The Achilles heel of Global Hydrological Models

R code

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Contents

1 Presentation

This document presents the workflow behind the paper "The Achilles heel of Global Hydrological Models", by A. Puy, S. Lo Piano, and A. Saltelli, whose abstract is the following:

Global Hydrological Models (GHM) compute irrigation water demands based on sub-models on crop types and calendars, soil evapotranspiration processes, irrigation efficiencies, weather data and irrigated areas. Here we demonstrate that such design is convoluted as irrigation water withdrawals are largely determined by irrigated areas only. We show that modeling water withdrawals as a function of irrigated areas eases the exploration of model uncertainties and allows the production of statistics on the model output, something unattainable by GHM due to their computational demands. The results suggest that GHM need to improve the balance between complexity and error and explicitly integrate uncertainties to provide more robust insights on agrarian strategies worldwide.

Once all datasets required for the analysis have been acquired from the appropriate sources, the results of the paper should be fully reproducible in any personal computer. Questions about the code or the computational design should be addressed to A. Puy (apuy@princeton.edu).

2 Preliminary functions

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

```
# LOAD PACKAGES ------------------------------------------------------------

# 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)
    }
  }
}

loadPackages(c("data.table", "sensobol", "ncdf4",
               "rworldmap", "sp", "countrycode",
               "IDPmisc", "boot", "parallel", "scales",
               "MASS", "doParallel", "complmrob",
               "mvoutlier", "sandwich", "lmtest", "mice",
               "ggridges", "broom", "naniar", "cowplot",
               "benchmarkme", "tidyverse"))

# SET CHECKPOINT -----------------------------------------------------------

dir.create(".checkpoint")
```

```r
library("checkpoint")

checkpoint("2020-05-17",
           R.version ="3.6.3",
           checkpointLocation = getwd())

# CUSTOM FUNCTION TO DEFINE THE PLOT THEMES ----------------------------------

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))
}
```

3 Read in datasets

In this section we will load all datasets and products required for the analysis. We will retrieve irrigation water withdrawal data from six Gobal Hydrological Models (GHM) (PCR-GLOBWB, H08, LPMjL, WaterGap, MPI-HM, DBHM) and from two FAO-based datasets (Aquastat and Aquastat without missing values).

For PCR-GLOBWB, H08, LPMjL and WaterGap we will use the `.nc` files compiled by Huang et al. (2018). For DBHM (Tang et al. 2007) and MPI-HM (Stacke and Hagemann 2012), we will rely on the `.nc` files available in the Inter-Sectoral Impact Model Intercomparison Project (ISIMI) webpage, https://www.isimip.org.

For the FAO-based datasets, we use the irrigation water withdrawal values reported by Aquastat (Frenken and Gillet 2012). We also use the dataset by Liu et al. (2016), which is similar to Aquastat's but without missing values.

3.1 Loading functions

Here we define some functions that will be applied later on to read in and clean the datasets just mentioned.

`country_code` will unify the country names and provide each country with its United Nations code to avoid any confusion during the processing of the data.

`coords2country` transforms the coordinates of the .nc files to the appropriate country names.

`get_nc_data` is tailored to specifically extract irrigation water withdrawal data at the country level from the datasets compiled by Huang et al. (2018). Note that inside the function there are calls to `country_code` and `coors2country` to transform each longitude and latitude value to a country name.

`open_nc_files` is tailored to specifically extract irrigation water withdrawal data at the country level from the datasets retrieved from ISIMIP. Again, it includes calls to `country_code` and `coors2country`.

```
# CREATE FUNCTIONS ------------------------------------------------------------

# Function to obtain UN code, Continent and Country names
country_code <- function(dt) {
  dt[, `:=` (Code = countrycode(dt[, Country],
                                origin = "country.name",
                                destination = "un"),
             Continent = countrycode(dt[, Country],
                                     origin = "country.name",
                                     destination = "continent"))]
  dt[, Country:= countrycode(dt[, Code],
                             origin = "un",
                             destination = "country.name")]
  setcolorder(dt, c("Country", "Continent", "Code", "Water.Withdrawn"))
  return(dt)
}

## Function to transform longitude and latitude to country.
# It is borrowed from Andy:
# https://stackoverflow.com/questions/14334970/convert-latitude-and-longitude-coordinates-to-c
coords2country = function(points) {
  countriesSP <- rworldmap::getMap(resolution = 'low')
  pointsSP = sp::SpatialPoints(points, proj4string=CRS(proj4string(countriesSP)))
  indices = sp::over(pointsSP, countriesSP)
  indices$ADMIN
  #indices$ISO3 # returns the ISO3 code
  #indices$continent   # returns the continent (6 continent model)
  #indices$REGION   # returns the continent (7 continent model)
}

# Function to load and extract data from .nc files produced
# by Huang et al. 2018
get_nc_data <- function(nc_file) {
  nc <- nc_open(nc_file)
  ww <- ncvar_get(nc, "withd_irr")
  lon <- ncvar_get(nc, "lon")
  lat <- ncvar_get(nc, "lat")
  water <- rowSums(ww[, 469:ncol(ww)]) # Obtain year values for 2010 only
  ww.df <- data.frame(cbind(lon, lat, water))
  countries <- coords2country(ww.df[1:nrow(ww.df), 1:2])
  df <- cbind(countries, ww.df)
  setDT(df)
  final <- df[, .(Water.Withdrawn = sum(water)), countries]
  setnames(final, "countries", "Country")
```

```
  country_code(final)
  out <- na.omit(final[order(Continent)])
  out[, Water.Withdrawn:= Water.Withdrawn / 1000] # From mm to m
  return(out)
}

# Function to load and extract data from .nc files from ISIMIP
open_nc_files <- function(file, dname) {
  ncin <- nc_open(file)
  # get longitude, latitude, time
  lon <- ncvar_get(ncin, "lon")
  lat <- ncvar_get(ncin, "lat")
  # Get variable
  tmp_array <- ncvar_get(ncin, dname)
  # Retrieve last 12 months
  # get last year
  m <- (dim(tmp_array)[3] - 11):dim(tmp_array)[3]
  tmp_slice <- lapply(m, function(m) tmp_array[, , m])
  # create dataframe -- reshape data
  # matrix (nlon*nlat rows by 2 cols) of lons and lats
  lonlat <- as.matrix(expand.grid(lon,lat))
  # vector of `tmp` values
  tmp_vec <- lapply(tmp_slice, function(x) as.vector(x))
  # create dataframe and add names
  tmp_df01 <- lapply(tmp_vec, function(x) data.frame(cbind(lonlat, x)))
  names(tmp_df01) <- m
  da <- lapply(tmp_df01, data.table) %>%
    rbindlist(., idcol = "month") %>%
    na.omit()
  # Convert coordinates to country
  countries <- coords2country(da[1:nrow(da), 2:3])
  df <- cbind(countries, da)
  setDT(df)
  out <- na.omit(df)[, .(Water.Withdrawn = sum(x)), countries]
  out[, Water.Withdrawn:= Water.Withdrawn * 10000]
  return(out)
}
```

3.2 Load GHM and FAO-based datasets

In this sections we will read in and clean all eight irrigation water withdrawal datasets. We first load the Aquastat dataset (`table4`), then the Aquastat without missing values (`liu.dt`), the `.nc` files from Huang et al. (2018) (PCR-GLOBWB, H08, LPMjL, WaterGap), and the `.nc` files from ISIMIP (DBHM, MPI-HM).

```
# READ IN DATASETS ON IRRIGATION WATER WITHDRAWAL ---------------------------------

# Define vector to reorder columns
```

```r
cols_order <- c("Continent", "Country", "Code", "Water.Dataset", "Water.Withdrawn")

# FAO data (Table 4) ----------------------------
# UNIT IS KM3/YEAR
table4.tmp <- fread("table_4.csv", skip = 3, nrows = 167) %>%
  .[, .(Country, Year, Water.withdrawal)] %>%
  setnames(., "Water.withdrawal", "Water.Withdrawn")

# Extract the selected years
table4.dt <- country_code(table4.tmp[Year %in% 1999:2012])[
  , Water.Dataset:= "Aquastat"][
    , Year:= NULL] %>%
  setcolorder(., cols_order)

# Liu et al. dataset ----------------------------
#UNIT IS 10^9 m3/year = km3/year
liu.dt <- fread("liu.csv")[, .(country, irr)] %>%
  setnames(., c("country", "irr"), c("Country", "Water.Withdrawn")) %>%
  country_code(.) %>%
  .[, Water.Dataset:= "Liu et al. 2016"] %>%
  setcolorder(., cols_order)


# Huang et al datasets --------------------------
names_nc_files <- c("withd_irr_lpjml.nc", "withd_irr_pcrglobwb.nc",
                    "withd_irr_h08.nc", "withd_irr_watergap.nc")
out.nc <- mclapply(names_nc_files, function(x) get_nc_data(x), mc.cores = detectCores() * 0.75)
names(out.nc) <- c("LPJmL", "PCR-GLOBWB", "H08", "WaterGap")
out.final <- rbindlist(out.nc, idcol = "Water.Dataset")

# ISIMIP datasets -------------------------------
files <- list("dbh_wfdei_nobc_hist_varsoc_co2_airrww_global_monthly_1971_2010.nc",
              "mpi-hm_miroc5_ewembi_picontrol_histsoc_co2_airrww_global_monthly_1861_2005.nc")

dname <- "airrww"

isimip.dt <- mclapply(files, function(x) open_nc_files(file = x, dname = dname),
                      mc.cores = detectCores() * 0.75)

names(isimip.dt) <- c("DBHM", "MPI-HM")

isimip.final <- rbindlist(isimip.dt, idcol = "Water.Dataset") %>%
  setnames(., "countries","Country") %>%
  country_code(.) %>%
  na.omit()

GHM.dt <- rbind(out.final, isimip.final) %>%
```

```
  .[order(Country)]

# The value for Gabon by MPI-HM is a clear outlier
GHM.dt[Country == "Gabon"]
```

```
##    Water.Dataset Country Continent Code Water.Withdrawn
## 1:         LPJmL   Gabon    Africa  266    1.644766e-02
## 2:    PCR-GLOBWB   Gabon    Africa  266    1.510275e-02
## 3:           H08   Gabon    Africa  266    1.280429e-02
## 4:      WaterGap   Gabon    Africa  266    1.791356e-02
## 5:          DBHM   Gabon    Africa  266    2.860231e-02
## 6:        MPI-HM   Gabon    Africa  266    1.909227e-08
```

```
# So what we do is to give it a NA
GHM.dt <- GHM.dt[, Water.Withdrawn:= ifelse(Country == "Gabon" &
                                              Water.Dataset == "MPI-HM", NA,
                                            Water.Withdrawn)] %>%
  setcolorder(., cols_order)
```

```
# CREATE THE FINAL IRRIGATION WATER WITHDRAWAL DATASET ----------------------------

water.dt <- rbind(liu.dt, table4.dt, GHM.dt)

# Check if there are duplicated countries
duplicated.countries <- water.dt[, .N, .(Country)][N > 8][, Country]

# Show duplicated countries
water.dt[Country %in% duplicated.countries]
```

```
##     Continent                 Country Code   Water.Dataset Water.Withdrawn
##  1:      Asia                  Cyprus  196 Liu et al. 2016     0.160000000
##  2:      Asia Palestinian Territories  275 Liu et al. 2016     0.250000000
##  3:      Asia                  Cyprus  196        Aquastat     0.148000000
##  4:      Asia Palestinian Territories  275        Aquastat     0.189000000
##  5:      Asia                  Cyprus  196           LPJmL     0.016139367
##  6:      Asia                  Cyprus  196           LPJmL     0.022694116
##  7:      Asia                  Cyprus  196      PCR-GLOBWB     0.014070284
##  8:      Asia                  Cyprus  196      PCR-GLOBWB     0.024366953
##  9:      Asia                  Cyprus  196             H08     0.016676997
## 10:      Asia                  Cyprus  196             H08     0.019444796
## 11:      Asia                  Cyprus  196        WaterGap     0.006359497
## 12:      Asia                  Cyprus  196        WaterGap     0.010202374
## 13:      Asia                  Cyprus  196            DBHM     0.315209567
## 14:      Asia                  Cyprus  196            DBHM     0.140490805
## 15:      Asia                  Cyprus  196          MPI-HM     0.110097728
## 16:      Asia                  Cyprus  196          MPI-HM     0.020111216
## 17:      Asia Palestinian Territories  275           LPJmL     0.245201230
## 18:      Asia Palestinian Territories  275           LPJmL     0.100188175
## 19:      Asia Palestinian Territories  275      PCR-GLOBWB     0.163368097
```

```
## 20:      Asia Palestinian Territories  275      PCR-GLOBWB     0.105801784
## 21:      Asia Palestinian Territories  275             H08     0.178804828
## 22:      Asia Palestinian Territories  275             H08     0.063406375
## 23:      Asia Palestinian Territories  275         WaterGap     0.187555342
## 24:      Asia Palestinian Territories  275         WaterGap     0.084385338
## 25:      Asia Palestinian Territories  275            DBHM     0.000000000
## 26:      Asia Palestinian Territories  275            DBHM     0.520364324
## 27:      Asia Palestinian Territories  275          MPI-HM     0.021298826
## 28:      Asia Palestinian Territories  275          MPI-HM     0.068825864
##     Continent                 Country Code   Water.Dataset Water.Withdrawn
```

```
# Compute mean
water.dt <- water.dt[, .(Water.Withdrawn = mean(Water.Withdrawn)),
                     .(Water.Dataset, Country, Code, Continent)]
```

3.3 Load FAO-GMIA dataset

```
# READ IN IRRIGATED AREA DATASET ------------------------------------------------

meier.dt <- fread("meier.csv") %>%
  setnames(., "Codes", "Code") %>%
  na.omit() %>%
  .[, .(Country, Continent, Code, `FAO-GMIA`)] %>%
  setnames(., "FAO-GMIA", "Irrigated.Area")
```

3.4 Plot FAO-GMIA against irrigation water withdrawal

```
# MERGE DATASETS ----------------------------------------------------------------

full.dt <- water.dt[, merge(.SD, meier.dt, by = c("Country", "Code", "Continent"),
                            all.y = TRUE), Water.Dataset] %>%
  .[!Continent == "Oceania"]

# Show countries with missing values in Water Withdrawal
full.dt[is.na(Water.Withdrawn), ] %>%
  .[, unique(Country)]
```

```
##  [1] "Bosnia and Herzegovina"
##  [2] "Burma"
##  [3] "Czech Republic"
##  [4] "Iran (Islamic Republic of)"
##  [5] "Korea, Republic of"
##  [6] "Lao People's Democratic Republic"
##  [7] "Libyan Arab Jamahiriya"
##  [8] "Palestine"
##  [9] "Republic of Moldova"
## [10] "Saint Lucia"
## [11] "Syrian Arab Republic"
```

```
## [12] "The former Yugoslav Republic of Macedonia"
## [13] "Trinidad and Tobago"
## [14] "United Republic of Tanzania"
## [15] "Viet Nam"
## [16] "Belize"
## [17] "Cape Verde"
## [18] "Croatia"
## [19] "Cuba"
## [20] "El Salvador"
## [21] "Grenada"
## [22] "Guyana"
## [23] "Haiti"
## [24] "Ireland"
## [25] "Lebanon"
## [26] "Luxembourg"
## [27] "Malaysia"
## [28] "Panama"
## [29] "Peru"
## [30] "Sudan"
## [31] "Suriname"
## [32] "Uruguay"
## [33] "Malta"
## [34] "Seychelles"
## [35] "Argentina"
## [36] "Canada"
## [37] "Portugal"
## [38] "Russia"
## [39] "Mauritius"
```

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

full.dt %>%
  na.omit() %>%
  ggplot(., aes(Irrigated.Area, Water.Withdrawn,
                color = Continent)) +
  geom_point(size = 0.7) +
  scale_x_log10(breaks = trans_breaks("log10", function(x) 10 ^ (4 * x)),
                labels = trans_format("log10", math_format(10 ^ .x))) +
  scale_y_log10(breaks = trans_breaks("log10", function(x) 10 ^ (2 * x)),
                labels = trans_format("log10", math_format(10 ^ .x))) +
  labs(x = "Irrigated area (ha)",
       y = expression(paste("Water withdrawal~", "", 10^9, m^3/year))) +
  facet_wrap(~Water.Dataset, ncol = 4) +
  theme_AP() +
  theme(legend.position = "top",
        strip.text = element_text(size = 6.7))
```

```
## Warning: Transformation introduced infinite values in continuous x-axis
```

```
## Warning: Transformation introduced infinite values in continuous y-axis
```

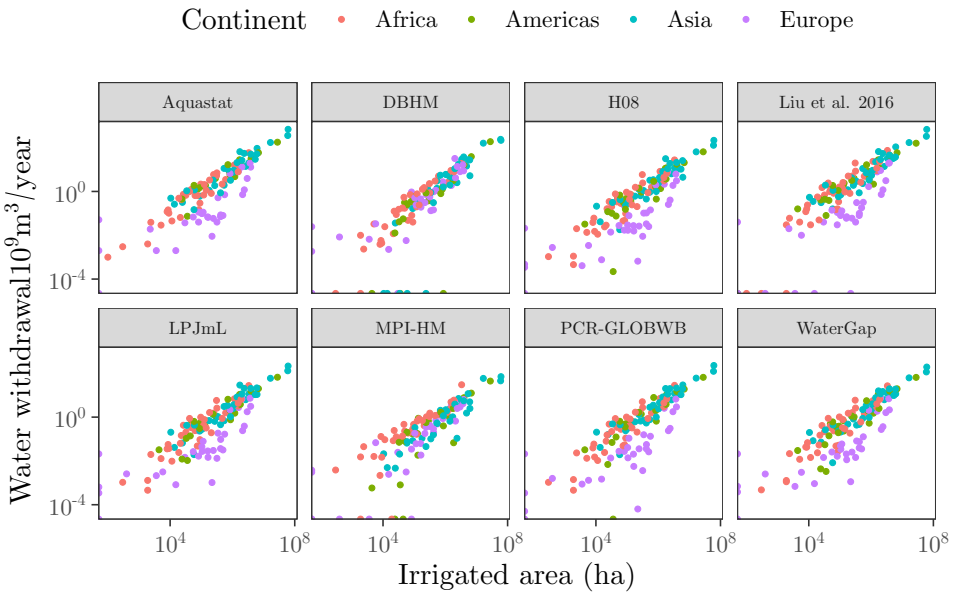


Figure 1: Scatterplots of irrigated areas reported by FAO-GMIA against irrigation water withdrawals.

```
# TRANSFORM DATASET ------------------------------------------------------------

cols <- c("Water.Withdrawn", "Irrigated.Area")
col_names <- c("Continent", "Water.Dataset", "Area.Dataset", "Regression",
               "Imputation.Method", "Iteration")
cols_group <- c("Continent", "Water.Dataset")
full.dt <- full.dt[, (cols):= lapply(.SD, log10), .SDcols = (cols)]
```

```
# EXPORT FULL DATASET WITH MISSING VALUES --------------------------------------

fwrite(full.dt, "full.dt.csv")
fwrite(water.dt, "water.dt.csv")
```

4 Missing values

```
# PLOT PERCENTAGE OF MISSING 2 -------------------------------------------------

full.dt[, sum(is.na(.SD) == TRUE) / .N,
        .(Continent, Water.Dataset),
        .SDcols = "Water.Withdrawn"] %>%
  ggplot(., aes(Continent, V1, fill = Water.Dataset)) +
  geom_bar(stat = "identity",
           position = position_dodge(0.7),
           color = "black") +
  labs(x = "",
       y = "Proportion of missing values") +
  scale_fill_discrete(name = "") +
```

```
  theme_AP() +
  theme(legend.position = "top")
```

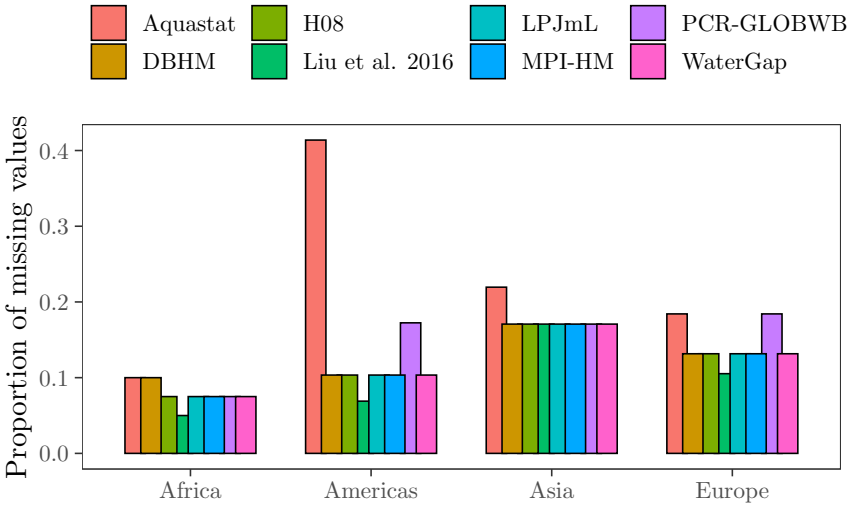


Figure 2: Proportion of missing values in irrigation water withdrawal per dataset.

```
##    Water.Dataset Country Code Continent Water.Withdrawn Irrigated.Area
## 1:             0       0    0         0               0              0
```

5 Regressions

```
# COMPUTE LINEAR REGRESSIONS ----------------------------------------------------

# Compute regressions in each combination
regressions <- full.imput %>%
  group_by(Continent, Water.Dataset, Imputation.Method, Iteration) %>%
  nest() %>%
  mutate(fit = map(.x = data, .f = ~lm(Water.Withdrawn ~ Irrigated.Area, data = .)),
         results = map(fit, glance),
         residuals = map(fit, augment))

# Extract r squared
results <- regressions %>%
  dplyr::select(Continent, Water.Dataset,
                Imputation.Method, Iteration, results) %>%
  unnest(results) %>%
  data.table() %>%
  .[, index:= paste(Continent, Water.Dataset,
                    Imputation.Method, Iteration, sep = "_")]

# Extract residuals
residuals <- regressions %>%
  dplyr::select(Continent, Water.Dataset,
```

```
                Imputation.Method, Iteration, residuals) %>%
  unnest(residuals) %>%
  data.table()

# PREDICT WATER WITHDRAWALS ----------------------------------------------------
size.gmia <- meier.dt[, .(Country, Continent, Irrigated.Area)] %>%
  .[!Irrigated.Area == 0] %>%
  .[, Irrigated.Area:= log10(Irrigated.Area)] %>%
  .[!Continent == "Oceania"] %>%
  .[order(Continent)]

countries <- split(size.gmia, size.gmia$Continent) %>%
  lapply(., function(x) x[, Country]) %>%
  lapply(., data.table)

areas <- split(size.gmia, size.gmia$Continent) %>%
  lapply(., function(x) x[, Irrigated.Area]) %>%
  lapply(., data.frame) %>%
  lapply(., function(x) setnames(x, "X..i..", "Irrigated.Area"))

tmp.regressions <- regressions %>%
  split(., .$Continent)

out <- list()
for(i in names(tmp.regressions)) {
  out[[i]] <- mutate(tmp.regressions[[i]],
                     pred = map(fit, .f = ~predict(., areas[[i]])))
}

water.predicted <- lapply(out, function(x) {
  select(x, Continent, Water.Dataset, Imputation.Method, Iteration, pred) %>%
  unnest(pred) %>%
  data.table()
})

out <- list()
for(i in names(water.predicted)) {
  out[[i]] <- water.predicted[[i]][, Country:= rep(countries[[i]][, V1],
                                                   times = nrow(water.predicted[[i]]) /
                                                           nrow(countries[[i]]))]
}

water.predicted <- rbindlist(water.predicted) %>%
  .[, pred:= 10 ^ pred]

# Compute quantiles
water.quantiles <- water.predicted[, .(min = min(pred),
```

```
                                        max = max(pred),
                                        q0.025 = quantile(pred, 0.025),
                                        q0.1 = quantile(pred, 0.1),
                                        q0.25 = quantile(pred, 0.25),
                                        q0.5 = quantile(pred, 0.5),
                                        q0.75 = quantile(pred, 0.75),
                                        q0.975 = quantile(pred, 0.975),
                                        q0.99 = quantile(pred, 0.99),
                                        q1 = quantile(pred, 1),
                                        mean = mean(pred),
                                        median = median(pred)),
                                    .(Continent, Country)] %>%
  .[order(Country, Continent)]
```

```
# PLOT PREDICTIONS AGAINST GHM AND FAO OUTPUTS -----------------------------------

water.tmp <- water.dt[Country %in% water.quantiles[, Country]]
Cont <- c("Africa", "Americas", "Asia", "Europe")
gg <- list()
for(i in Cont) {
  gg[[i]] <- water.quantiles[Continent == i] %>%
    ggplot(., aes(reorder(Country, median), median)) +
    geom_point() +
    geom_point(data = water.tmp[Continent == i],
               aes(Country, Water.Withdrawn, color = Water.Dataset)) +
    geom_errorbar(aes(ymin = min,
                      ymax = max)) +
    scale_y_log10(breaks = trans_breaks("log10", function(x) 10 ^ (2 * x)),
                  labels = trans_format("log10", math_format(10 ^ .x))) +
    scale_color_discrete(name = "Water dataset") +
    labs(y = expression(paste("Water withdrawal ", " ", "(", 10^9, m^3/year, "", ")")),
         x = "") +
    coord_flip() +
    theme_AP()
}
gg
```

```
## $Africa

## Warning: Transformation introduced infinite values in continuous y-axis

##
## $Americas

## Warning: Transformation introduced infinite values in continuous y-axis

##
## $Asia

## Warning: Transformation introduced infinite values in continuous y-axis
```

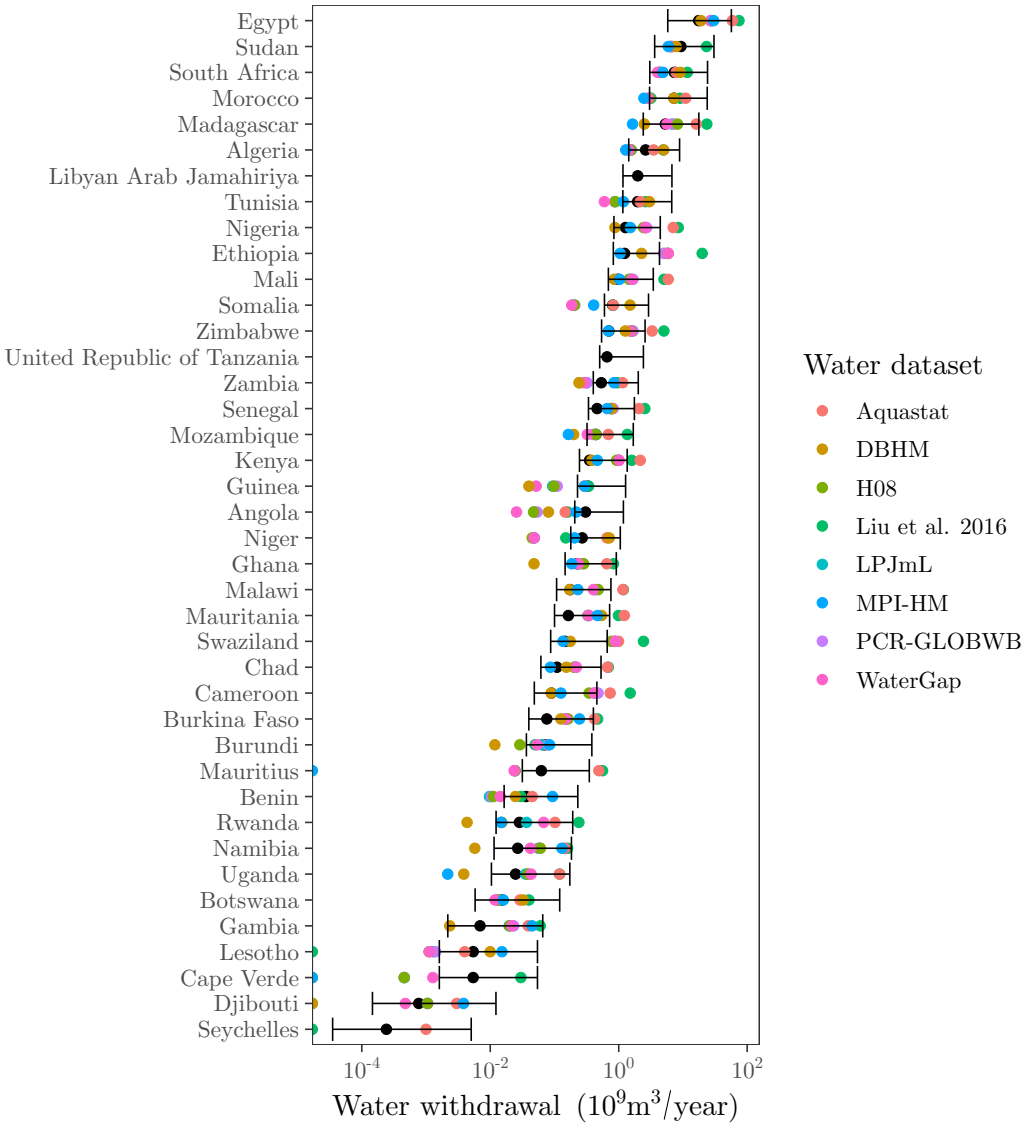


Figure 3: Validation of our approach. The black dots and the error bars show the range of irrigation water withdrawal values predicted from irrigated areas only. The colored dots show the irrigation water withdrawal values outputted by Global Hydrological Models and FAO-based datasets.

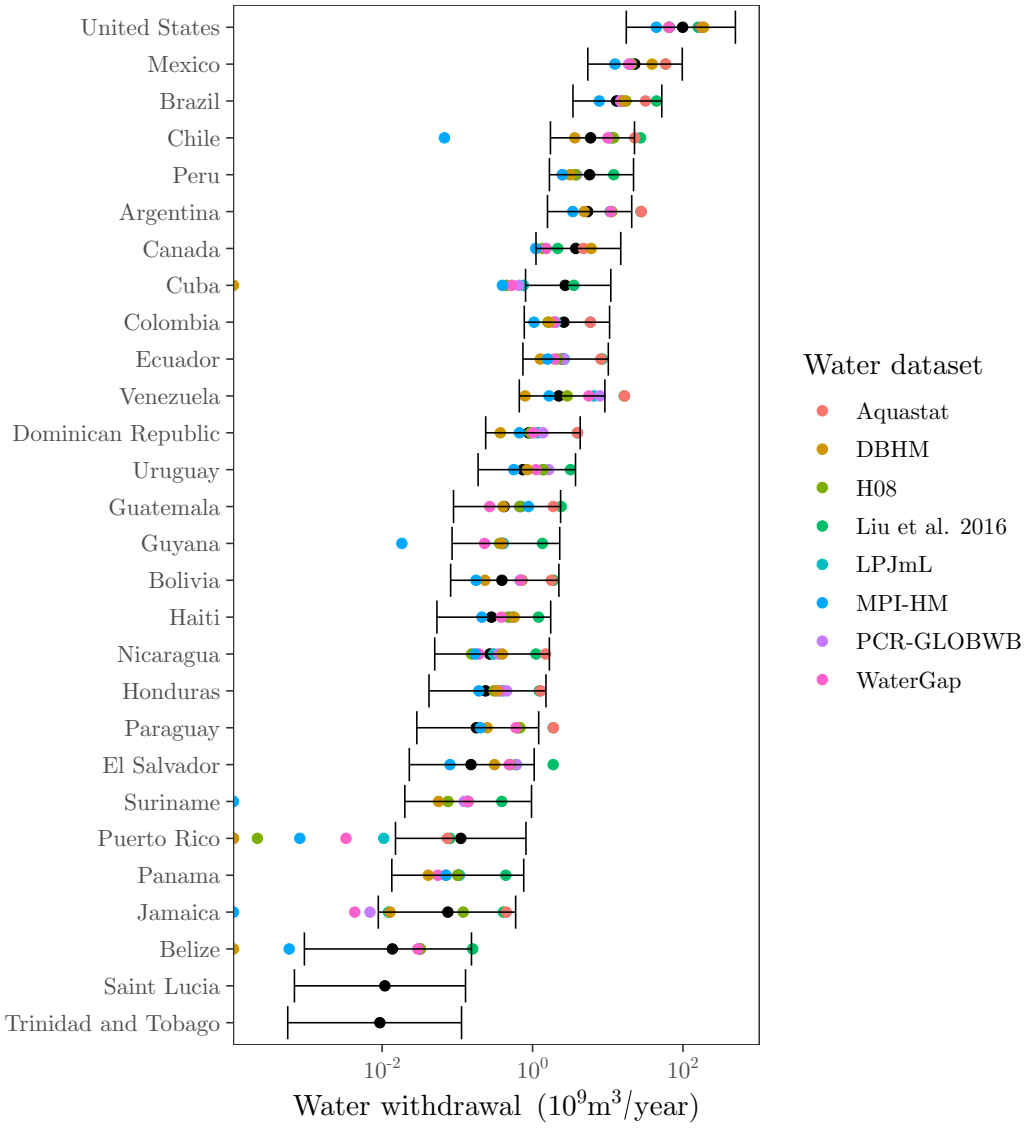


Figure 4: Validation of our approach. The black dots and the error bars show the range of irrigation water withdrawal values predicted from irrigated areas only. The colored dots show the irrigation water withdrawal values outputted by Global Hydrological Models and FAO-based datasets.

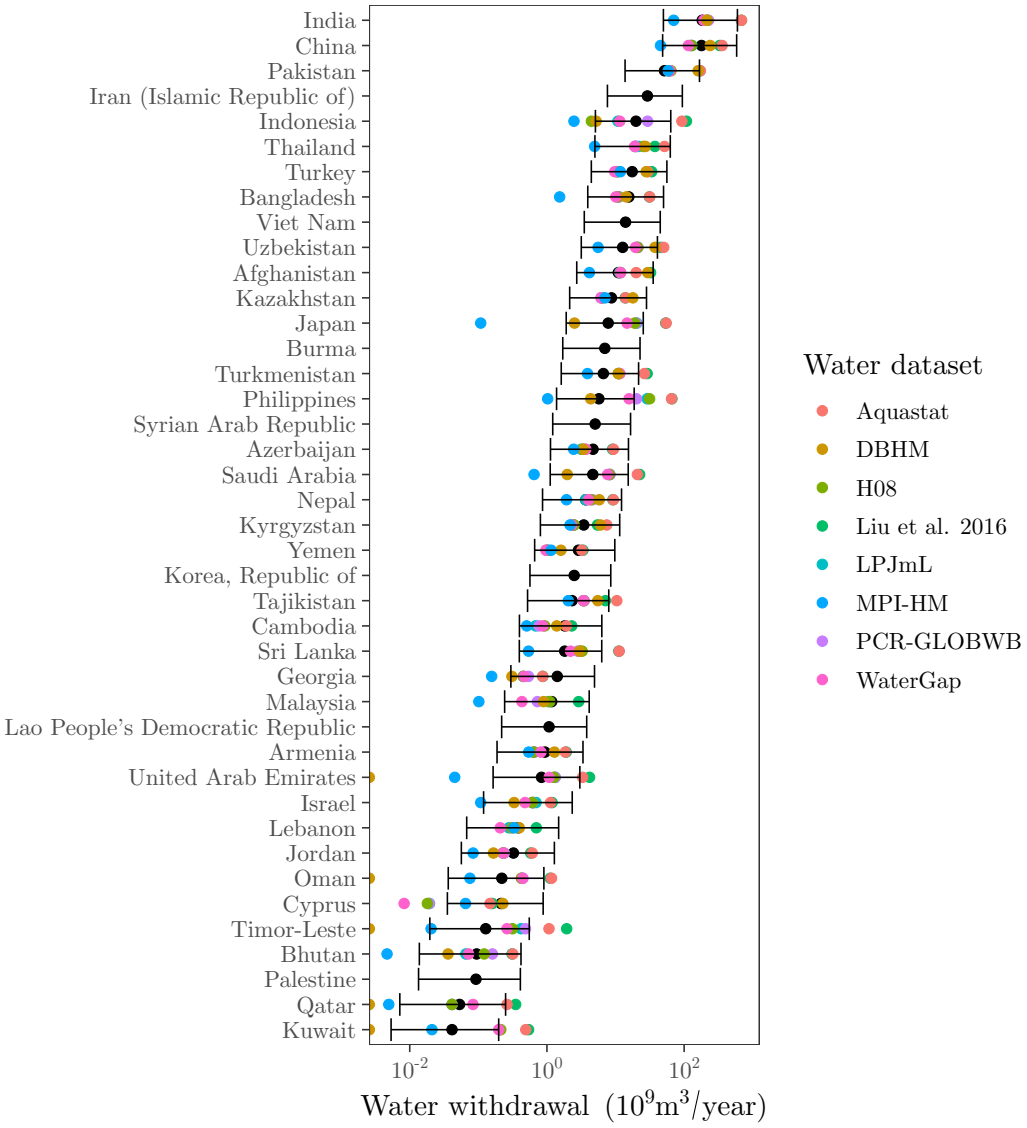


Figure 5: Validation of our approach. The black dots and the error bars show the range of irrigation water withdrawal values predicted from irrigated areas only. The colored dots show the irrigation water withdrawal values outputted by Global Hydrological Models and FAO-based datasets.

```
##
## $Europe

## Warning: Transformation introduced infinite values in continuous y-axis
```

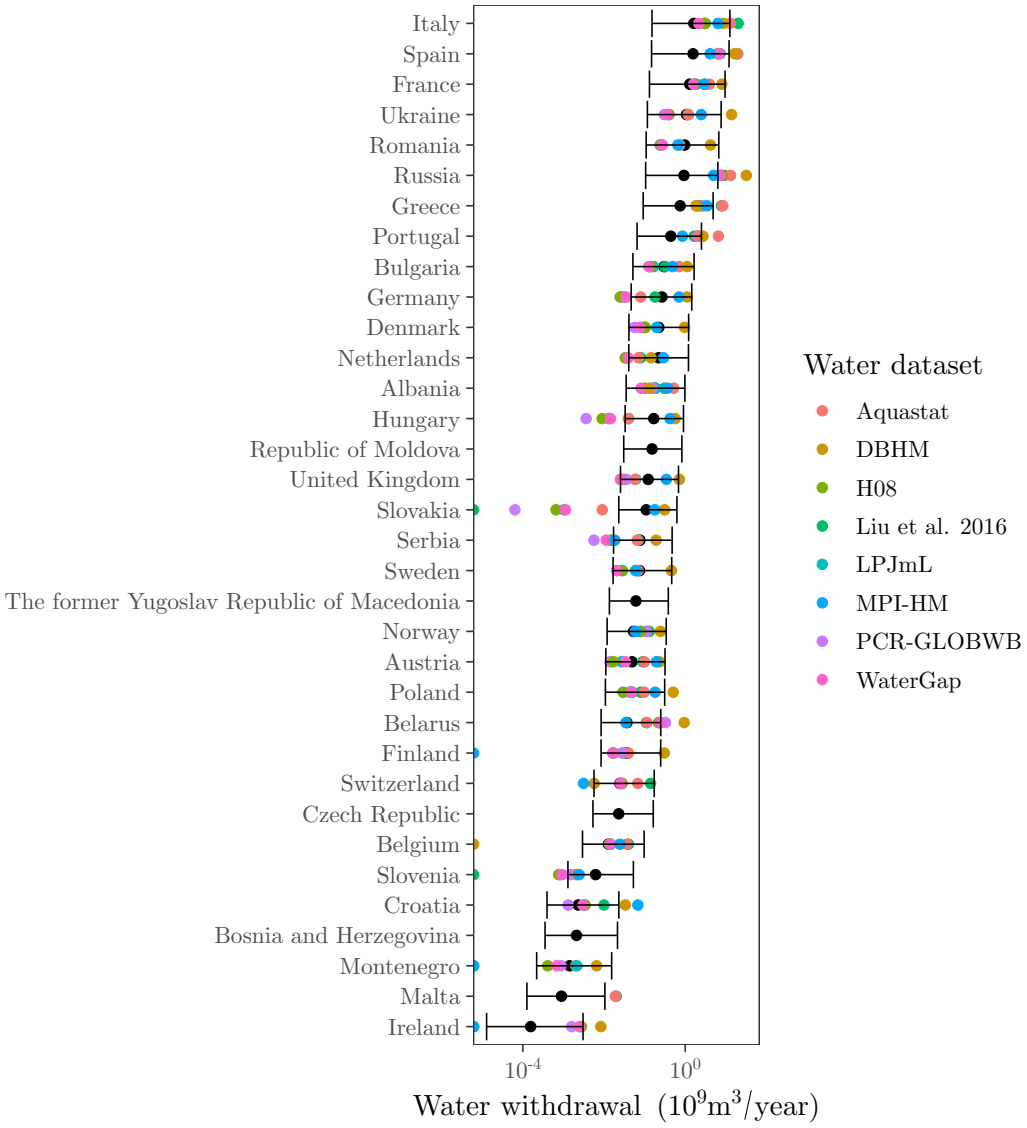


Figure 6: Validation of our approach. The black dots and the error bars show the range of irrigation water withdrawal values predicted from irrigated areas only. The colored dots show the irrigation water withdrawal values outputted by Global Hydrological Models and FAO-based datasets.

6 Lookup table

Here we define the lookup table that we will use to select the β value according to the conditions set by the triggers in the sample matrix (see below).

```
# CREATE LOOKUP TABLE ------------------------------------------------------------

lookup <- setkey(results, index)
```

```r
# EXPORT DATASETS ---------------------------------------------------------------

fwrite(full.imput, "full.imput.csv")
fwrite(results, "results.csv")
fwrite(residuals, "residuals.csv")
fwrite(lookup, "lookup.csv")
fwrite(water.quantiles, "water.quantiles.csv")
```

7 Run the model

7.1 Define settings

```r
# DEFINE THE SETTINGS OF THE SAMPLE MATRIX --------------------------------------

Continents <- c("Africa", "Americas", "Asia", "Europe")

# Create a vector with the name of the columns
parameters <- paste("X", 1:3, sep = "")

# Select sample size
n <- 2 ^ 13

# Define order
order <- "third"
```

7.2 Sample matrix

```r
# CREATE THE SAMPLE MATRIX ------------------------------------------------------

# Create an A, B and AB matrices for each continent
sample.matrix <- lapply(Continents, function(Continents)
  sobol_matrices(N = n,
                 params = parameters,
                 order = order) %>%
    data.table())

# Name the slots, each is a continent
names(sample.matrix) <- Continents

# Name the columns
sample.matrix <- lapply(sample.matrix, setnames, parameters)
```

```r
# TRANSFORM THE SAMPLE MATRIX ---------------------------------------------------

# Function to transform sample matrix to appropriate distributions
transform_sample_matrix <- function(dt) {
  dt[, X1:= floor(X1 * (8 - 1 + 1)) + 1] %>%
```

```
    .[, X1:= ifelse(X1 == 1, "LPJmL",
                    ifelse(X1 == 2, "H08",
                           ifelse(X1 == 3, "PCR-GLOBWB",
                                  ifelse(X1 == 4, "WaterGap",
                                         ifelse(X1 == 5, "Aquastat",
                                                ifelse(X1 == 6, "Liu et al. 2016",
                                                       ifelse(X1 == 7, "DBHM", "MPI-HM"))))))]
    .[, X2:= floor(X2 * (length(imputation.methods) - 1 + 1)) + 1] %>%
    .[, X2:= ifelse(X2 == 1, imputation.methods[1],
                    ifelse(X2 == 2, imputation.methods[2], imputation.methods[3]))] %>%
    .[, X3:= floor(X3 * (m.iterations - 1 + 1)) + 1]
}

sample.matrix <- lapply(sample.matrix, transform_sample_matrix)
sample.matrix.dt <- rbindlist(sample.matrix, idcol = "Continent")
```

```
# PRINT SAMPLE MATRIX ------------------------------------------------------------

print(sample.matrix.dt)
```

```
##         Continent              X1        X2 X3
##      1:    Africa        Aquastat norm.boot 21
##      2:    Africa            DBHM      norm 31
##      3:    Africa      PCR-GLOBWB  norm.nob 11
##      4:    Africa        WaterGap norm.boot 26
##      5:    Africa          MPI-HM  norm.nob  6
##     ---
## 294908:    Europe        WaterGap norm.boot 30
## 294909:    Europe          MPI-HM      norm 10
## 294910:    Europe             H08 norm.boot 40
## 294911:    Europe Liu et al. 2016  norm.nob 20
## 294912:    Europe            DBHM      norm 33
```

7.3 The model

The model is simply a one-line function that runs in the sample matrix as follows: at the v-th row, it creates a vector with all the conditions set by $X_1^{(v)}, ..., X_6^{(v)}$, and uses this vector to extract from the lookup table the $\beta^{(v)}$ value according to these conditions.

```
# THE MODEL ----------------------------------------------------------------

model <- function(X) lookup[.(paste0(X[, 1:4], collapse = "_"))][, r.squared]
```

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

# Set number of cores at 75%
n_cores <- floor(detectCores() * 0.75)

# Create cluster
```

```r
cl <- makeCluster(n_cores)
registerDoParallel(cl)

# Run model in parallel
r.squared <- foreach(i=1:nrow(sample.matrix.dt),
             .packages = "data.table",
             .combine = "c") %dopar%
  {
    model(sample.matrix.dt[i])
  }

# Stop parallel cluster
stopCluster(cl)
```

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

sample.matrix.dt <- cbind(sample.matrix.dt, r.squared)

# Select the A and B matrix only (for uncertainty analysis)
AB.dt <- sample.matrix.dt[, .SD[1:(n * 2)], Continent]

# Export results
fwrite(sample.matrix.dt, "sample.matrix.dt.csv")
fwrite(AB.dt, "AB.dt.csv")
```

8 Uncertainty analysis

```r
# COMPUTE QUANTILES AND MEAN ------------------------------------------------------

AB.dt[, .(q0.025 = quantile(r.squared, 0.025),
          q0.1 = quantile(r.squared, 0.1),
          q0.25 = quantile(r.squared, 0.25),
          q0.5 = quantile(r.squared, 0.5),
          q0.75 = quantile(r.squared, 0.75),
          q0.975 = quantile(r.squared, 0.975),
          q0.99 = quantile(r.squared, 0.99),
          q1 = quantile(r.squared, 1),
          mean = mean(r.squared),
          median = median(r.squared)), Continent]
```

```
##    Continent    q0.025      q0.1     q0.25      q0.5     q0.75    q0.975
## 1:    Africa 0.8215929 0.8372900 0.8517387 0.8663348 0.8878623 0.9133331
## 2:  Americas 0.6762378 0.7291203 0.7937019 0.8659180 0.8984204 0.9456457
## 3:      Asia 0.8334491 0.8478166 0.8598476 0.8722937 0.8846674 0.9299792
## 4:    Europe 0.4958679 0.5863070 0.6621637 0.7199073 0.7899133 0.8783011
##        q0.99        q1      mean    median
## 1: 0.9181754 0.9211349 0.8684724 0.8663348
```

```
## 2: 0.9498877 0.9563170 0.8435401 0.8659180
## 3: 0.9350349 0.9400244 0.8739635 0.8722937
## 4: 0.8845060 0.9002252 0.7165019 0.7199073
```

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

# Plot r2
unc.plot <- ggplot(AB.dt, aes(r.squared)) +
      geom_histogram(color = "black", fill = "white") +
      theme_AP() +
      labs(x = expression(italic(r) ^ 2),
           y = "Density") +
      scale_y_continuous(breaks = pretty_breaks(n = 2)) +
      scale_x_continuous(breaks = pretty_breaks(n = 3)) +
      facet_wrap(~Continent, ncol = 1) +
      theme(panel.spacing.x = unit(4, "mm"))

unc.plot
```

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

```
# PLOT UNCERTAINTY IN EACH GHM AND FAO-BASED DATASET --------------------------

unc.GHM <- AB.dt %>%
  ggplot(., aes(reorder(X1, r.squared), r.squared, fill = Continent)) +
  geom_boxplot(position = position_dodge(0.6),
               outlier.size = 0.3) +
  theme_AP() +
  labs(y = expression(italic(r)^2),
       x = "") +
  scale_x_discrete(labels = c("PCR-GLOBWB" = expression(bold(PCR-GLOBWB)),
                              "DBHM" = expression(bold(DBHM)),
                              "MPI-HM" = expression(bold(MPI-HM)),
                              "LPJmL" = expression(bold(LPJmL)),
                              "H08" = expression(bold(H08)),
                              "WaterGap" = expression(bold(WaterGap)))) +
  theme(legend.position = "none") +
  coord_flip()

# Get legend
legend <- get_legend(unc.GHM + theme(legend.position = "top"))
```

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

bottom <- plot_grid(unc.plot, unc.GHM, ncol = 2,
                    rel_widths = c(0.5, 1), labels = "auto")
```

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

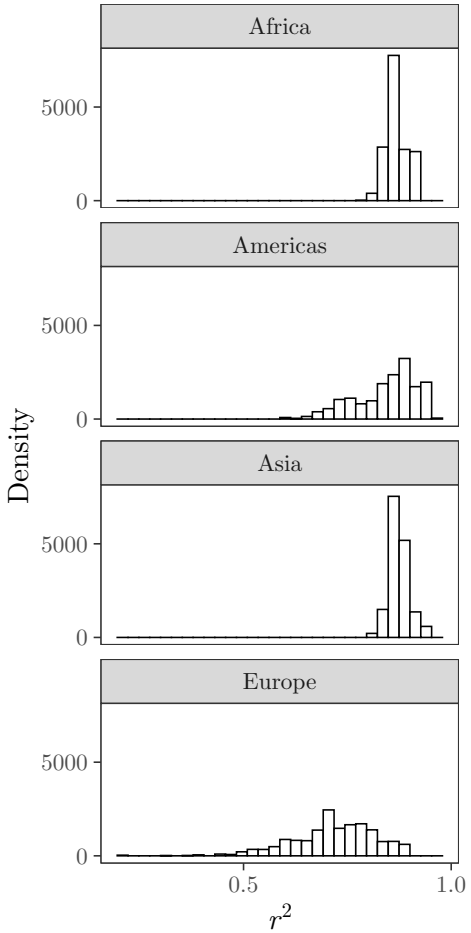


Figure 7: Uncertainty in the model output. a) Uncertainty in the model goodness of fit. All sources of uncertainty have been taken into account except the selection between OLS and OLS robust (trigger X2). Robust OLS does not allow to compute r^2. b) Uncertainty in the slope.

```
all <- plot_grid(legend, bottom, ncol = 1, rel_heights = c(0.1, 1))
```

```
# PLOT CUMULATIVE EMPIRICAL DISTRIBUTION FOR R2 ----------------------------------

ggplot(AB.dt, aes(r.squared, colour = Continent)) +
  stat_ecdf() +
  labs(x = "$r^2$",
       y = "y") +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  theme_AP()
```

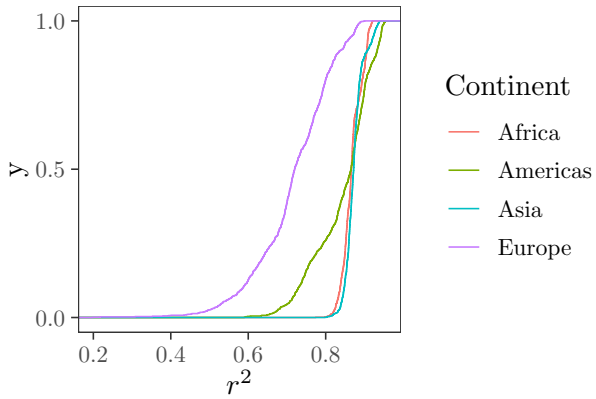


Figure 8: Cumulative empirical distribution for r^2.

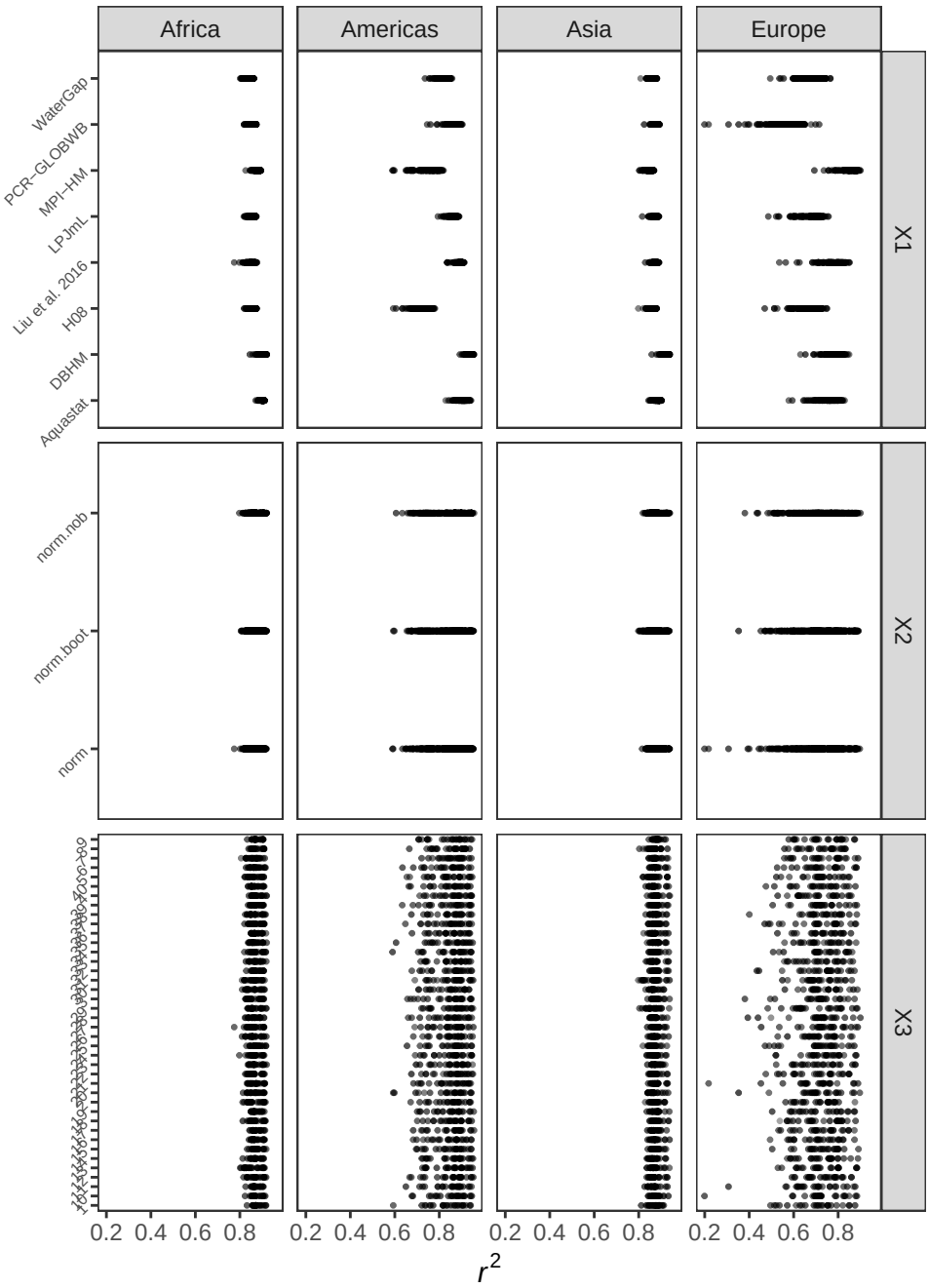
9 Sensitivity analysis

```
# PLOT SCATTERPLOTS OF PARAMETERS VS MODEL OUTPUT ---------------------------------

AB.dt <- AB.dt[, X3:= factor(X3, levels = as.factor(1:m.iterations))]

scatter.dt <- melt(AB.dt[, .SD[1:n], Continent],
                   measure.vars = paste("X", 1:3, sep = ""))

# R squared
ggplot(scatter.dt, aes(r.squared, value)) +
  geom_point(alpha = 0.1, size = 0.5) +
  facet_grid(variable ~ Continent,
             scales = "free_y") +
  labs(y = "",
       x = expression(italic(r)^2)) +
  scale_x_continuous(breaks = pretty_breaks(n = 3)) +
  scale_color_manual(values = c("#00BFC4", "#F8766D")) +
  theme_AP() +
  theme(axis.text.y = element_text(angle = 45, hjust = 1, size = 6),
        legend.position = "top")
```




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

# Number of bootstrap replicas
R <- 1000

parameters.recoded <- c("$X_1$", "$X_2$", "$X_3$")

# Sobol' indices for r2
indices <- sample.matrix.dt[, sobol_indices(Y = r.squared,
                                            N = n,
                                            params = parameters.recoded,
```

```
                                          first = "jansen",
                                          R = R,
                                          boot = TRUE,
                                          parallel = "multicore",
                                          ncpus = n_cores,
                                          order = order),
                            Continent]
```

```
# PRINT AND EXPORT SENSITIVITY INDICES ----------------------------------------

print(indices[sensitivity %in% c("Si", "Ti")])
```

```
##     Continent     original          bias   std.error      low.ci    high.ci
##  1:    Africa  0.720619411 -7.994611e-05 0.005197866  0.71051173 0.73088699
##  2:    Africa  0.010697268 -1.196400e-04 0.013049718 -0.01476007 0.03639388
##  3:    Africa  0.044124350  2.275565e-04 0.013815199  0.01681950 0.07097409
##  4:    Africa  0.893166906 -4.469596e-04 0.013910263  0.86635025 0.92087748
##  5:    Africa  0.165582325  1.452862e-04 0.003899822  0.15779353 0.17308055
##  6:    Africa  0.265048916 -2.040609e-04 0.005130178  0.25519801 0.27530794
##  7:  Americas  0.874486367 -1.626353e-05 0.003309601  0.86801593 0.88098933
##  8:  Americas -0.001168093  3.415676e-04 0.012566921 -0.02614037 0.02312105
##  9:  Americas  0.011018352  6.343718e-04 0.013281883 -0.01564803 0.03641599
## 10:  Americas  0.968019902 -3.192744e-04 0.013565312  0.94175165 0.99492670
## 11:  Americas  0.087442878  1.321420e-04 0.002739294  0.08194182 0.09267965
## 12:  Americas  0.122352770  2.560315e-05 0.003128528  0.11619536 0.12845897
## 13:      Asia  0.730515628 -6.397168e-05 0.005942775  0.71893198 0.74222722
## 14:      Asia -0.001026535 -2.264506e-04 0.013728241 -0.02770694 0.02610677
## 15:      Asia  0.038043782 -2.956189e-04 0.014099072  0.01070573 0.06597308
## 16:      Asia  0.846120801  8.057625e-04 0.013521626  0.81881314 0.87181694
## 17:      Asia  0.185832640  9.646047e-05 0.004890859  0.17615027 0.19532209
## 18:      Asia  0.265703075 -1.946358e-04 0.005593892  0.25493388 0.27686154
## 19:    Europe  0.729714816 -2.159044e-04 0.006452730  0.71728360 0.74257784
## 20:    Europe  0.003395427 -5.595039e-04 0.014352104 -0.02417468 0.03208454
## 21:    Europe  0.013724452  3.706511e-05 0.016291964 -0.01824428 0.04561905
## 22:    Europe  0.946109350  4.783269e-05 0.015915523  0.91486767 0.97725537
## 23:    Europe  0.179895778 -2.034249e-04 0.005998639  0.16834209 0.19185632
## 24:    Europe  0.264681637 -1.261745e-04 0.006426923  0.25221127 0.27740435
##     Continent     original          bias   std.error      low.ci    high.ci
##     sensitivity parameters
##  1:          Si      $X_1$
##  2:          Si      $X_2$
##  3:          Si      $X_3$
##  4:          Ti      $X_1$
##  5:          Ti      $X_2$
##  6:          Ti      $X_3$
##  7:          Si      $X_1$
##  8:          Si      $X_2$
##  9:          Si      $X_3$
```

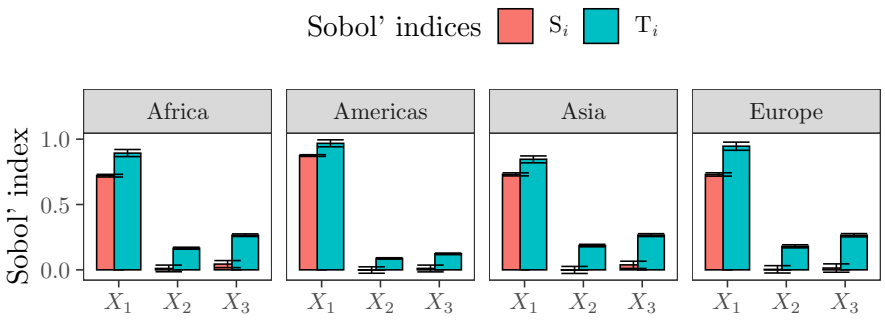
```
## 10:          Ti      $X_1$
## 11:          Ti      $X_2$
## 12:          Ti      $X_3$
## 13:          Si      $X_1$
## 14:          Si      $X_2$
## 15:          Si      $X_3$
## 16:          Ti      $X_1$
## 17:          Ti      $X_2$
## 18:          Ti      $X_3$
## 19:          Si      $X_1$
## 20:          Si      $X_2$
## 21:          Si      $X_3$
## 22:          Ti      $X_1$
## 23:          Ti      $X_2$
## 24:          Ti      $X_3$
##     sensitivity parameters
```

```r
fwrite(indices, "indices.csv")
```

```r
# PLOT UNCERTAINTY AND SOBOL' INDICES ------------------------------------------

bottom <- indices[sensitivity %in% c("Si", "Ti")] %>%
  ggplot(., aes(parameters, original, fill = sensitivity)) +
    geom_bar(stat = "identity",
             position = position_dodge(0.6),
             color = "black") +
    geom_errorbar(aes(ymin = low.ci,
                      ymax = high.ci),
                  position = position_dodge(0.6)) +
    scale_y_continuous(breaks = scales::pretty_breaks(n = 3)) +
    facet_wrap(~Continent,
               ncol = 4) +
    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")

bottom
```




```
# MERGE UNCERTAINTY AND SENSITIVITY ANALYSIS PLOTS ---------------------------------

plot_grid(all, bottom, align = "hv", rel_heights = c(0.8, 0.4),
          labels = c("", "c"), ncol = 1)
```

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

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

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

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

```
##    Continent        V1
## 1:    Africa 0.7754410
## 2:  Americas 0.8843366
## 3:      Asia 0.7675329
## 4:    Europe 0.7468347
```

```
# PLOT SOBOL' INDICES (SECOND AND THIRD ORDER) -------------------------------------

indices[sensitivity == "Sij" | sensitivity == "Sijk"] %>%
  .[low.ci > 0] %>%
  .[, sensitivity:= ifelse(sensitivity %in% "Sij", "$S_{ij}$",
                           "$S_{ijk}$")] %>%
  ggplot(., aes(reorder(parameters, original), original, color = Continent)) +
  geom_point(position = position_dodge(0.6)) +
  geom_errorbar(aes(ymax = high.ci, ymin = low.ci),
                position = position_dodge(0.6)) +
  geom_hline(yintercept = 0,
             lty = 2,
             color = "red") +
  facet_grid(~sensitivity,
             scales = "free_x",
             space = "free_x") +
  scale_color_discrete(name = "Continent") +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  labs(x = "",
       y = "Sobol' index") +
```

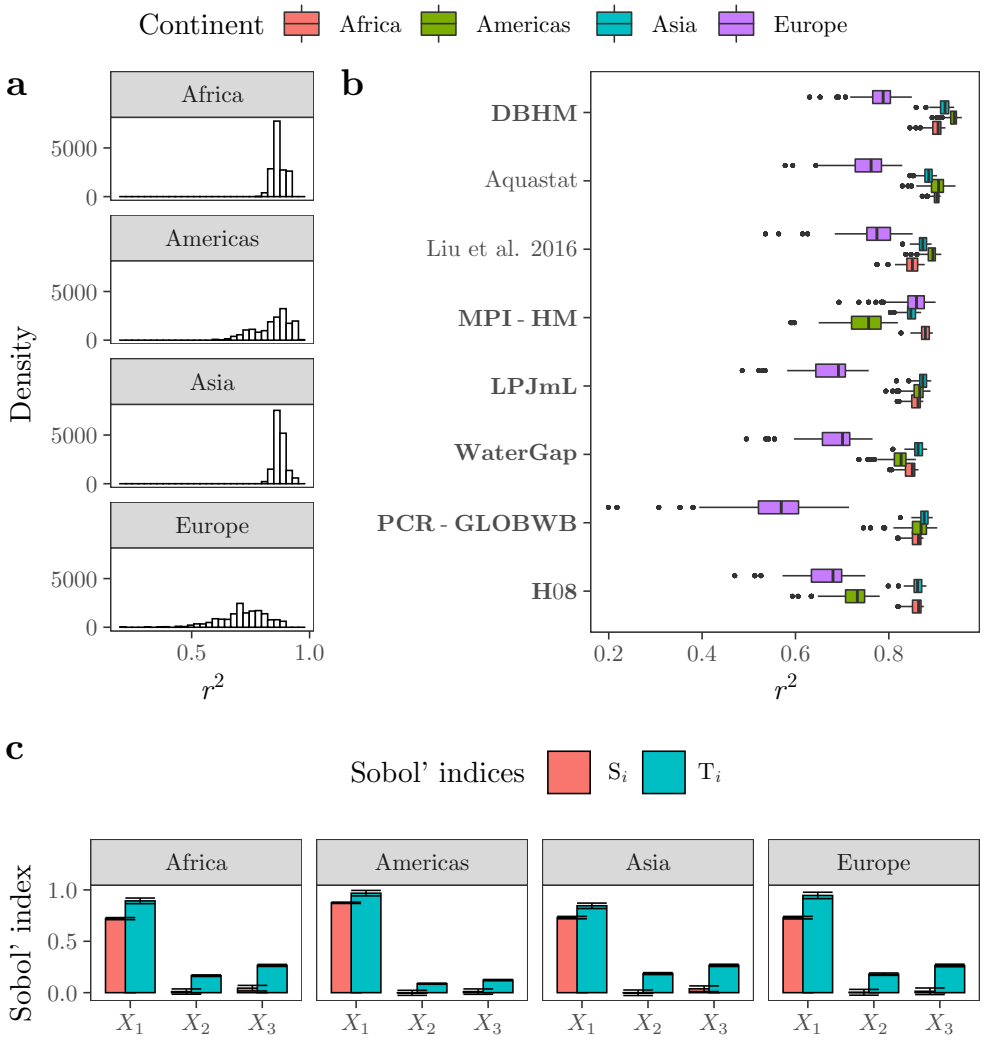


Figure 9: Uncertainty and sensitivity analysis. a) Empirical distribution for r^2 at the continental level. b) Boxplots of r^2 values obtained when regressions where run with GHM (in bold) and FAO-based datasets. c) Sobol' indices. S_i and T_i refer respectively to Sobol' first and total order indices. S_i measures the influence of a parameter in the model output, while T_i measures the influence of a parameter jointly with its interactions.

```
theme_AP()
```

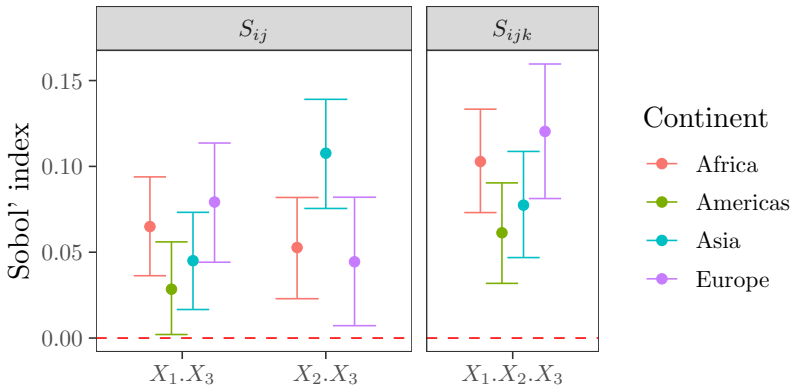


Figure 10: High-order interactions between the triggers.

10 Session information

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

sessionInfo()
```

```
## R version 3.6.3 (2020-02-29)
## Platform: x86_64-apple-darwin15.6.0 (64-bit)
## Running under: macOS Catalina 10.15.5
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/3.6/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/3.6/Resources/lib/libRlapack.dylib
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
## [1] parallel  stats     graphics  grDevices utils     datasets  methods
## [8] base
##
## other attached packages:
##  [1] checkpoint_0.4.9  forcats_0.5.0     stringr_1.4.0     dplyr_0.8.5
##  [5] purrr_0.3.4       readr_1.3.1       tidyr_1.0.2       tibble_3.0.1
##  [9] ggplot2_3.3.0     tidyverse_1.3.0   benchmarkme_1.0.3 cowplot_1.0.0
## [13] naniar_0.5.0      broom_0.5.6       ggridges_0.5.2    mice_3.8.0
## [17] lmtest_0.9-37     zoo_1.8-7         sandwich_2.5-1    mvoutlier_2.0.9
## [21] sgeostat_1.0-27   complmrob_0.7.0   doParallel_1.0.15 iterators_1.0.12
## [25] foreach_1.5.0     MASS_7.3-51.5     scales_1.1.1      boot_1.3-24
## [29] IDPmisc_1.1.20    countrycode_1.1.1 rworldmap_1.3-6   sp_1.4-1
## [33] ncdf4_1.17        sensobol_0.3      data.table_1.12.8
##
## loaded via a namespace (and not attached):
##   [1] colorspace_1.4-1      ellipsis_0.3.0        class_7.3-16
##   [4] modeltools_0.2-23     rio_0.5.16            visdat_0.5.3
##   [7] mclust_5.4.6          fs_1.4.1              pls_2.7-2
##  [10] rstudioapi_0.11       cvTools_0.3.2         flexmix_2.3-15
##  [13] fansi_0.4.1           lubridate_1.7.8       mvtnorm_1.1-0
##  [16] xml2_1.3.1            ranger_0.12.1         codetools_0.2-16
##  [19] splines_3.6.3         sROC_0.1-2            robustbase_0.93-6
##  [22] knitr_1.28            jsonlite_1.6.1        spam_2.5-1
##  [25] robCompositions_2.2.1 dbplyr_1.4.3          cluster_2.1.0
##  [28] kernlab_0.9-29        httr_1.4.1            rrcov_1.5-2
##  [31] compiler_3.6.3        backports_1.1.6       assertthat_0.2.1
##  [34] Matrix_1.2-18         cli_2.0.2             htmltools_0.4.0
##  [37] tools_3.6.3           dotCall64_1.0-0       gtable_0.3.0
##  [40] glue_1.4.0            maps_3.3.0            Rcpp_1.0.4.6
##  [43] carData_3.0-3         cellranger_1.1.0      vctrs_0.2.4
```

```
##  [46] zCompositions_1.3.4   nlme_3.1-147          fpc_2.2-5
##  [49] gbRd_0.4-11           xfun_0.13             laeken_0.5.1
##  [52] rvest_0.3.5           openxlsx_4.1.4        lifecycle_0.2.0
##  [55] DEoptimR_1.0-8        VIM_5.1.1             hms_0.5.3
##  [58] RColorBrewer_1.1-2    fields_10.3           yaml_2.2.1
##  [61] curl_4.3              NADA_1.6-1.1          reshape_0.8.8
##  [64] stringi_1.4.6         maptools_0.9-9        pcaPP_1.9-73
##  [67] e1071_1.7-3           zip_2.0.4             bibtex_0.4.2.2
##  [70] benchmarkmeData_1.0.3 truncnorm_1.0-8       Rdpack_0.11-1
##  [73] rlang_0.4.5           pkgconfig_2.0.3       prabclus_2.3-2
##  [76] evaluate_0.14         lattice_0.20-41       tidyselect_1.0.0
##  [79] GGally_1.5.0          plyr_1.8.6            magrittr_1.5
##  [82] R6_2.4.1              generics_0.0.2        DBI_1.1.0
##  [85] withr_2.2.0           pillar_1.4.3          haven_2.2.0
##  [88] foreign_0.8-76        survival_3.1-12       abind_1.4-5
##  [91] nnet_7.3-13           modelr_0.1.6          crayon_1.3.4
##  [94] car_3.0-7             rmarkdown_2.1         grid_3.6.3
##  [97] readxl_1.3.1          reprex_0.3.0          vcd_1.4-7
## [100] digest_0.6.25         diptest_0.75-7        stats4_3.6.3
## [103] munsell_0.5.0
```

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

```
## Machine:
```

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

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

```
## Num cores:
```

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

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

```
## Num threads:
```

```
## [1] 16
```

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

```
## RAM:
```

```
## 34.4 GB
```

References

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