Discrepancy measures for sensitivity analysis in mathematical modeling

R code

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Contents

1 Preliminary functions

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

# 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)
    }
  }
}

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.margin=margin(0, 0, 0, 0),
          legend.box.margin=margin(-7,-7,-7,-7),
          legend.key = element_rect(fill = "transparent",
                                    color = NA),
          strip.background = element_rect(fill = "white"))
}

# Load the packages
loadPackages(c("sensobol", "data.table", "tidyverse", "parallel",
               "RcppAlgos", "scales", "doParallel", "benchmarkme",
               "cowplot", "wesanderson", "benchmarkme"))

# CPP CODE ---------------------------------------------------------------------

# Source cpp code ------------------------------
cpp_functions <- c("cpp_functions.cpp", "L2star_functions.cpp",
                   "L2_functions.cpp", "L2centered_functions.cpp",
                   "L2wraparound_functions.cpp", "L2modified_functions.cpp")

for(i in 1:length(cpp_functions)) {
  Rcpp::sourceCpp(cpp_functions[i])
}
```

2 Goal

We aim at checking whether discrepancy measures can be used as a sensitivity measure to reliably rank parameters in terms of their influence in the model output. To that aim, we explore how well the symmetric L2-discrepancy measure ranks the most important parameters of a set of functions, including for the moment the Oakley and O'Hagan 2004 and the Bratley et al. 1992 functions, and compare its efficacy with that of the Jansen estimator. We do the comparison on Savage-score transformed ranks (Iman and Conover 1987).

The discrepancy is computed directly on the plane of the X_i, Y scatterplots where X_i is a coordinate $(0, 1)$ of the input hypercube and Y is the output rescaled in $0, 1$. For each of the k scatterplots, the points are sorted by one of the X_i. The idea is that a ''pattern" (=effect) corresponds to a deviation from a uniform distribution of points (noise) for a non-influential variable: the largest the effect, the larger the discrepancy, e.g., there are areas in the plot where points are denser and areas where they are more rarefied.

One might wonder why use a discrepancy measure when there are the Sobol' indices. The reply is that many do not understand the theory behind them (and the same applies to moment independent methods or VARS), while everyone understands scatterplots. 'Explaining' discrepancy as a measure of the non-uniformity of the scatterplots appears an avenue likely to appeal to some users.

3 Required functions

3.1 C++ functions

3.2 Savage ranks function

```
# SAVAGE SCORES FUNCTION ------------------------------------------------------

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)
}
```

3.3 Discrepancy function

```
# DISCREPANCY FUNCTION --------------------------------------------------------

# This is based on the function discrepancyCriteria_cpp of
# the sensitivity package

# Function to rescale ---------------------------
rescale_fun <- function(x) (x - min(x)) / (max(x) - min(x))

# Function ------------------------------------
```

```r
discrepancy_fun <- function (design, type) {

  X <- as.matrix(design)
  dimension <- ncol(X)
  n <- nrow(X)

  # Reescale if needed-------

  if (min(X) < 0 || max(X) > 1) {

    X <- apply(X, 2, rescale_fun)
  }

  # Compute discrepancy

  if (type == "symmetric") {

    P <- 1 + 2 * X - 2 * X^2
    s1 <- DisS2_Rowprod(t(P), dimension)
    s2 <- DisS2_Crossprod(c(t(X)), dimension)
    R <- sqrt(((4/3)^dimension) - ((2/n) * s1) + ((2^dimension/n^2) * s2))

  } else if (type == "star") {

    dL2 <- DisL2star_Crossprod(t(X), dimension)
    R <- sqrt(3^(-dimension) + dL2)

  } else if (type == "L2") {

    P <- X * (1 - X)
    s1 <- DisL2_Rowprod(t(P), dimension)
    s2 <- DisL2_Crossprod(c(t(X)), dimension)
    R <- sqrt(12^(-dimension) - (((2^(1 - dimension))/n) * s1) + ((1/n^2) * s2))

  } else if (type == "centered") {

    P <- 1 + 0.5 * abs(X - 0.5) - 0.5 * (abs(X - 0.5)^2)
    s1 <- DisC2_Rowprod(t(P), dimension)
    s2 <- DisC2_Crossprod(c(t(X)), dimension)
    R <- sqrt(((13/12)^dimension) - ((2/n) * s1) + ((1/n^2) * s2))

  } else if (type == "wraparound") {

    s1 <- DisW2_Crossprod(t(X), dimension)
    R <- sqrt(-(4/3)^dimension + (1/n^2) * s1)

  } else if (type == "modified") {
```

```
    P <- 3 - X^2
    s1 <- DisM2_Rowprod(t(P), dimension)
    s2 <- DisM2_Crossprod(c(t(X)), dimension)
    R <- sqrt(((4/3)^dimension) - (((2^(1 - dimension))/n) * s1) + ((1/n^2) * s2))

  }
  return(R)
}

# Discrepancy function --------------------------
discrepancy <- function(mat, y, params, type) {
  value <- sapply(1:ncol(mat), function(j) {
    design <- cbind(mat[, j], y)
    value <- discrepancy_fun(design = design, type = type)
  })
  return(value)
}
```

3.4 Jansen estimator

```
# FUNCTION TO COMPUTE JANSEN TI ------------------------------------------------

jansen_ti <- function(d, N, params) {
  m <- matrix(d, nrow = N)
  k <- length(params)
  Y_A <- m[, 1]
  Y_AB <- m[, -1]
  f0 <- (1 / length(Y_A)) * sum(Y_A)
  VY <- 1 / length(Y_A) * sum((Y_A - f0) ^ 2)
  value <- (1 / (2 * N) * Rfast::colsums((Y_A - Y_AB) ^ 2)) / VY
  return(value)
}
```

```
# LIST OF FUNCTIONS ------------------------------------------------------------

# NEW FUNCTIONS ----------------------------------

f1_fun <- function(x) 10 * x[, 1] + 0.2 * x[, 2]^3

f2_fun <- function(x) 2 * x[, 1] - x[, 2]^2

f3_fun <- function(x) x[, 1]^2 + x[, 2]^4 + x[, 1] * x[, 2] + x[, 2] * x[, 3]^4

f4_fun <- function(x) 0.2 * exp(x[, 1] - 3) + 2.2 * abs(x[, 2]) + 1.3 * x[, 2]^6 -
  2 * x[, 2]^2 - 0.5 * x[, 2]^4 - 0.5 * x[, 1]^4 + 2.5 * x[, 1]^2 + 0.7 * x[, 1]^3 +
  3 / ((8 * x[, 1] - 2)^2 + (5 * x[, 2] - 3)^2 + 1) + sin(5 * x[, 1]) * cos(3 * x[, 1]^2)
```

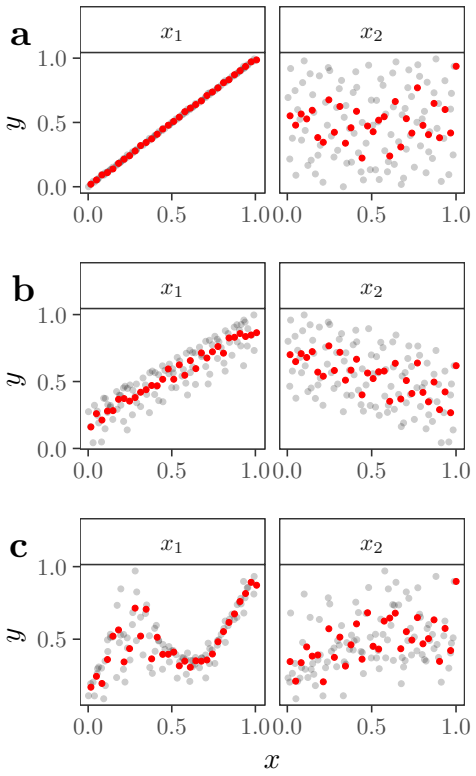
```r
f6_fun <- function(x) 0.2 * exp(x[, 1] + 2 * x[, 2])

fun_vec <- paste("f", 1:4, "_fun", sep = "")

f_list <- list(f1_fun, f2_fun, f3_fun, f4_fun)
names(f_list) <- fun_vec

# RUN FUNCTIONS ------------------------------------------------------------

output <- ind <- list()

for (i in names(f_list)) {

  if(i == "f3_fun") {

    k <- 3

  } else {

    k <- 2
  }
  params <- paste("$x_", 1:k, "$", sep = "")
  N <- 100
  mat <- sobol_matrices(N = N, params = params, scrambling = 1)
  y <- f_list[[i]](mat)
  y <- rescale_fun(y)
  ind[[i]] <- sobol_indices(Y = y, N = N, params = params)
  output[[i]] <- plot_scatter(data = mat, N = N, Y = y, params = params) +
    labs(x = "$x$", y = "$y$") +
    scale_x_continuous(breaks = pretty_breaks(n = 3)) +
    scale_y_continuous(breaks = pretty_breaks(n = 3)) +
    theme(plot.margin = unit(c(0, 0.2, 0, 0), "cm"))
}

ind
```

```
## $f1_fun
##
## First-order estimator: saltelli | Total-order estimator: jansen
##
## Total number of model runs: 400
##
## Sum of first order indices: 1.002007
##        original sensitivity parameters
## 1: 1.0003862784          Si      $x_1$
## 2: 0.0016209664          Si      $x_2$
## 3: 1.0135578141          Ti      $x_1$
```

```
## 4: 0.0003635617          Ti      $x_2$
##
## $f2_fun
##
## First-order estimator: saltelli | Total-order estimator: jansen
##
## Total number of model runs: 400
##
## Sum of first order indices: 0.9938603
##     original sensitivity parameters
## 1: 0.8111121          Si      $x_1$
## 2: 0.1827481          Si      $x_2$
## 3: 0.8062738          Ti      $x_1$
## 4: 0.2011789          Ti      $x_2$
##
## $f3_fun
##
## First-order estimator: saltelli | Total-order estimator: jansen
##
## Total number of model runs: 500
##
## Sum of first order indices: 0.9551073
##      original sensitivity parameters
## 1: 0.39436570          Si      $x_1$
## 2: 0.51742917          Si      $x_2$
## 3: 0.04331248          Si      $x_3$
## 4: 0.46291049          Ti      $x_1$
## 5: 0.49048129          Ti      $x_2$
## 6: 0.04838575          Ti      $x_3$
##
## $f4_fun
##
## First-order estimator: saltelli | Total-order estimator: jansen
##
## Total number of model runs: 400
##
## Sum of first order indices: 0.7475612
##      original sensitivity parameters
## 1: 0.65955374          Si      $x_1$
## 2: 0.08800745          Si      $x_2$
## 3: 0.85677289          Ti      $x_1$
## 4: 0.32296577          Ti      $x_2$
```

```r
# PLOT LIST OF FUNCTIONS ------------------------------

plot_list <- list(output[[1]] + labs(x = "", y = "$y$"),
                  output[[2]] + labs(x = "", y = "$y$"),
                  output[[4]])
```

```
scat_plot <- plot_grid(plotlist = plot_list, ncol = 1, labels = "auto")
scat_plot
```



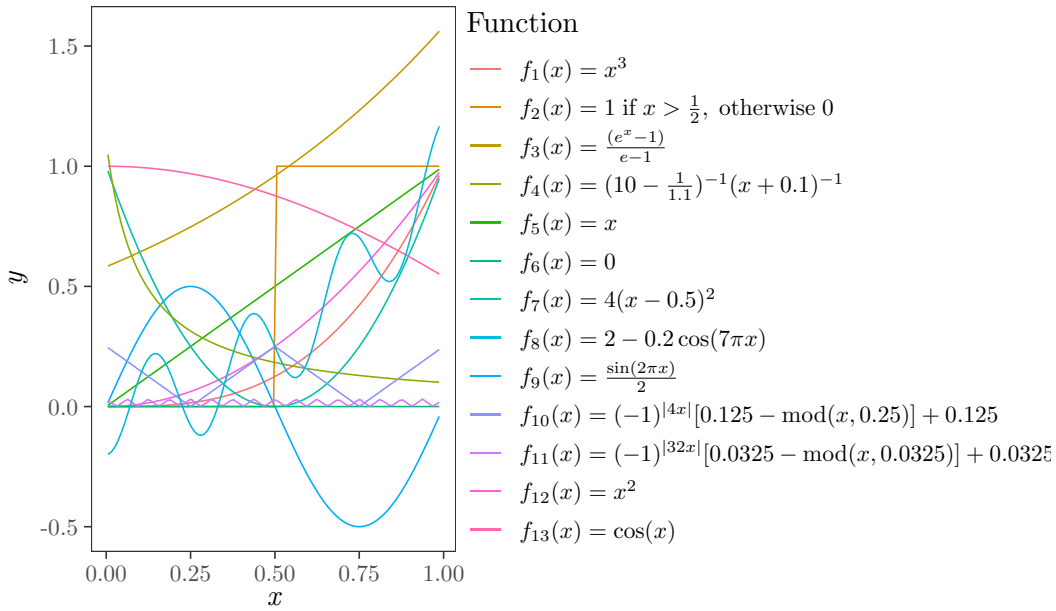
4 The metamodel

```
# RANDOM FUNCTIONS AND DISTRIBUTIONS ------------------------------------------

# Functions -----------------------------------
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),
  Piecewise.large = function(x) ((-1) ^ as.integer(4 * x) *
                                   (0.125 - (x %% 0.25)) + 0.125),
  Piecewise.small = function(x) ((-1) ^ as.integer(32 * x) *
                                   (0.03125 - 2 * (x %% 0.03125)) + 0.03125) / 2,
  Oscillation = function(x) x ^ 2 - 0.2 * cos(7 * pi * x)
```

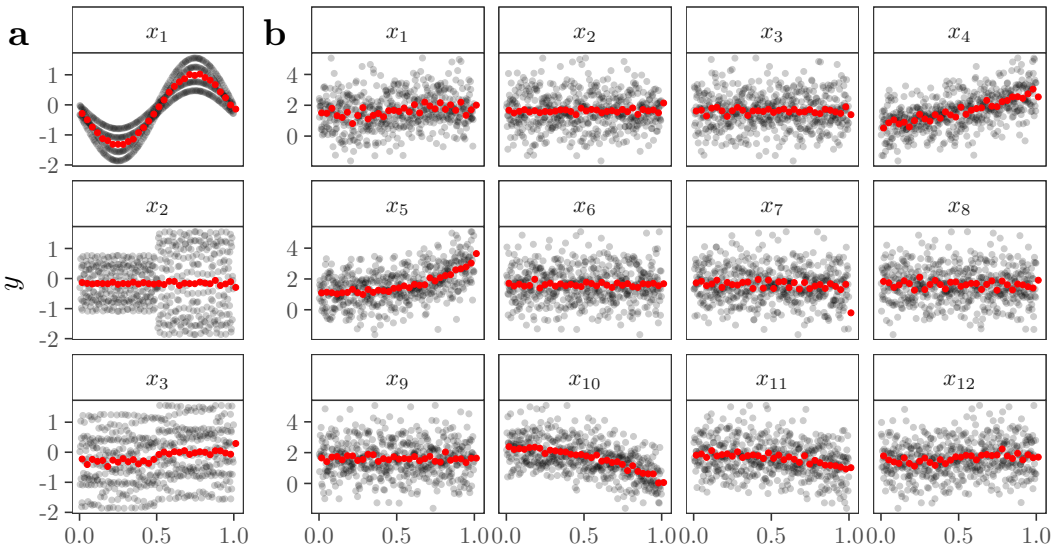
```
)

# Random distributions  ------------------------
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) logitnorm::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 METAFUNCTION ----------------------------------------------------------

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("$f_1(x) = x^3$",
                                  "$f_2(x) = 1 \\hspace{1mm} \\mbox{if} \\hspace{1mm} x > \\fra
                                  "$f_3(x) = \\frac{(e^x - 1)}{e-1}$",
                                  "$f_4(x) = (10-\\frac{1}{1.1})^{-1}(x + 0.1)^{-1}$",
                                  "$f_5(x) = x$",
                                  "$f_6(x) = 0$",
                                  "$f_7(x) = 4(x - 0.5)^2$",
                                  "$f_8(x) = 2 - 0.2 \\cos(7 \\pi x)$",
                                  "$f_9(x) = \\frac{\\sin(2 \\pi x)}{2}$",
                                  "$f_{10}(x) = (-1)^ {|4x|} [0.125- \\mbox{mod}(x, 0.25)] + 0
```

```
                                    "$f_{11}(x) = (-1)^ {|32x|} [0.0325-\\mbox{mod}(x, 0.0325)] +
                                    "$f_{12}(x) = x^2$",
                                    "$f_{13}(x) = \\cos(x)$")) +
  theme_AP() +
  theme(legend.text.align = 0)
```




```
# PLOT SCATTERS FROM METAFUNCTION ------------------------------------------

k_epsilon <- list(c(3, 2), c(12, 6))
out <- list()

for(i in 1:length(k_epsilon)) {
  N <- 2^9
  params <- paste("$x_{", 1:k_epsilon[[i]][[1]], "}$", sep = "")
  mat <- sobol_matrices(N = N, params = params)
  y <- metafunction(mat, epsilon = k_epsilon[[i]][[2]])
  out[[i]] <- plot_scatter(data = mat, N = N, Y = y, params = params) +
    scale_x_continuous(breaks = pretty_breaks(n = 3)) +
    theme(plot.margin = unit(c(0, 0.1, 0, 0), "cm")) +
    labs(x = "", y = "$y$")

}

scatters_plot <- plot_grid(out[[1]] + facet_wrap(~variable, ncol = 1),
          out[[2]] + facet_wrap(~variable, ncol = 4) + labs(y = ""),
          ncol = 2, labels = "auto", rel_widths = c(0.24, 0.76))

scatters_plot
```



4.1 Define the model

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

model_fun <- function(tau, epsilon, base.sample.size, cost.discrepancy, phi, k) {

  params <- paste("X", 1:k, sep = "")

  if (tau == 1) {

    type <- "R"

  } else if (tau == 2) {

    type <- "QRN"
  }
  set.seed(epsilon)
  discrepancy.mat <- sobol_matrices(matrices = "A", N = cost.discrepancy,
                                    params = params,
                                    type = type)

  set.seed(epsilon)
  jansen.mat <- sobol_matrices(matrices = c("A", "AB"), N = base.sample.size,
                               params = params,
                               type = type)

  all.matrices <- rbind(discrepancy.mat, jansen.mat)
  set.seed(epsilon)
  transformed.all.matrices <- random_distributions(X = all.matrices, phi = phi)

  y <- sensobol::metafunction(data = transformed.all.matrices, epsilon = epsilon)
```

```
  type <- c("symmetric", "star", "L2", "centered", "wraparound", "modified")

  discrepancy.value <- lapply(type, function(x)
    discrepancy(mat = all.matrices[1:cost.discrepancy, ],
                y = y[1:cost.discrepancy], params = params, type = x))


  jansen.value <- jansen_ti(d = y[(cost.discrepancy + 1):length(y)],
                            N = base.sample.size, params = params)

  savage.discrepancy <- lapply(discrepancy.value, savage_scores)
  jansen.discrepancy <- savage_scores(jansen.value)

  out <- lapply(savage.discrepancy, function(x)
    cor(x, jansen.discrepancy))

  return(out)
}
```

4.2 Run the model

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

N <- 2^10
params <- c("epsilon", "phi", "k", "tau", "base.sample.size")
mat <- sobol_matrices(matrices = "A", N = N, params = params)

# Define distributions -------------------------

mat[, "epsilon"] <- floor(qunif(mat[, "epsilon"], 1, 200))
mat[, "phi"] <- floor(mat[, "phi"] * 8) + 1
mat[, "k"] <- floor(qunif(mat[, "k"], 3, 50))
mat[, "tau"] <- floor(mat[, "tau"] * 2) + 1
mat[, "base.sample.size"] <- floor(qunif(mat[, "base.sample.size"], 10, 100))

cost.jansen <- mat[, "base.sample.size"] * (mat[, "k"] + 1)
cost.discrepancy <- cost.jansen

final.mat <- cbind(mat, cost.jansen, cost.discrepancy)
```

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

y <- mclapply(1:nrow(final.mat), function(i) {
  model_fun(tau = final.mat[i, "tau"],
            epsilon = final.mat[i, "epsilon"],
            base.sample.size = final.mat[i, "base.sample.size"],
            cost.discrepancy = final.mat[i, "cost.discrepancy"],
```

```
            phi = final.mat[i, "phi"],
            k = final.mat[i, "k"])},
  mc.cores = floor(detectCores() * 0.75))
```

4.3 Arrange model output

```
# ARRANGE DATA ------------------------------------------------------------

y <- lapply(y, unlist)
output <- data.table(do.call(rbind, y))
discrepancy_methods <- c("symmetric", "star", "L2", "centered",
                         "wraparound", "modified")
colnames(output) <- discrepancy_methods

final.output <- data.table(cbind(final.mat, output))

# Write model output
fwrite(final.output, "final.output.csv")
```

5 Model for discretization

5.1 Define the model

```
# DISCRETIZATION FUNCTIONS ------------------------------------------------

plot_ti <- function(ind, params) {

  out <- data.table(ind) %>%
    .[, parameters:= params] %>%
    ggplot(., aes(parameters, ind)) +
    geom_bar(stat = "identity", fill = "#00BFC4", color = "black") +
    labs(x = "", y = "$T_i$") +
    theme_AP()

  return(out)
}

# FUNCTION TO DISCRETIZE THE BRATLEY ET AL. FUNCTION ----------------------

discretization_fun <- function(N, k, epsilon, plot.scatterplot = FALSE,
                               plot.jansen = FALSE, savage.scores = TRUE) {

  params <- paste("$x_", 1:k, "$", sep = "")
  mat <- sobol_matrices(N = N, params = params, matrices = c("A", "AB"))
  mat2 <- mat # mat2 = matrix for discretization
```

```
  # Determine how many parameters to discretize (n.discrete),
  # which parameters to discretize (n.parameters), and the
  # number of levels (n.levels)
  set.seed(epsilon)
  n.discrete <- sample(1:ceiling(k / 2), size = 1)
  set.seed(epsilon)
  n.parameters <- sample(1:k, size = n.discrete)
  set.seed(epsilon)
  n.levels <- sample(2:5, size = 1)

  # Discretization of the sampled parameters
  mat2[, n.parameters] <- floor(mat2[, n.parameters] * n.levels) + 1

  # Compute output and sobol indices (Jansen estimator)
  y <- bratley1992_Fun(mat2)
  ind2 <- jansen_ti(d = y, N = N, params = params)

  # Conditional
  if (plot.scatterplot == TRUE) {
    out <- plot_scatter(data = mat2, N = N, Y = y, params = params)
  }
  if (plot.jansen == TRUE) {
    out <- plot_ti(ind = ind2, params = params)
  }
  if(savage.scores == TRUE) {
    sobol_ranks <- savage_scores(ind2)

    # Compute discrepancy
    type <- c("symmetric", "star", "L2", "centered", "wraparound", "modified")
    discrepancy.out <- lapply(type, function(x)
      discrepancy(mat = mat[1:N, ], y = y[1:N], params = params, type = x))

    discrepancy.ranks <- lapply(discrepancy.out, savage_scores)
    # Correlation on savage scores
    out <- lapply(discrepancy.ranks, function(x) cor(sobol_ranks, x))
  }
  return(out)
}
```

5.2 Run the model

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

N <- 2^9
params <- c("k", "epsilon")
mat <- sobol_matrices(matrices = "A", N = N, params = params)
```

```r
# Define distributions -------------------------

mat[, "epsilon"] <- floor(qunif(mat[, "epsilon"], 1, N))
mat[, "k"] <- floor(qunif(mat[, "k"], 6, 50))

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

y.discrete <- mclapply(1:nrow(mat), function(i) {
  discretization_fun(N = 2^12,
                     k = mat[i, "k"],
                     epsilon = mat[i, "epsilon"],
                     plot.scatterplot = FALSE,
                     plot.jansen = FALSE,
                     savage.scores = TRUE)},
  mc.cores = floor(detectCores() * 0.75))
```

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

y.discrete <- lapply(y.discrete, unlist)
output <- data.table(do.call(rbind, y.discrete))
discrepancy_methods <- c("symmetric", "star", "L2", "centered",
                         "wraparound", "modified")
colnames(output) <- discrepancy_methods

final.output.discrete <- data.table(cbind(mat, output))

melt(final.output.discrete, measure.vars = discrepancy_methods) %>%
  .[, .(mean = mean(value, na.rm = TRUE),
        median = median(value, na.rm = TRUE)), variable] %>%
  .[order(-median)]
```

```
##      variable      mean    median
## 1: wraparound 0.7359107 0.8223486
## 2:  symmetric 0.6722620 0.7701982
## 3:   centered 0.5956070 0.7384221
## 4:         L2 0.6365500 0.7201984
## 5:       star 0.5889423 0.6375529
## 6:   modified 0.5889365 0.6375529
```

```r
# EXPORT OUTPUT DISCRETE -----------------------------------------------------

fwrite(final.output.discrete, "final.output.discrete.csv")
```

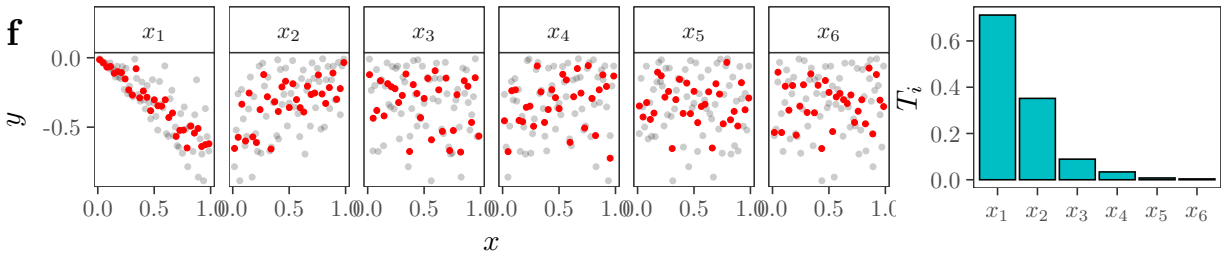
```r
# RUN MODEL TO GET SCATTERPLOTS ----------------------------------------------

N.scatter <- 2^6
N.indices <- 2^10
row.selected <- 63
```

```r
y.scatters <- discretization_fun(N = N.scatter,
                                 k = mat[row.selected, "k"],
                                 epsilon = mat[i, "epsilon"],
                                 plot.scatterplot = TRUE,
                                 plot.jansen = FALSE,
                                 savage.scores = FALSE)

# RUN MODEL TO GET JANSEN TI ------------------------------------------------

y.indices <- discretization_fun(N = N.indices,
                      k = mat[row.selected, "k"],
                      epsilon = mat[i, "epsilon"],
                      plot.scatterplot = FALSE,
                      plot.jansen = TRUE,
                      savage.scores = FALSE)
```

5.3 Bratley et al. function

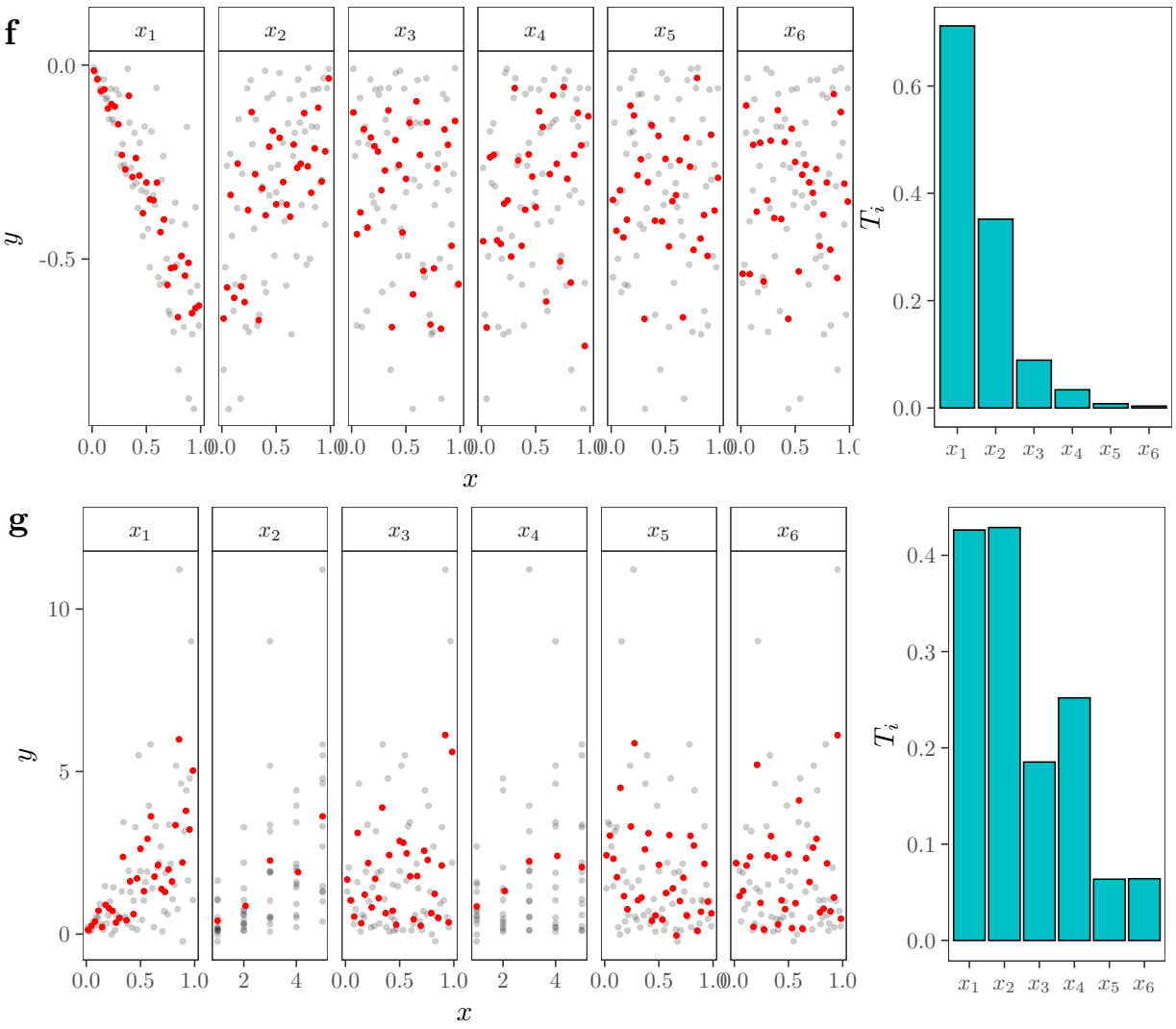
```r
# PLOT ORIGINAL BRATLEY ET AL. FUNCTION -------------------------------------

# Settings ------------------------------
N <- 2^6
k <- 6
params <- paste("$x_", 1:k,"$", sep = "")
matrices <- c("A", "AB")

# Compute -------------------------------
mat <- sobol_matrices(N = N, params = params, matrices = matrices)
y <- bratley1992_Fun(mat)
ind <- jansen_ti(d = y, N = N, params = params)

# Plot scatter --------------------------
bratley_scatter <- plot_scatter(data = mat, N = N, Y = y, params = params) +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  facet_wrap(~variable, ncol = 6) +
  labs(x = "$x$", y = "$y$") +
  theme(plot.margin = unit(c(0, 0.1, 0, 0), "cm"))

# Plot Ti -------------------------------
bratley_ti <- plot_ti(ind = ind, params = params) +
  theme(plot.margin = unit(c(0, 0.1, 0, 0), "cm")) +
  labs(x = "", y = "$T_i$") +
  scale_x_discrete(guide = guide_axis(n.dodge = 1))

# Merge ---------------------------------
bratley_plots <- plot_grid(bratley_scatter, bratley_ti, labels = c("f", ""),
```

```
                          ncol = 2, rel_widths = c(0.73, 0.27))
bratley_plots
```



5.4 Plot Bratley et al.

```
# PLOT BRATLEY ET AL. DISCRETIZED ------------------------------------------

bottom.plots <- plot_grid(y.scatters +
                            facet_wrap(~variable, ncol = 6 ,scales = "free_x") +
                            scale_x_continuous(breaks = pretty_breaks(n = 3)) +
                            scale_y_continuous(breaks = pretty_breaks(n = 3))  +
                            labs(x = "$x$", y = "$y$"),
                          y.indices,
                          ncol = 2, rel_widths = c(0.73, 0.27))

all.bottom.plots <- plot_grid(bratley_plots, bottom.plots, ncol = 1, labels = c("", "g"),
                              rel_heights = c(0.47, 0.53))
all.bottom.plots
```

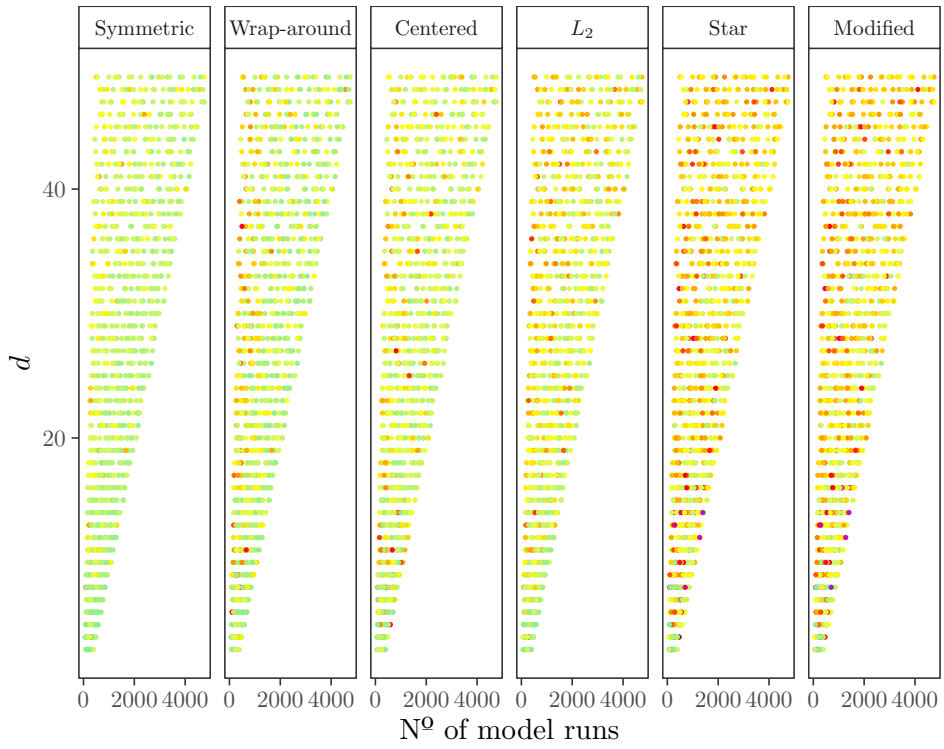


5.5 Plot uncertainty meta-model

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


# SCATTERPLOT -----------------------------------

supp.labs <- c("Symmetric", "Star", "$L_2$", "Centered", "Wrap-around", "Modified")
names(supp.labs) <- discrepancy_methods

# SCATTERPLOT -----------------------------------

a <- melt(final.output, measure.vars = discrepancy_methods) %>%
  .[, variable:= factor(variable, levels =   c("symmetric", "wraparound",
                                               "centered", "L2",
                                               "star","modified"))] %>%
  ggplot(., aes(cost.discrepancy, k, color = value)) +
```

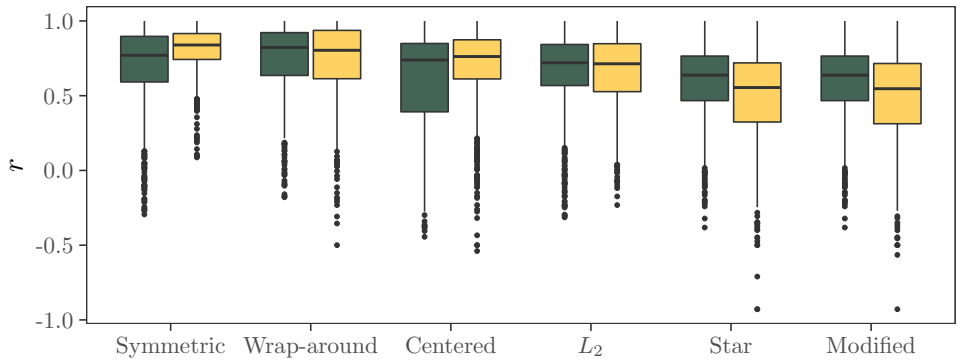
```
  geom_point(size = 0.4) +
  scale_colour_gradientn(colours = c("black", "purple", "red", "orange",
                                     "yellow", "lightgreen"),
                         name = expression(italic(r)),
                         breaks = pretty_breaks(n = 3)) +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  labs(x = "Nº of model runs", y = "$d$") +
  facet_wrap(~variable, ncol = 6, labeller = labeller(variable = supp.labs)) +
  theme_AP() +
  theme(legend.position = "none",
        strip.background = element_rect(fill = "white"),
        strip.text.x = element_text(size = 8))

# BOXPLOTS -------------------------------------

discrete.dt <- melt(final.output.discrete, measure.vars = discrepancy_methods) %>%
  .[, Function:= "Bratley et al. 1992"] %>%
  .[, .(variable, value, Function)]

final.dt <- melt(final.output, measure.vars = discrepancy_methods) %>%
  .[, Function:= "Meta-model"] %>%
  .[, .(variable, value, Function)]

b <- rbind(discrete.dt, final.dt) %>%
  ggplot(., aes(reorder(variable, -value), value, fill = Function)) +
  geom_boxplot(outlier.size = 0.5) +
  scale_x_discrete(labels = supp.labs) +
  scale_fill_manual(values = wes_palette(2, name = "Chevalier1")) +
  labs(x = "", y = "$r$") +
  theme_AP() +
  theme(legend.position = "none",
        plot.margin = unit(c(0, 0.1, 0, 0), "cm"))
```

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

a
```



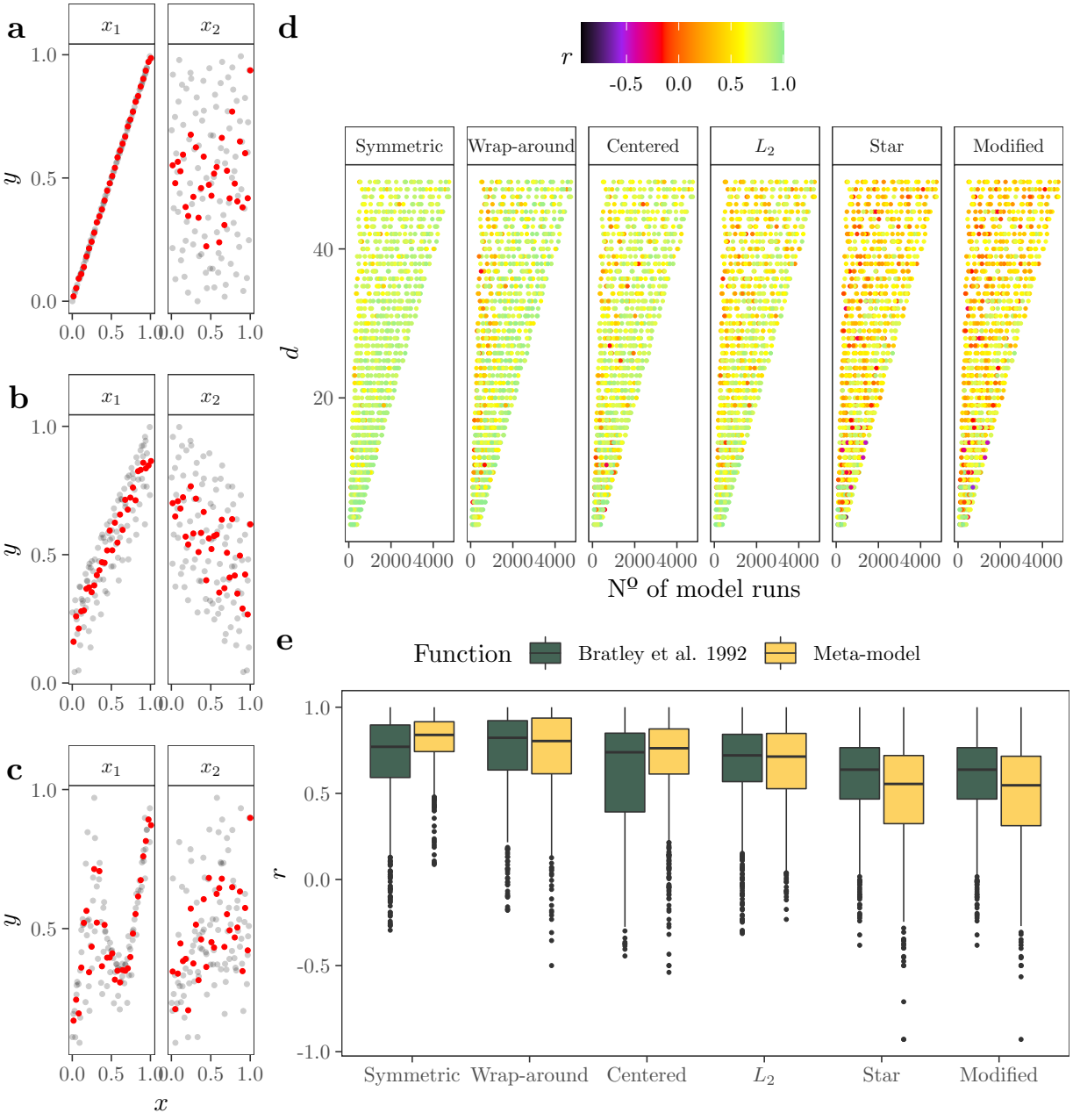

```
# PLOT BOXPLOTS ----------------------------------------------------------------
```

b

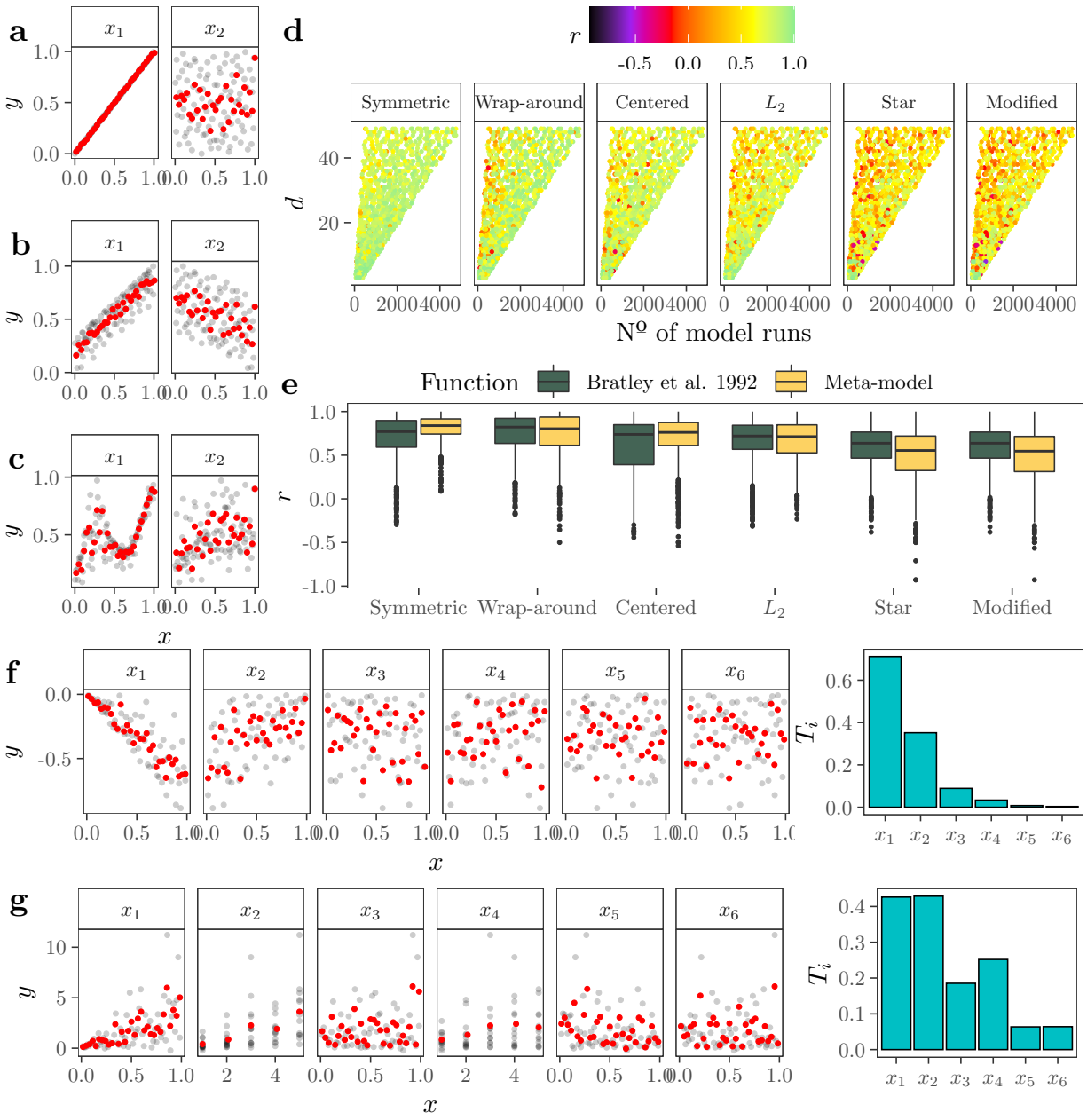



```
# MERGE ALL PLOTS ----------------------------------------------------------

legend <- get_legend(a + theme(legend.position = "top",
                               legend.margin=margin(0, 0, 0, 0),
                               legend.box.margin=margin(-7,-7,-7,-7)))

legend.boxplot <- get_legend(b + theme(legend.position = "top",
                               legend.margin=margin(0, 0, 0, 0),
                               legend.box.margin=margin(-7,-7,-7,-7)))

boxplots.plot <- plot_grid(legend.boxplot, b, ncol = 1, rel_heights = c(0.15, 0.85),
                           labels = c("e", ""))
scatters.plot <- plot_grid(legend, a, ncol = 1, rel_heights = c(0.18, 0.82),
```

```
                          labels = c("d", ""))
da <- plot_grid(scatters.plot, boxplots.plot, ncol = 1, rel_heights = c(0.55, 0.45))

full.plot <- plot_grid(scat_plot, da, ncol = 2, rel_widths = c(0.25, 0.75))
full.plot
```




```
plot_grid(full.plot, all.bottom.plots, ncol = 1, rel_heights = c(0.6, 0.45),
          labels = c("", ""))
```




```
# STATISTICS ------------------------------------------------------------------

rbind(discrete.dt, final.dt) %>%
  .[, .(mean = mean(value), median = median(value)), .(Function, variable)] %>%
  .[order(-mean, variable)]
```

```
##                Function   variable      mean    median
##  1:          Meta-model  symmetric 0.8115546 0.8391197
##  2:          Meta-model wraparound 0.7400277 0.8036229
##  3: Bratley et al. 1992 wraparound 0.7359107 0.8223486
##  4:          Meta-model   centered 0.7028626 0.7618533
##  5: Bratley et al. 1992  symmetric 0.6722620 0.7701982
##  6:          Meta-model         L2 0.6652102 0.7133971
```

```
##  7: Bratley et al. 1992         L2 0.6365500 0.7201984
##  8: Bratley et al. 1992   centered 0.5956070 0.7384221
##  9: Bratley et al. 1992       star 0.5889423 0.6375529
## 10: Bratley et al. 1992   modified 0.5889365 0.6375529
## 11:          Meta-model       star 0.5000740 0.5545182
## 12:          Meta-model   modified 0.4916879 0.5466692
```

6 Session information

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

sessionInfo()
```

```
## R version 4.2.0 (2022-04-22)
## Platform: aarch64-apple-darwin20 (64-bit)
## Running under: macOS Monterey 12.4
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.2-arm64/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.2-arm64/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] wesanderson_0.3.6 cowplot_1.1.1     benchmarkme_1.0.7 doParallel_1.0.17
##  [5] iterators_1.0.14  foreach_1.5.2     scales_1.2.0      RcppAlgos_2.5.3
##  [9] forcats_0.5.1     stringr_1.4.0     dplyr_1.0.9       purrr_0.3.4
## [13] readr_2.1.2       tidyr_1.2.0       tibble_3.1.7      ggplot2_3.3.6
## [17] tidyverse_1.3.1   data.table_1.14.2 sensobol_1.1.1
##
## loaded via a namespace (and not attached):
##  [1] Rcpp_1.0.8.3          lattice_0.20-45       lubridate_1.8.0
##  [4] gmp_0.6-5             assertthat_0.2.1      digest_0.6.29
##  [7] utf8_1.2.2            R6_2.5.1              cellranger_1.1.0
## [10] backports_1.4.1       reprex_2.0.1          evaluate_0.15
## [13] httr_1.4.3            pillar_1.7.0          Rdpack_2.3
## [16] rlang_1.0.2           readxl_1.4.0          rstudioapi_0.13
## [19] Matrix_1.4-1          tikzDevice_0.12.3.1   rmarkdown_2.14
## [22] munsell_0.5.0         broom_0.8.0           compiler_4.2.0
## [25] modelr_0.1.8          xfun_0.31             pkgconfig_2.0.3
## [28] htmltools_0.5.2       tidyselect_1.1.2      codetools_0.2-18
## [31] fansi_1.0.3           crayon_1.5.1          tzdb_0.3.0
## [34] dbplyr_2.1.1          withr_2.5.0           rbibutils_2.2.8
## [37] grid_4.2.0            jsonlite_1.8.0        gtable_0.3.0
## [40] lifecycle_1.0.1       DBI_1.1.2             magrittr_2.0.3
## [43] cli_3.3.0             stringi_1.7.6         fs_1.5.2
## [46] benchmarkmeData_1.0.4 xml2_1.3.3            ellipsis_0.3.2
## [49] generics_0.1.2        vctrs_0.4.1           tools_4.2.0
## [52] glue_1.6.2            hms_1.1.1             fastmap_1.1.0
## [55] yaml_2.3.5            colorspace_2.0-3      filehash_2.4-3
```

```
## [58] rvest_1.0.2           knitr_1.39            haven_2.5.0
```

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

```
## Machine:
```

```
## [1] "Apple M1 Max"
```

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

```
## Num cores:
```

```
## [1] 10
```

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

```
## Num threads:
```

```
## [1] 10
```

References

Iman, Ronald L., and W. J. Conover. 1987. "A measure of top-down correlation." *Technometrics* 29 (3): 351–57.