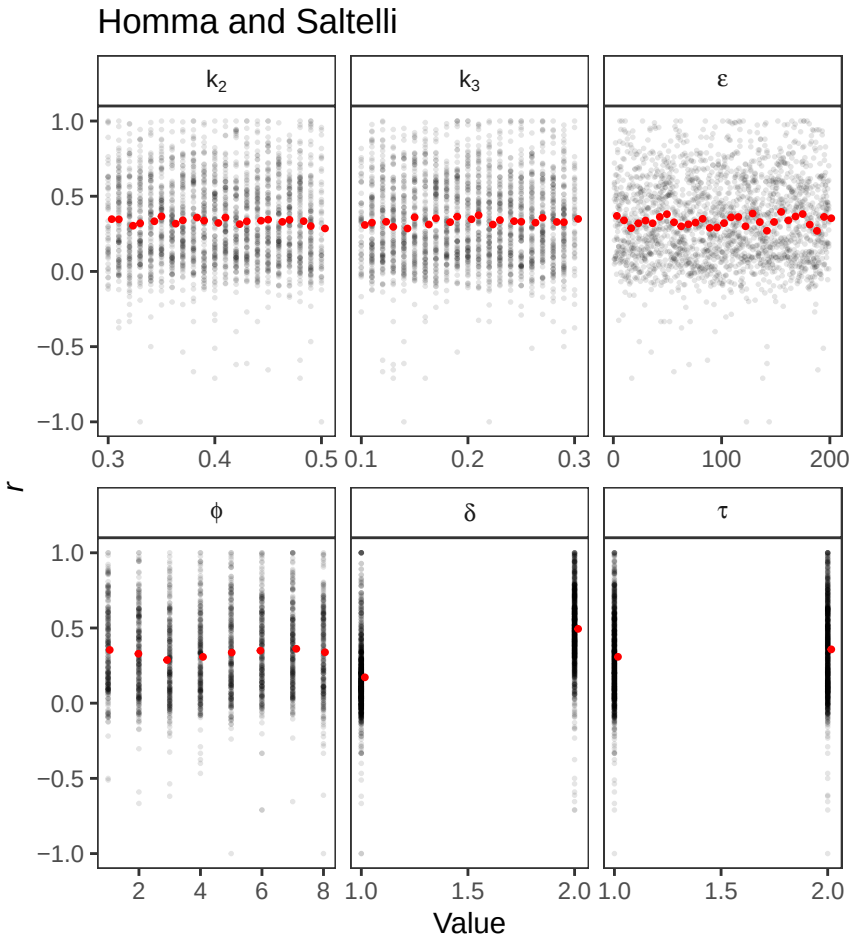
```
## $`Azzini and Rosati`
```



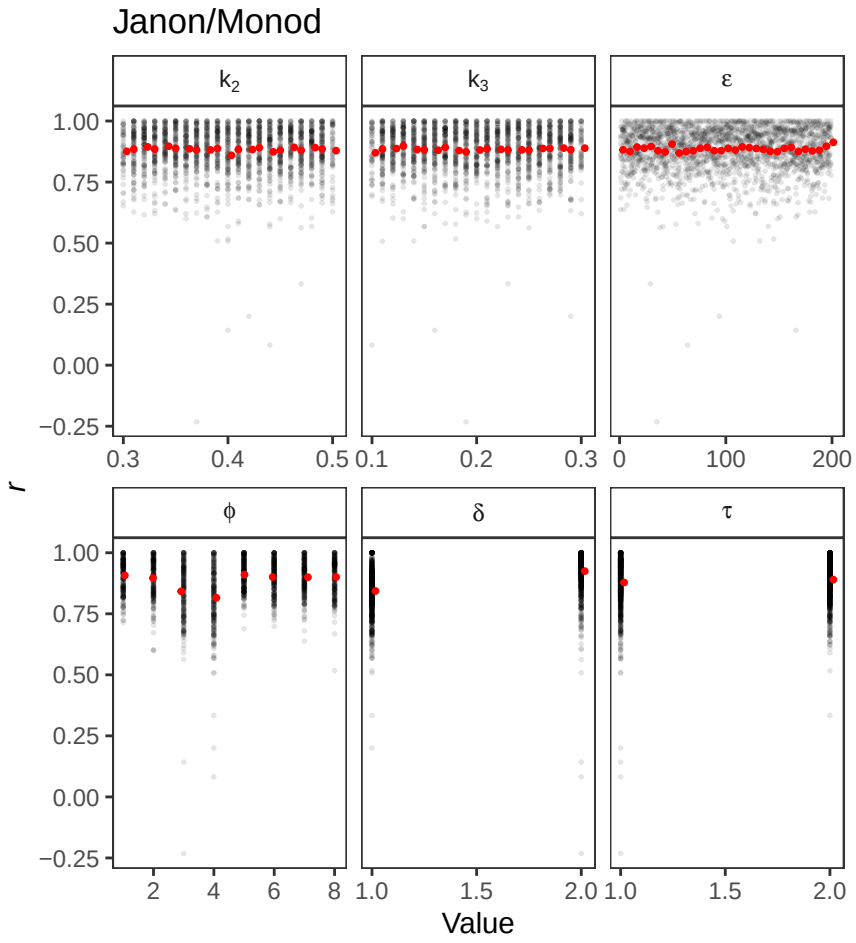

```
##
## $`Glen and Isaacs`
```



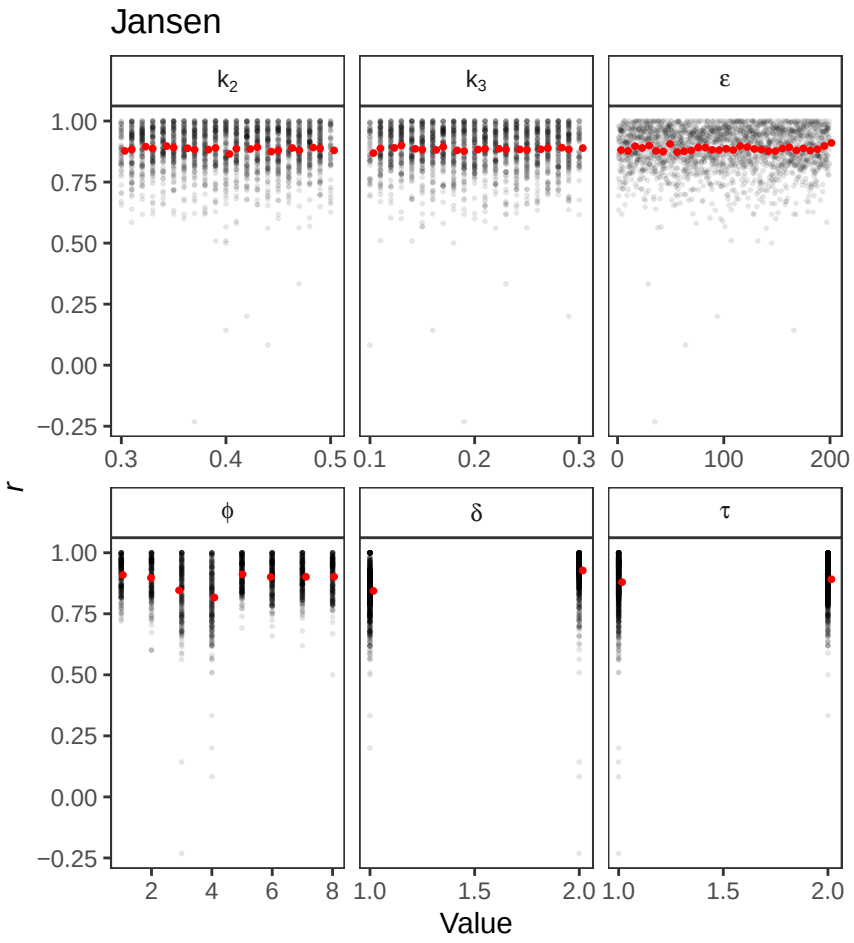

```
##
## $`Homma and Saltelli`
```


Homma and Saltelli
k2
k3
ε
ϕ
δ
τ
r
1.0
0.5
0.0
−0.5
−1.0
0.3
0.4
0.5
0.1
0.2
0.3
0
100
200
2
4
6
8
1.0
1.5
2.0
Value

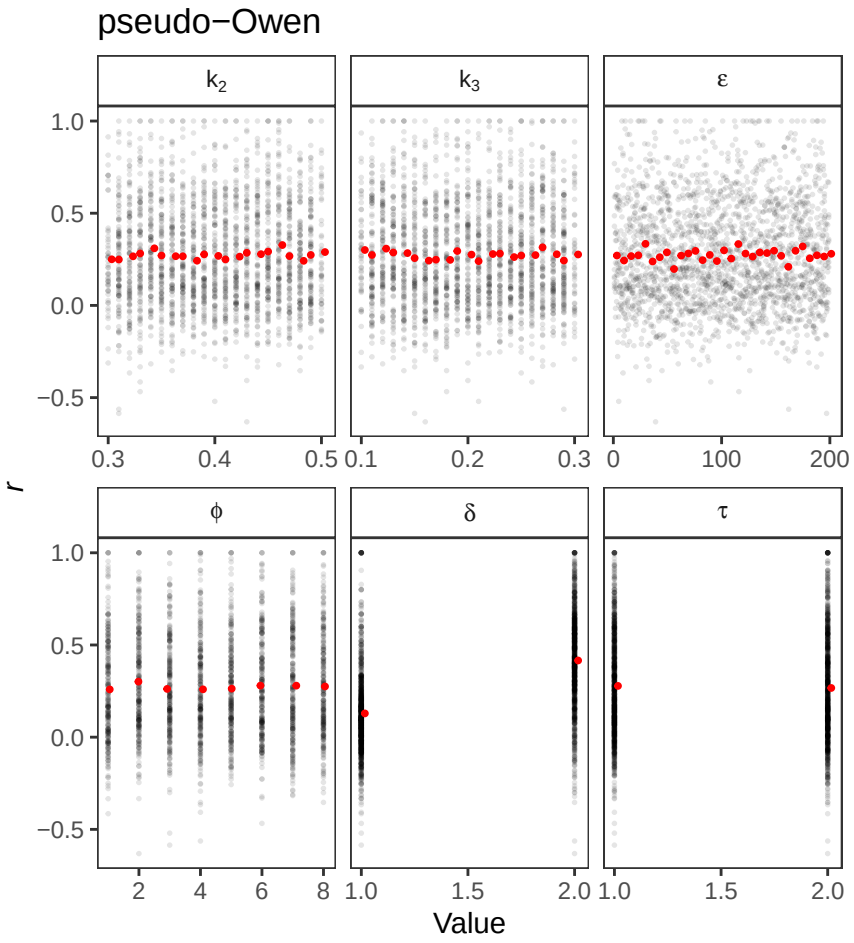
```
##
## $`Janon/Monod`
```



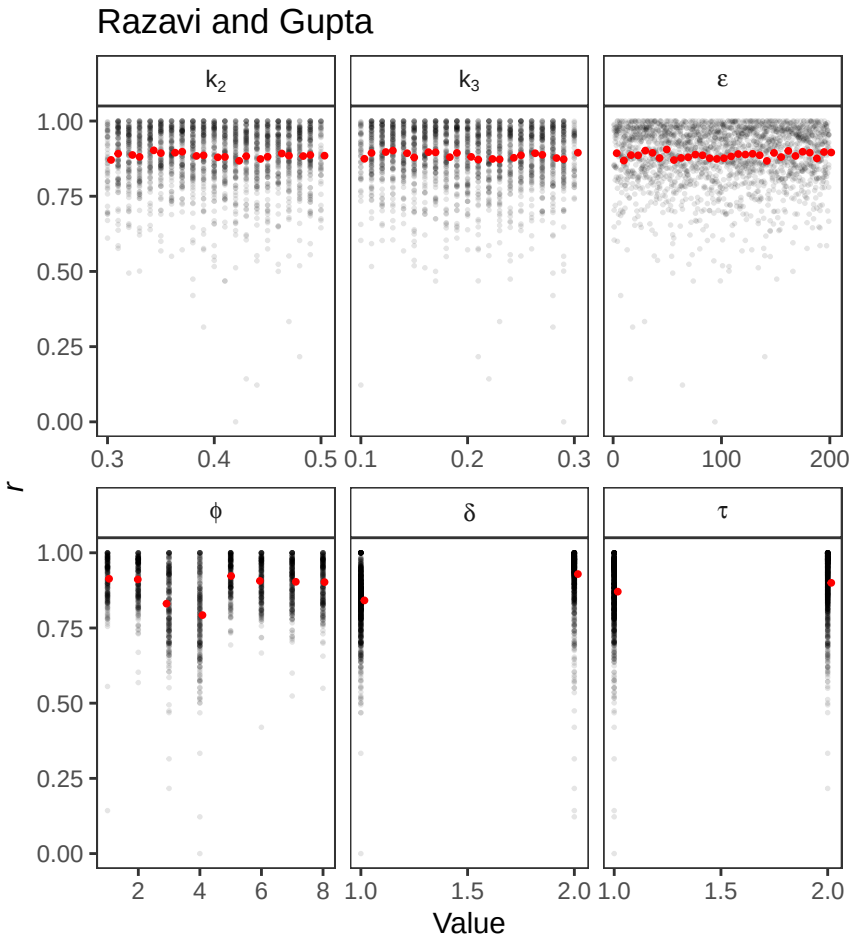

```
##
## $Jansen
```


Jansen
k2
k3
ε
ϕ
δ
τ
r
1.00
0.75
0.50
0.25
0.00
−0.25
0.3
0.4
0.5
0.1
0.2
0.3
0
100
200
2
4
6
8
1.0
1.5
2.0
Value

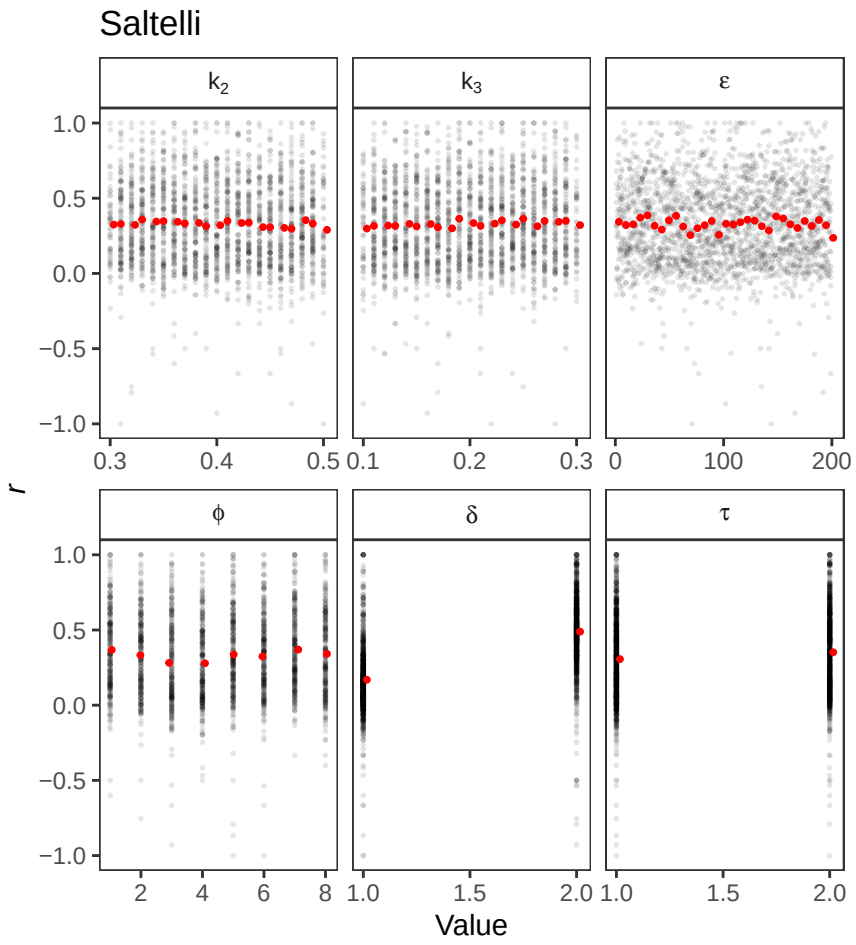
```
##
## $`pseudo-Owen`
```




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

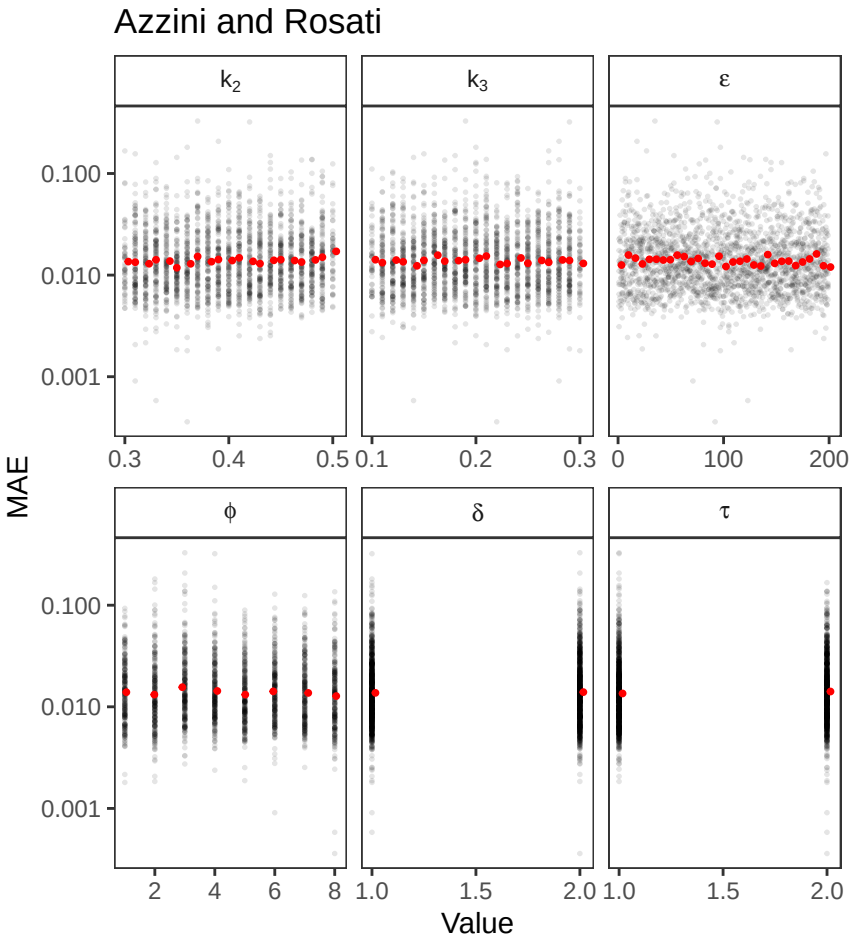

Razavi and Gupta
k2
k3
ε
ϕ
δ
τ
r
1.00
0.75
0.50
0.25
0.00
0.3
0.4
0.5
0.1
0.2
0.3
0
100
200
2
4
6
8
1.0
1.5
2.0
Value

```
##
## $Saltelli
```

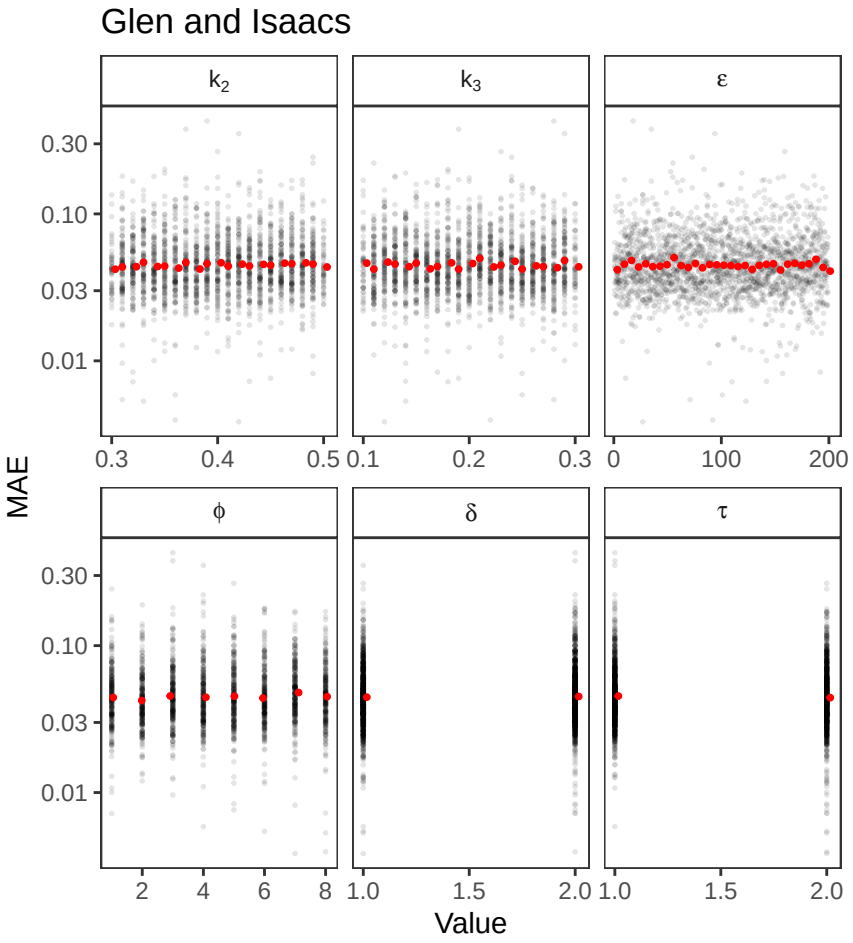



```
gg.mae
```

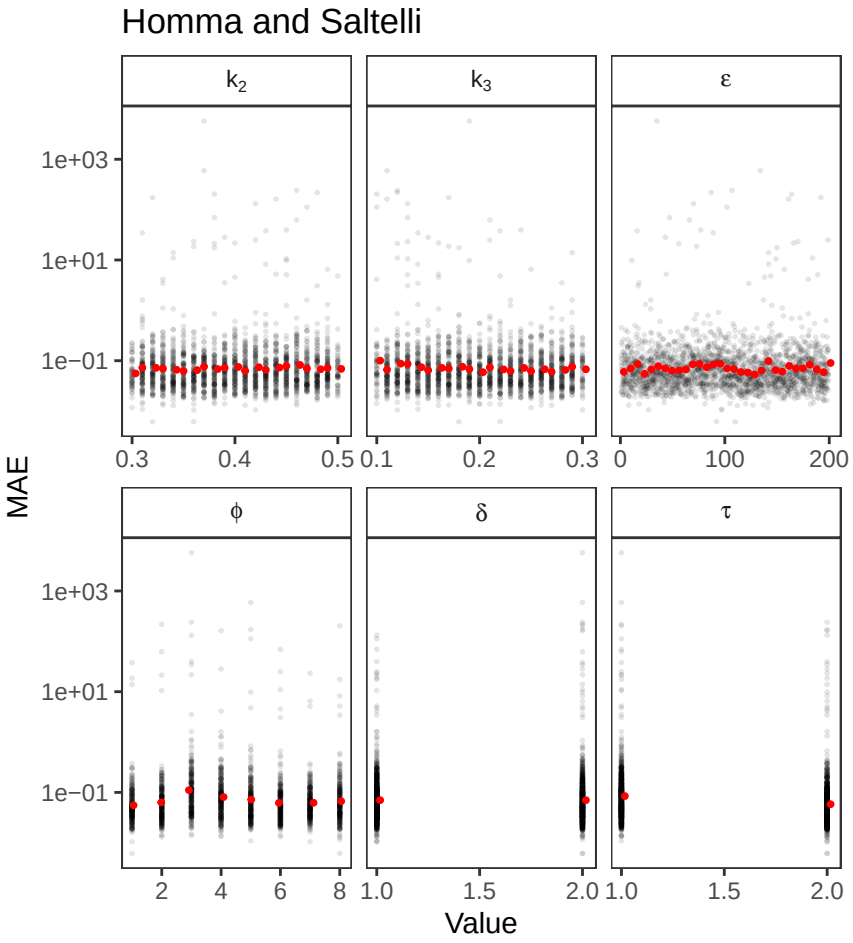
```
## $`Azzini and Rosati`
```



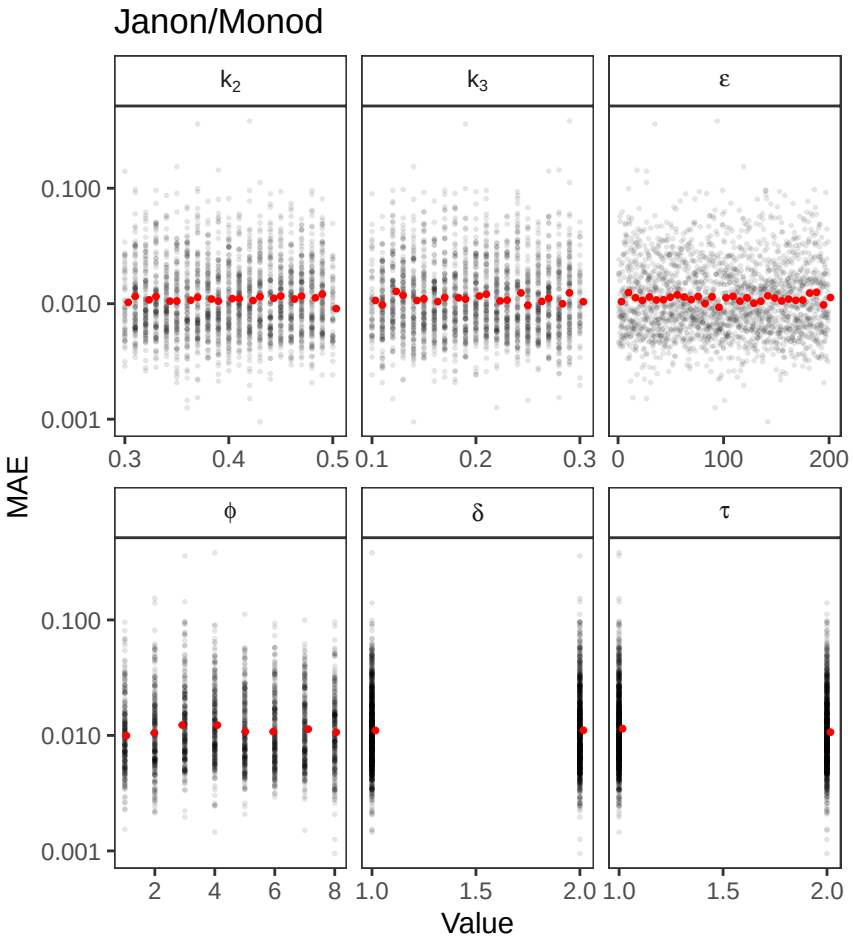

```
##
## $`Glen and Isaacs`
```



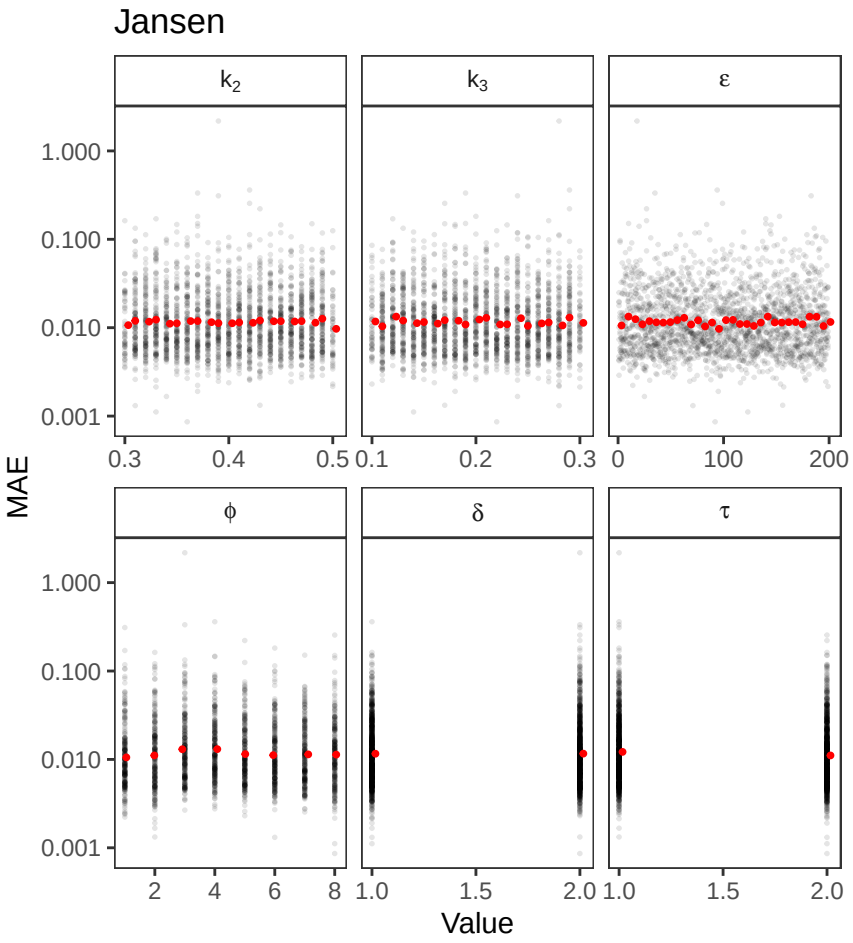

```
##
## $`Homma and Saltelli`
```


Homma and Saltelli
k2
k3
ε
ϕ
δ
τ
1e+03
1e+01
1e−01
MAE
0.3
0.4
0.5
0.1
0.2
0.3
0
100
200
2
4
6
8
1.0
1.5
2.0
Value

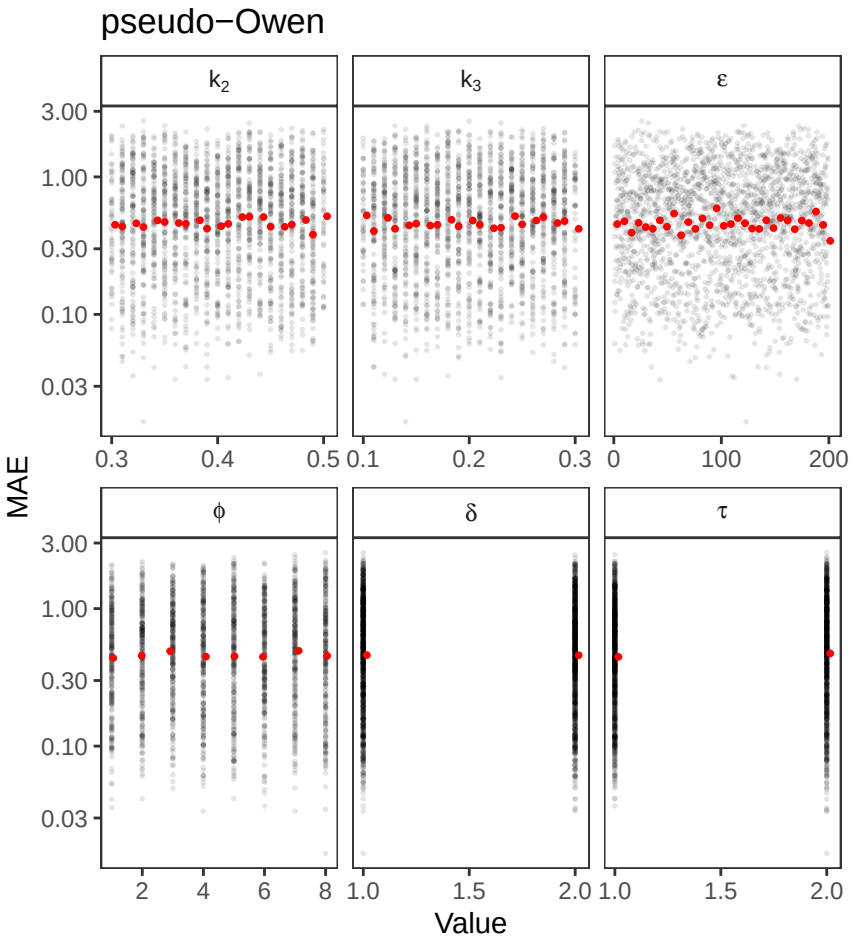
```
##
## $`Janon/Monod`
```


Janon/Monod
k2
k3
ε
ϕ
δ
τ
MAE
Value
0.100
0.010
0.001
0.3
0.4
0.5
0.1
0.2
0.3
0
100
200
2
4
6
8
1.0
1.5
2.0

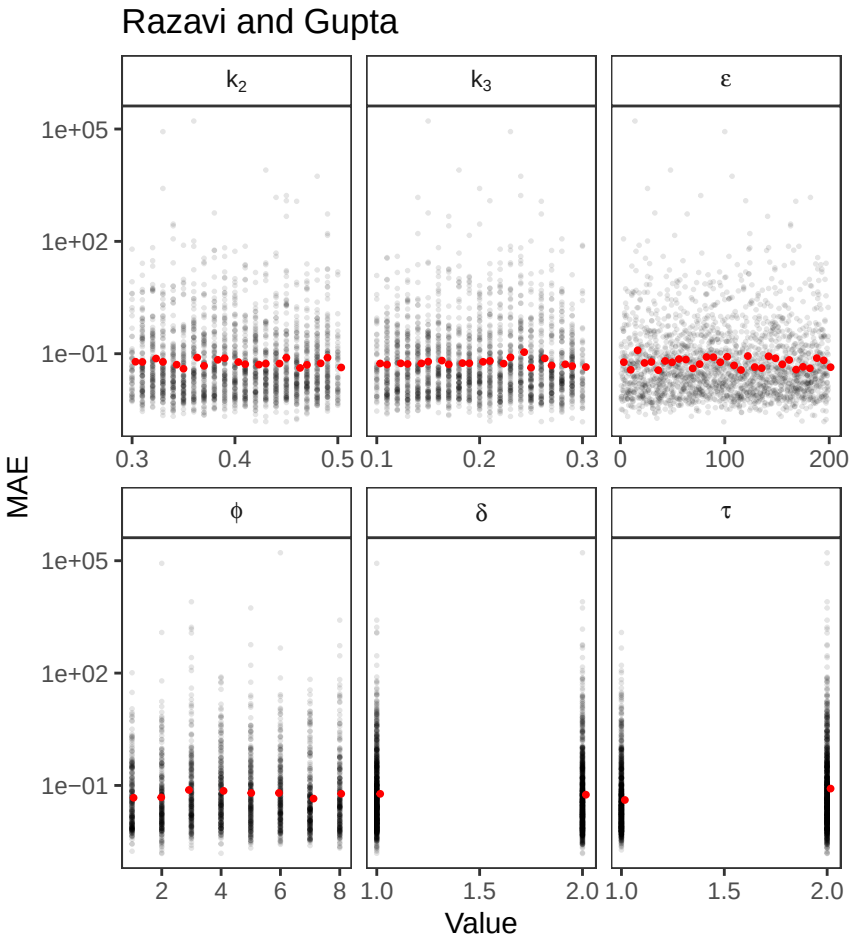
```
##
## $Jansen
```


Jansen
k2
k3
ε
ϕ
δ
τ
1.000
0.100
0.010
0.001
MAE
0.3
0.4
0.5
0.1
0.2
0.3
0
100
200
2
4
6
8
1.0
1.5
2.0
Value

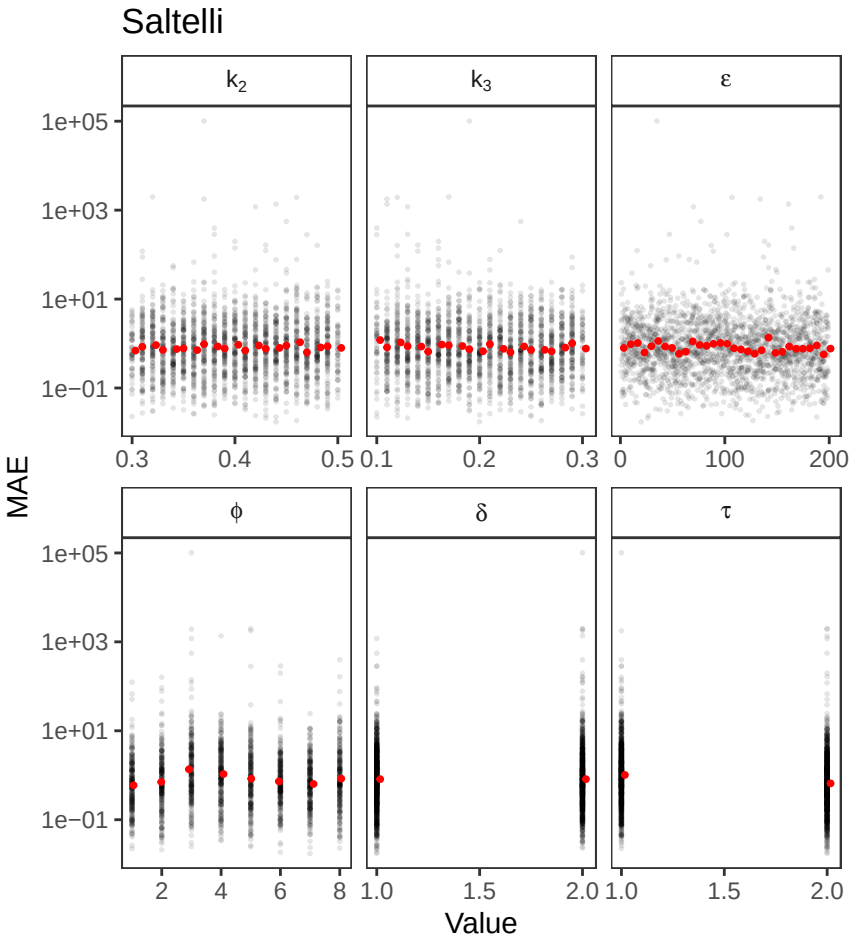
```
##
## $`pseudo-Owen`
```




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


Razavi and Gupta
k2
k3
ε
ϕ
δ
τ
MAE
1e+05
1e+02
1e−01
0.3
0.4
0.5
0.1
0.2
0.3
0
100
200
2
4
6
8
1.0
1.5
2.0
Value

```
##
## $Saltelli
```



5.2 Sobol' indices

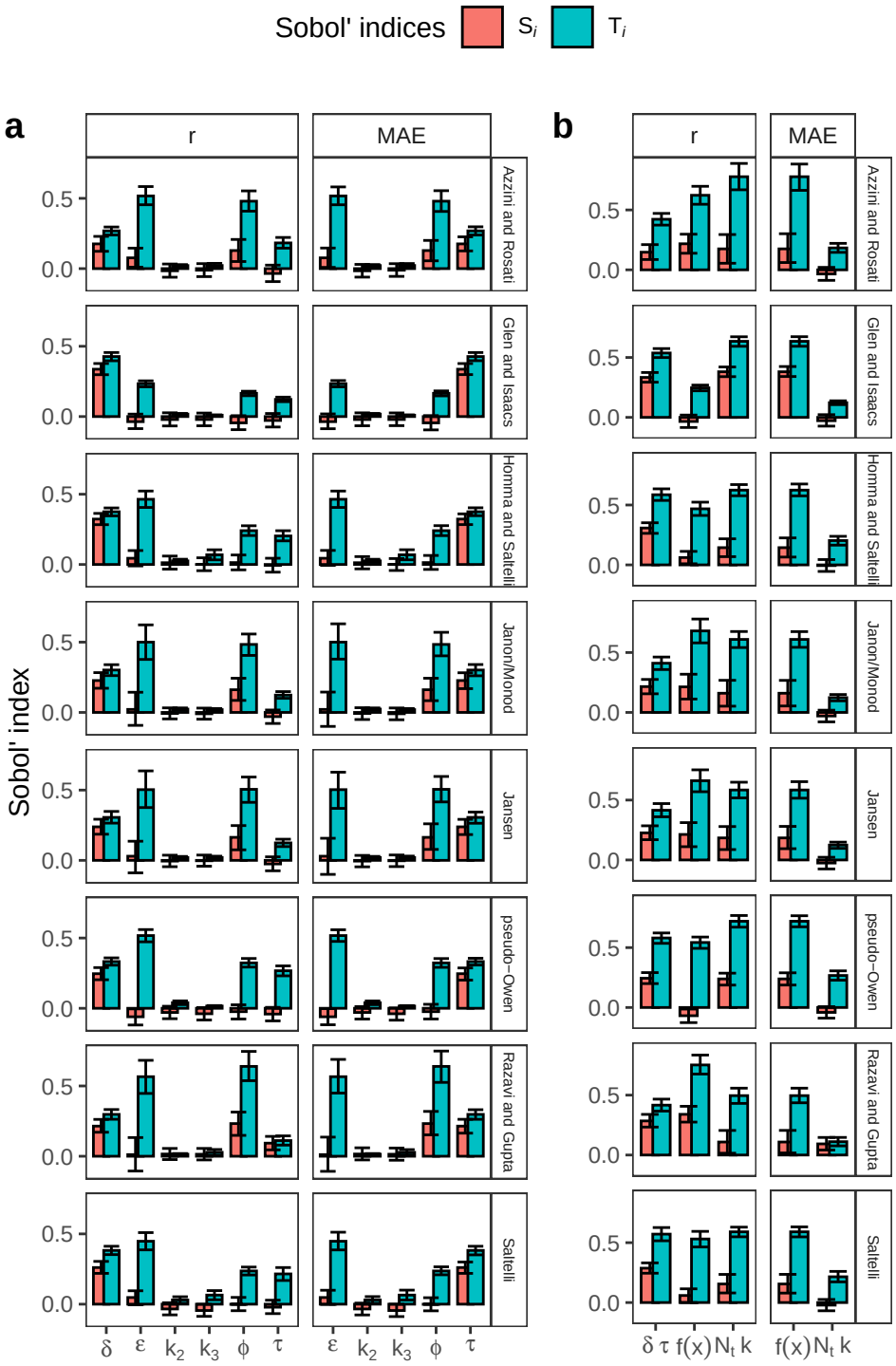
```
# SOBOL' INDICES ------------------------------------------------------------------

out <- list()
for(i in c("r", "MAE")) {
  if(i == "r") {
    params <- c("k[2]", "k[3]", "epsilon", "phi", "delta",
                "tau", "N[t]~k", "f(x)", "delta~tau")
  } else {
    params <- c("k[2]", "k[3]", "epsilon", "phi",
                "tau", "N[t]~k", "f(x)")
  }
  out[[i]] <- full.output[, sobol_indices(Y = value,
                                          N = N,
                                          params = params,
                                          first = "jansen",
                                          boot = TRUE,
                                          R = R,
                                          order = order),
                          estimator]
```

```
}

ind <- rbindlist(out, idcol = "type")
ind <- ind[, group:= ifelse(parameters %in% c("N[t]~k", "f(x)", "delta~tau"),
                            "Cluster", "Individual")] %>%
  .[, type:= factor(type, levels = c("r", "MAE"))]
```

5.3 Plot Sobol' indices

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

a <- lapply(c("Individual", "Cluster"), function(x)
  plot_sobol(ind[group == x]) +
    facet_grid(estimator~type,
               space = "free_x",
               scales = "free_x") +
    scale_x_discrete(labels = ggplot2:::parse_safe) +
    theme(strip.text.y = element_text(size = 6),
          legend.position = "none"))
```

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

legend <- get_legend(a[[1]] + theme(legend.position = "top"))
bottom <- plot_grid(a[[1]], a[[2]] + labs(x = "", y = ""), labels = "auto",
                    rel_widths = c(0.6, 0.4))
plot_grid(legend, bottom, ncol = 1, rel_heights = c(0.1, 0.9))
```



6 Session information

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

sessionInfo()
```

```
## R version 4.0.3 (2020-10-10)
## Platform: x86_64-apple-darwin17.0 (64-bit)
## Running under: macOS Catalina 10.15.7
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.0/Resources/lib/libRblas.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.0/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_0.4.10        ggrepel_0.9.1            sensobol_1.0.2
##  [4] logitnorm_0.8.38         benchmarkme_1.0.7        cowplot_1.1.1
##  [7] scales_1.1.1             data.table_1.14.0        Rfast_2.0.1
## [10] RcppZiggurat_0.1.6       doParallel_1.0.16        iterators_1.0.13
## [13] foreach_1.5.1            forcats_0.5.1            stringr_1.4.0
## [16] dplyr_1.0.6              purrr_0.3.4              readr_1.4.0
## [19] tidyr_1.1.3              tibble_3.1.1             ggplot2_3.3.3
## [22] tidyverse_1.3.1          RcppArmadillo_0.10.4.0.0 Rcpp_1.0.6
##
## loaded via a namespace (and not attached):
##  [1] lattice_0.20-44       lubridate_1.7.10      assertthat_0.2.1
##  [4] digest_0.6.27         utf8_1.2.1            R6_2.5.0
##  [7] cellranger_1.1.0      backports_1.2.1       reprex_2.0.0
## [10] evaluate_0.14         httr_1.4.2            pillar_1.6.0
## [13] Rdpack_2.1.1          rlang_0.4.11          readxl_1.3.1
## [16] rstudioapi_0.13       Matrix_1.3-3          rmarkdown_2.8
## [19] munsell_0.5.0         broom_0.7.6           compiler_4.0.3
## [22] modelr_0.1.8          xfun_0.22             pkgconfig_2.0.3
## [25] htmltools_0.5.1.1     tidyselect_1.1.1      codetools_0.2-18
## [28] fansi_0.4.2           crayon_1.4.1          dbplyr_2.1.1
## [31] withr_2.4.2           rbibutils_2.1.1       grid_4.0.3
## [34] jsonlite_1.7.2        gtable_0.3.0          lifecycle_1.0.0
## [37] DBI_1.1.1             magrittr_2.0.1        cli_2.5.0
## [40] stringi_1.5.3         fs_1.5.0              benchmarkmeData_1.0.4
## [43] xml2_1.3.2            ellipsis_0.3.2        generics_0.1.0
## [46] vctrs_0.3.8           tools_4.0.3           glue_1.4.2
## [49] hms_1.0.0             yaml_2.2.1            colorspace_2.0-1
## [52] rvest_1.0.0           knitr_1.33            haven_2.4.1
```

```
## 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
```

Becker, William. 2020. "Metafunctions for benchmarking in sensitivity analysis." *Reliability Engineering and System Safety* 204: 107189. https://doi.org/10.1016/j.ress.2020.107189.