Validation, calibration, etc

R code

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Contents

```
# PRELIMINARY FUNCTIONS ###################################################

# Load the packages
sensobol::load_packages(c("data.table", "tidyverse", "openxlsx", "tm", "stringr",
                          "pdftools", "tidytext", "scales", "cowplot",
                          "ggrepel", "tidyquant"))

# Create custom theme
# 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),
          strip.background = element_rect(fill = "white"),
          legend.margin = margin(0.5, 0.1, 0.1, 0.1),
          legend.box.margin = margin(0.2,-4,-7,-7),
          plot.margin = margin(3, 4, 0, 4),
          legend.text = element_text(size = 6.5),
          axis.title = element_text(size = 10),
          axis.text.x = element_text(size = 7),
          axis.text.y = element_text(size = 7),
          axis.title.x = element_text(size = 7.3),
          axis.title.y = element_text(size = 7.3),
          strip.text.x = element_text(size = 7.4),
          strip.text.y = element_text(size = 7.4),
          legend.key.width = unit(0.4, "cm"),
          legend.key.height = unit(0.5, "lines"),
          legend.title = element_text(size = 7.5))
}
```

```
# FUNCTIONS TO CLEAN THE TEXT #############################################
```

```r
# Function to remove words from text
removeWords <- function(str, stopwords) {
  x <- unlist(strsplit(str, " "))
  paste(x[!x %in% stopwords], collapse = " ")
}

# Function to remove punctuation, citations, numbers, stopwords in english,
# bring to lowercase and strip whitespace, and especial characters, etc...
clear_text <- function(x, stem = TRUE) {

  y <- tolower(x)
  y <- str_replace_all(y, "[[:punct:]]", " ") # Remove punctuation characters
  y <- tm::removeNumbers(y)
  y <- tm::removeWords(y, stopwords::stopwords(language = "en"))
  y <- str_remove_all(y, "[^[\\da-zA-Z ]]")# Remove all non-alphanumerical
  y <- gsub("\\s[A-Za-z](?= )", " ", y, perl = TRUE) # Remove isolated letters
  #y <- tm::stripWhitespace(y)
  y <- str_squish(y)

  if (stem == TRUE) {
    y <- stemDocument(y) # Stem the document and keep only the root of the word
  }

  return(y)
}

# READ DATA ###################################################################

dt <- data.table(read.xlsx("final.dt.xlsx"))
dt[, keywords.large:= tolower(keywords.large)]
dt[, abstract.cleaned:= clear_text(abstract.large, stem = FALSE)]

# TERMS TO SEARCH #############################################################

keywords <- c("validation", "verification", "calibration", "confirmation", "evaluation",
              "benchmarking")
keywords.stemmed <- stemDocument(keywords)

# keywords.stemmed <- c(
#  "calibration", "verification", "validation", "evaluation",
#  "calibrations", "verifications", "validations", "evaluations",
#  "calibrated", "verified", "validated", "evaluated",
#  "calibrating", "verifying", "validating", "evaluating",
#  "calibrative", "verificative", "validative", "evaluative",
#  "calibratively", "verificatively", "validatively", "evaluatively"
# )
```

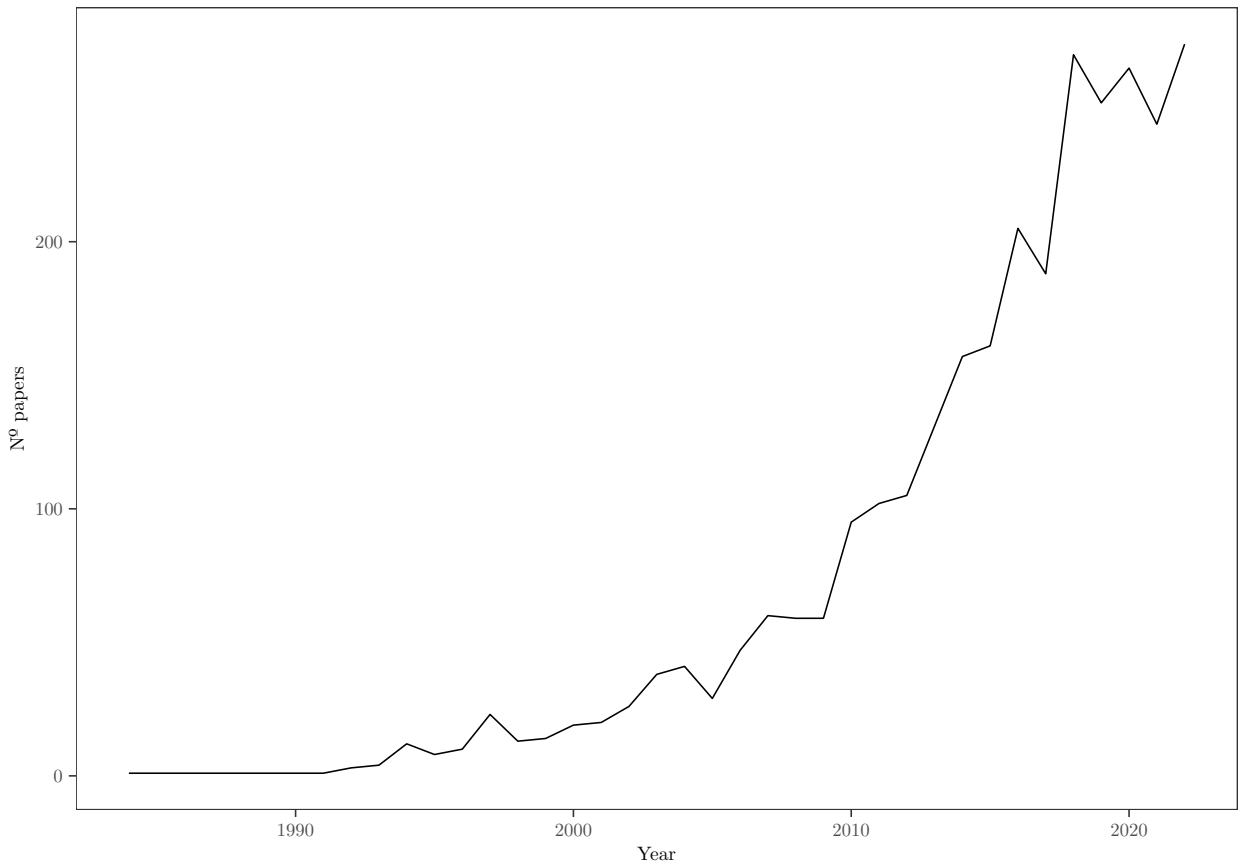
```r
# SEARCHING FOR TERMS ############################################################

# Check which papers include keywords in abstract, keywords or title -----------
selected_cols <- c("title", "abstract", "keywords")
#selected_cols <- c("title.large", "abstract.large", "keywords.large")
out <- list()

for(i in 1:length(keywords.stemmed)) {

  out[[i]] <- dt[, lapply(.SD, function(x)
    str_detect(x, keywords.stemmed[i])), .SDcols = (selected_cols)]

}

# ARRANGE DATA ###################################################################

names(out) <- keywords.stemmed

valid.dt <- lapply(out, function(x) rowSums(x, na.rm = TRUE) > 0L) %>%
  do.call(cbind, .) %>%
  data.table() %>%
  .[, any.column:= rowSums(.SD) > 0]

full.dt <- cbind(dt, valid.dt)
full.dt.cols <- data.frame(full.dt[, .SD, .SDcols = keywords.stemmed])

# DESCRIPTIVE STATISTICS #########################################################

full.dt[, lapply(.SD, sum), .SDcols = keywords.stemmed]
```

```
##    valid verif calibr confirm evalu benchmark
##    <int> <int>  <int>   <int> <int>     <int>
## 1:   536    76    743      74  1065        86
```

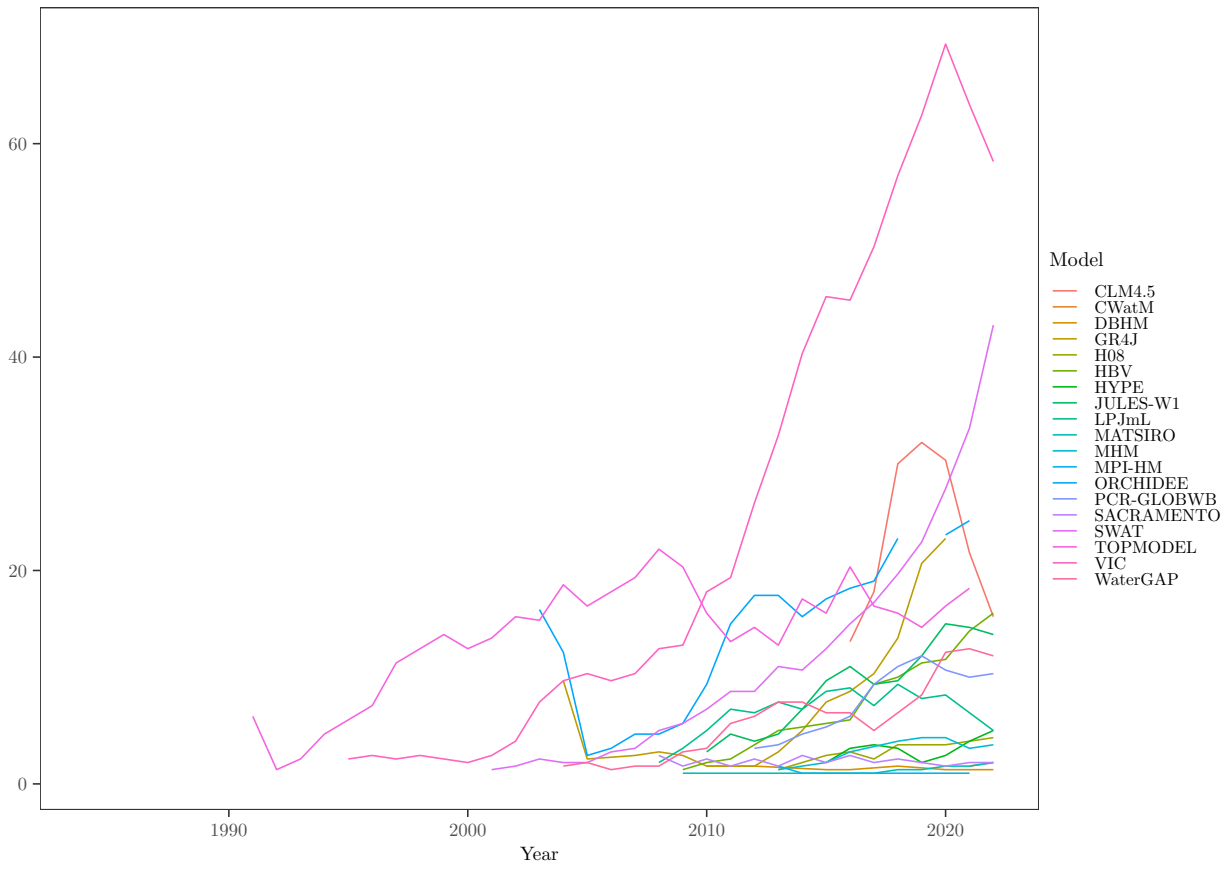
```r
# Count number of papers with mentions to validation, validation + verification,
# validation + calibration, etc ------------------------------------------------

# Function to count the number of TRUE values shared between columns
count_shared_true <- function(data, cols) {
  sum(rowSums(data[, cols]) == length(cols))
}

# Create an empty list to store results
results_list <- list()

# Loop through all combinations of columns and count shared TRUE values
for (size in 2:length(keywords.stemmed)) {
```

```
  for (cols_combination in combn(ncol(full.dt.cols), size, simplify = FALSE)) {

    shared_true_count <- count_shared_true(data = full.dt.cols, cols = cols_combination)
    col_names <- colnames(full.dt.cols)[cols_combination]

    # Append results to the list
    results_list <- c(results_list, list(data.table(combination = paste(col_names, collapse =
  }
}

# Combine the list of data.tables into a single data.table
comb_dt <- rbindlist(results_list)
```

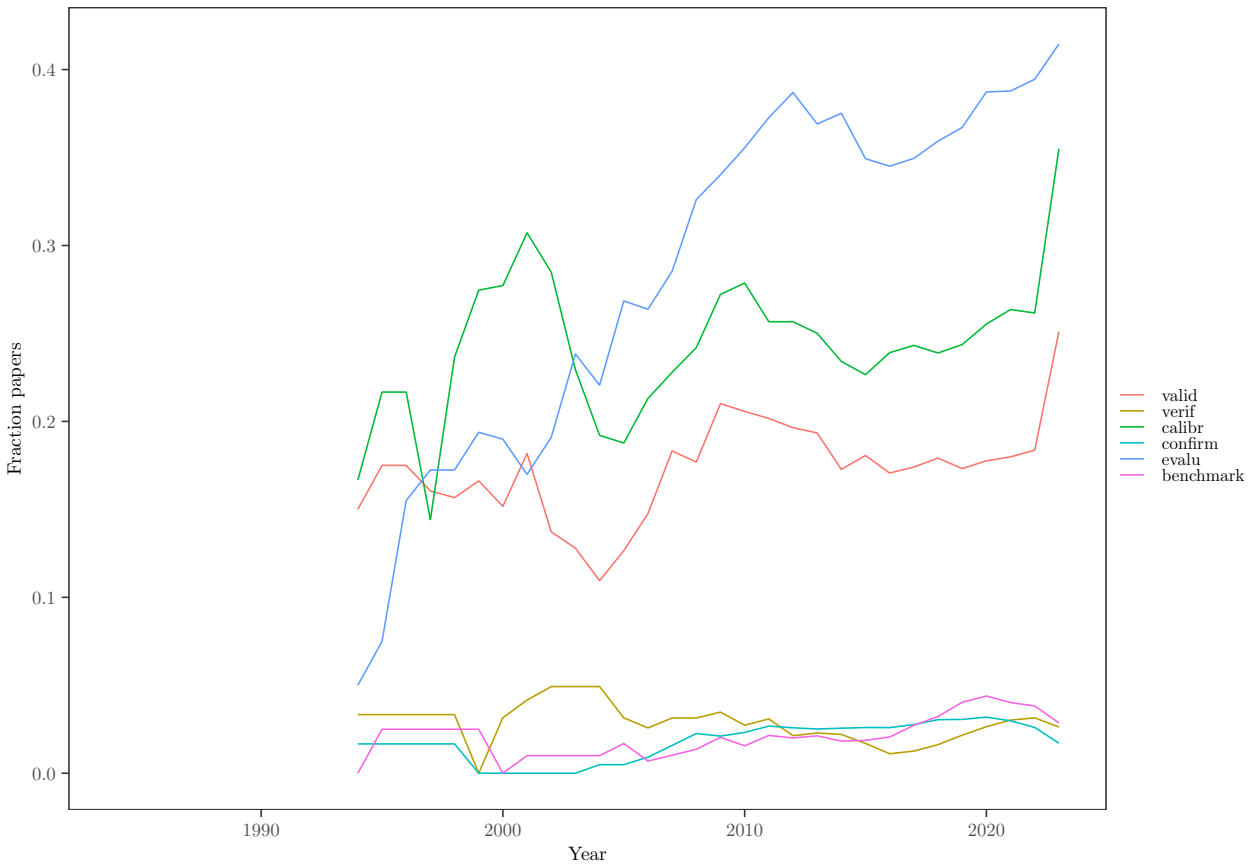
```
# PLOTS ##########################################################################

plot.year <- full.dt[, .N, year] %>%
  .[!year == 2023] %>%
  ggplot(., aes(year, N)) +
  geom_line() +
  labs(x = "Year", y = "Nº papers") +
  theme_AP()

plot.year
```



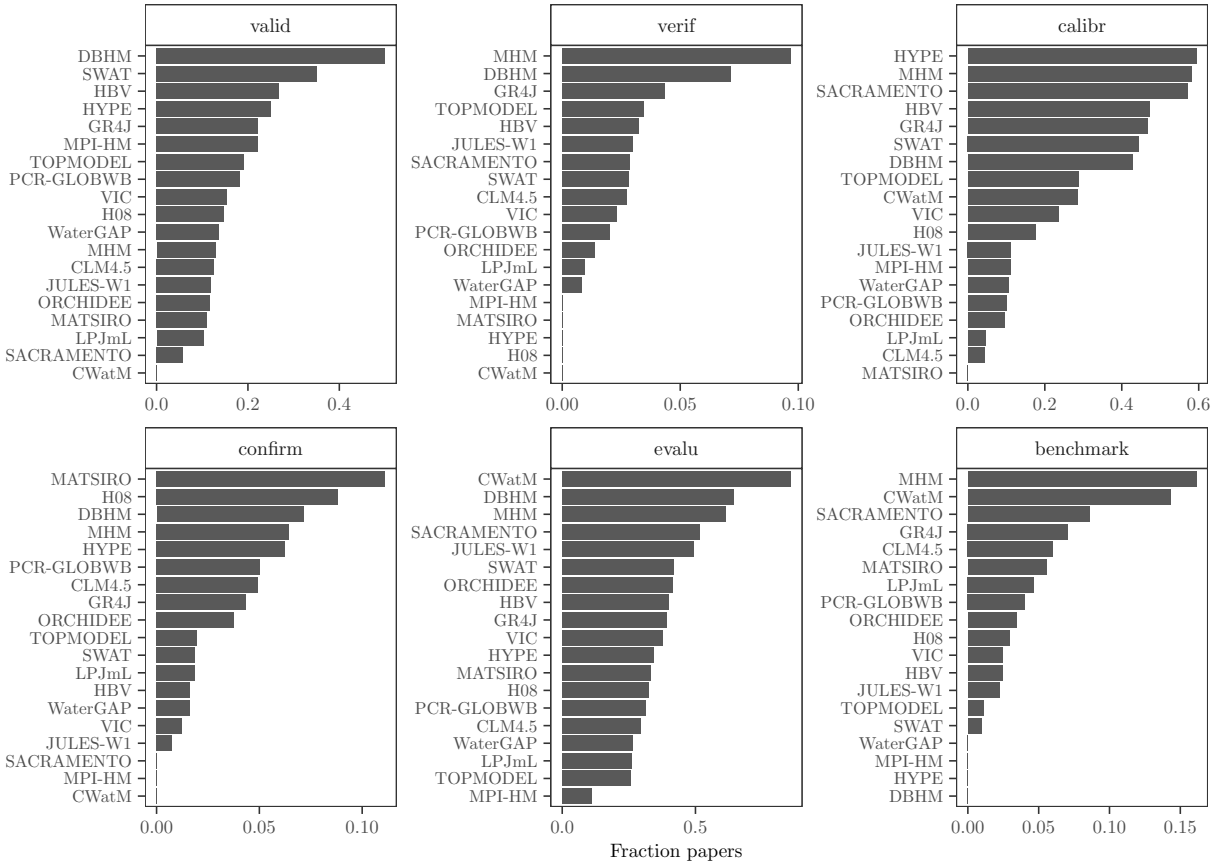

```
plot.model.year <- full.dt[, .N, .(Model, year)] %>%
  .[!year == 2023] %>%
  ggplot(., aes(year, N, color = Model)) +
  geom_ma(ma_fun = SMA, n = 3, lty = 1) +
  labs(x = "Year", y = "") +
  theme_AP()

plot.model.year
```



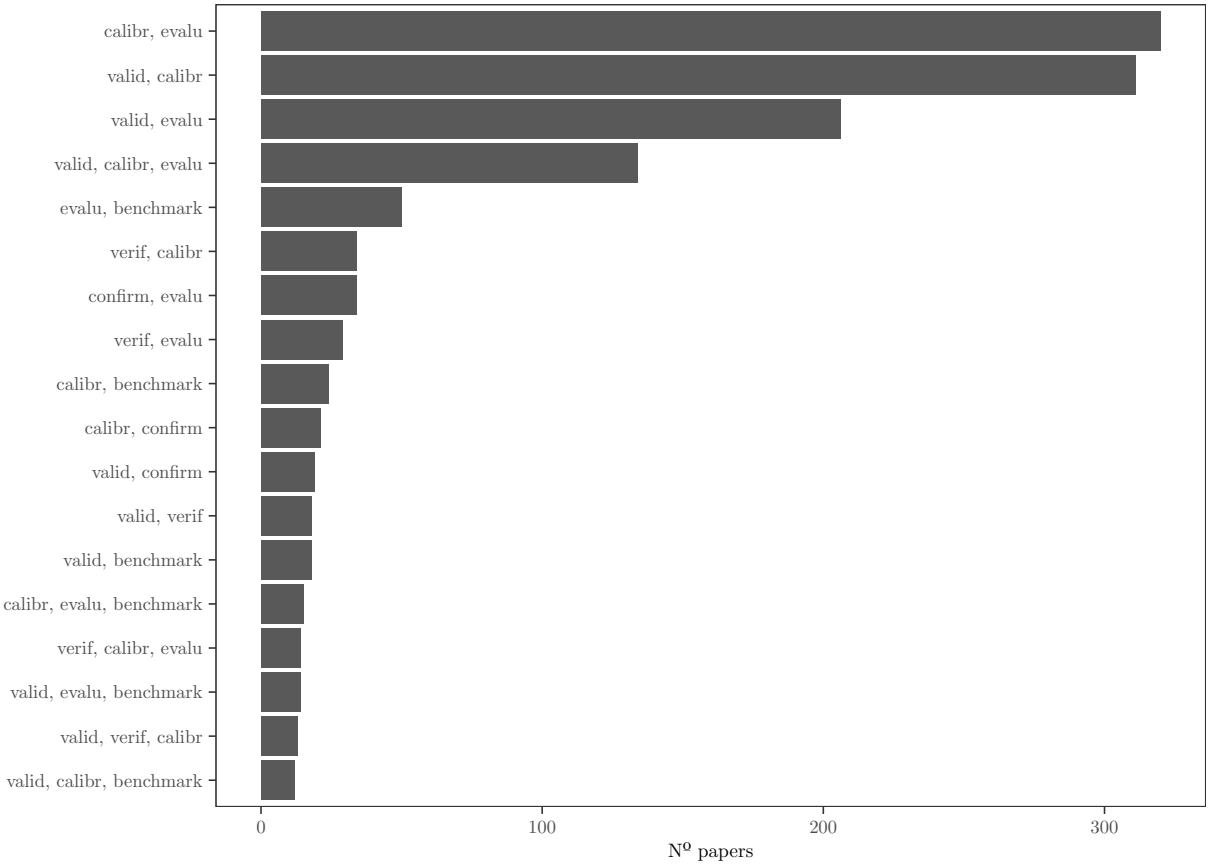

```
plot.keywords.time <- merge(full.dt, full.dt[, .(total.papers = .N), year], by = "year") %>%
  melt(., measure.vars = keywords.stemmed) %>%
  .[, sum(value, na.rm = TRUE), .(variable, year, total.papers)] %>%
  .[, fraction:= V1 / total.papers] %>%
  ggplot(., aes(year, fraction, color = variable)) +
  scale_color_discrete(name = "") +
  geom_ma(ma_fun = SMA, n = 5, lty = 1) +
  theme_AP() +
  labs(x = "Year", y = "Fraction papers")

plot.keywords.time
```



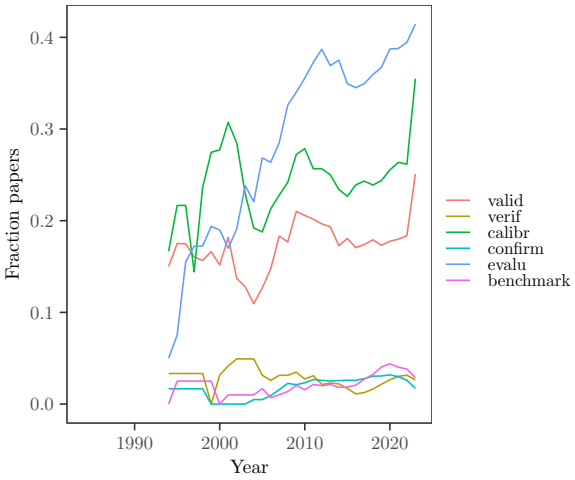

```
tmp <- merge(full.dt, full.dt[, .(total.papers = .N), Model], by = "Model") %>%
  melt(., measure.vars = keywords.stemmed) %>%
  .[, sum(value, na.rm = TRUE), .(variable, Model, total.papers)] %>%
  .[, fraction:= V1 / total.papers] %>%
  mutate(variable = as.factor(variable),
       name = reorder_within(Model, fraction, variable))

plot.keyword.per.model <- tmp %>%
  ggplot(., aes(name, fraction)) +
  geom_bar(stat = "identity") +
  coord_flip() +
  facet_wrap(~variable, scales = "free") +
  scale_x_reordered() +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  theme_AP() +
  labs(x = "", y = "Fraction papers") +
  theme(axis.text.y = element_text(size = 6.5))

plot.keyword.per.model
```




```
plot.keyword.comb <- comb_dt[N > 10] %>%
  ggplot(., aes(reorder(combination, N), N)) +
  geom_bar(stat = "identity") +
  coord_flip() +
  theme_AP() +
  theme(axis.text.y = element_text(size = 7)) +
  labs(x = "", y = "Nº papers")

plot.keyword.comb
```

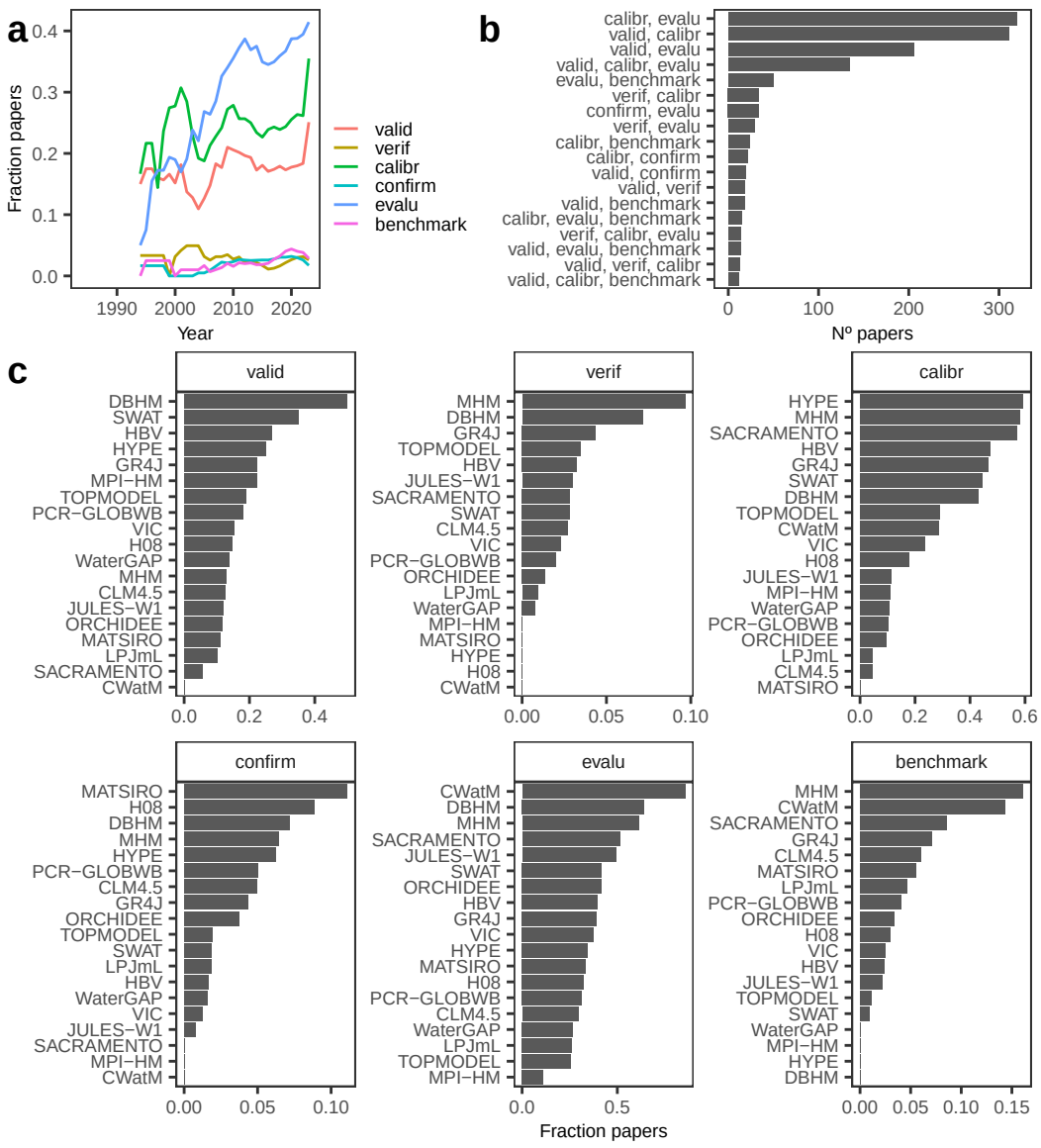



```
plot.keywords.time
```

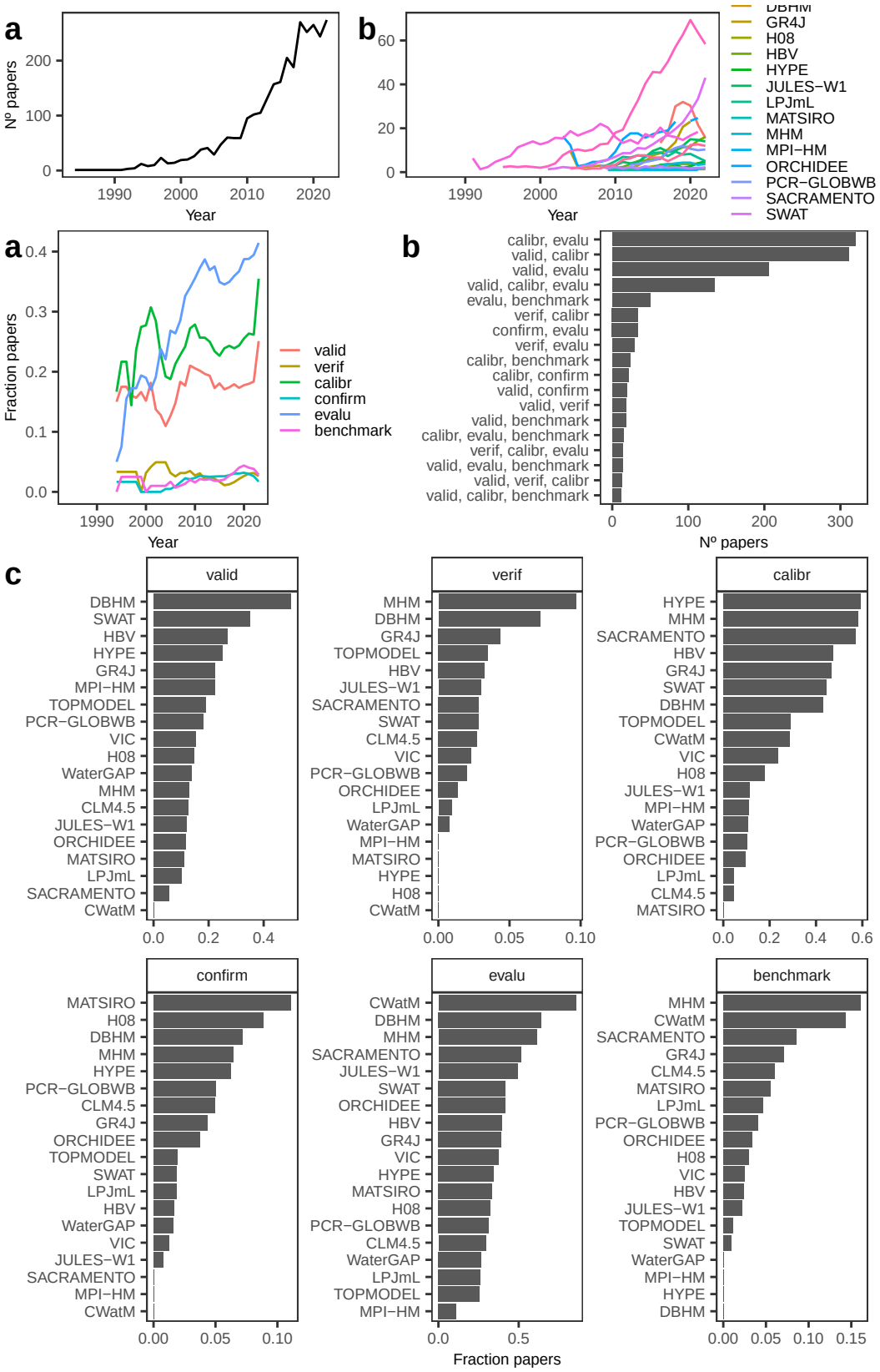



```
# MERGE DESCRIPTIVE PLOTS ##########################################################

top <- plot_grid(plot.keywords.time, plot.keyword.comb, ncol = 2, labels = "auto",
                 rel_widths = c(0.45, 0.55))

plot.merged <- plot_grid(top, plot.keyword.per.model, ncol = 1,
                         labels = c("", "c"), rel_heights = c(0.3, 0.7))
```

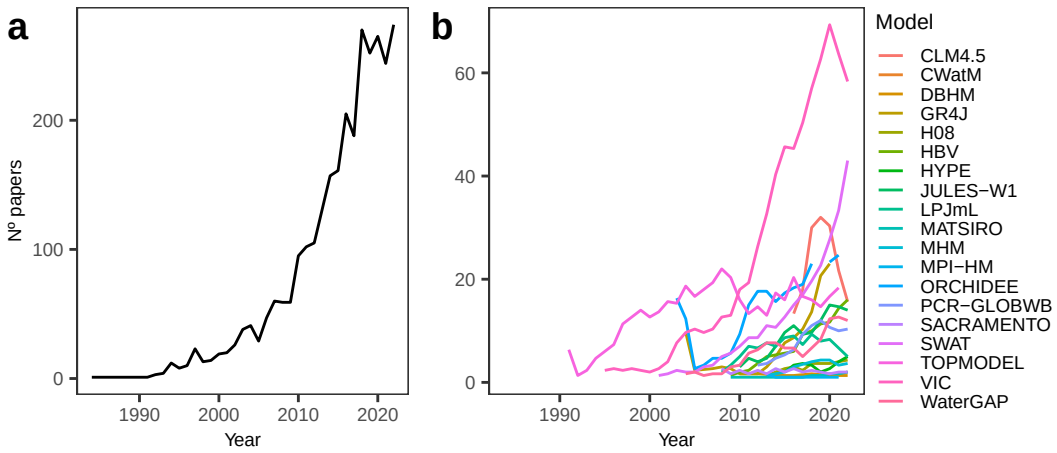
```
plot.merged
```




```
toppest <- plot_grid(plot.year, plot.model.year, ncol = 2, labels = "auto",
                     rel_widths = c(0.4, 0.6))

top <- plot_grid(plot.keywords.time, plot.keyword.comb, ncol = 2, labels = "auto",
                 rel_widths = c(0.45, 0.55))

both.top <- plot_grid(toppest, top, ncol = 1, rel_heights = c(0.4, 0.6))

plot.merged <- plot_grid(both.top, plot.keyword.per.model, ncol = 1,
                         labels = c("", "c"), rel_heights = c(0.4, 0.6))

plot.merged
```


a
Nº papers
Year
b
DBHM
GR4J
H08
HBV
HYPE
JULES−W1
LPJmL
MATSIRO
MHM
MPI−HM
ORCHIDEE
PCR−GLOBWB
SACRAMENTO
SWAT
a
Fraction papers
valid
verif
calibr
confirm
evalu
benchmark
b
calibr, evalu
valid, calibr
valid, evalu
valid, calibr, evalu
evalu, benchmark
verif, calibr
confirm, evalu
verif, evalu
calibr, benchmark
calibr, confirm
valid, confirm
valid, verif
valid, benchmark
calibr, evalu, benchmark
verif, calibr, evalu
valid, evalu, benchmark
valid, verif, calibr
valid, calibr, benchmark
Nº papers
c
valid
verif
calibr
confirm
evalu
benchmark
Fraction papers

```
toppest
```

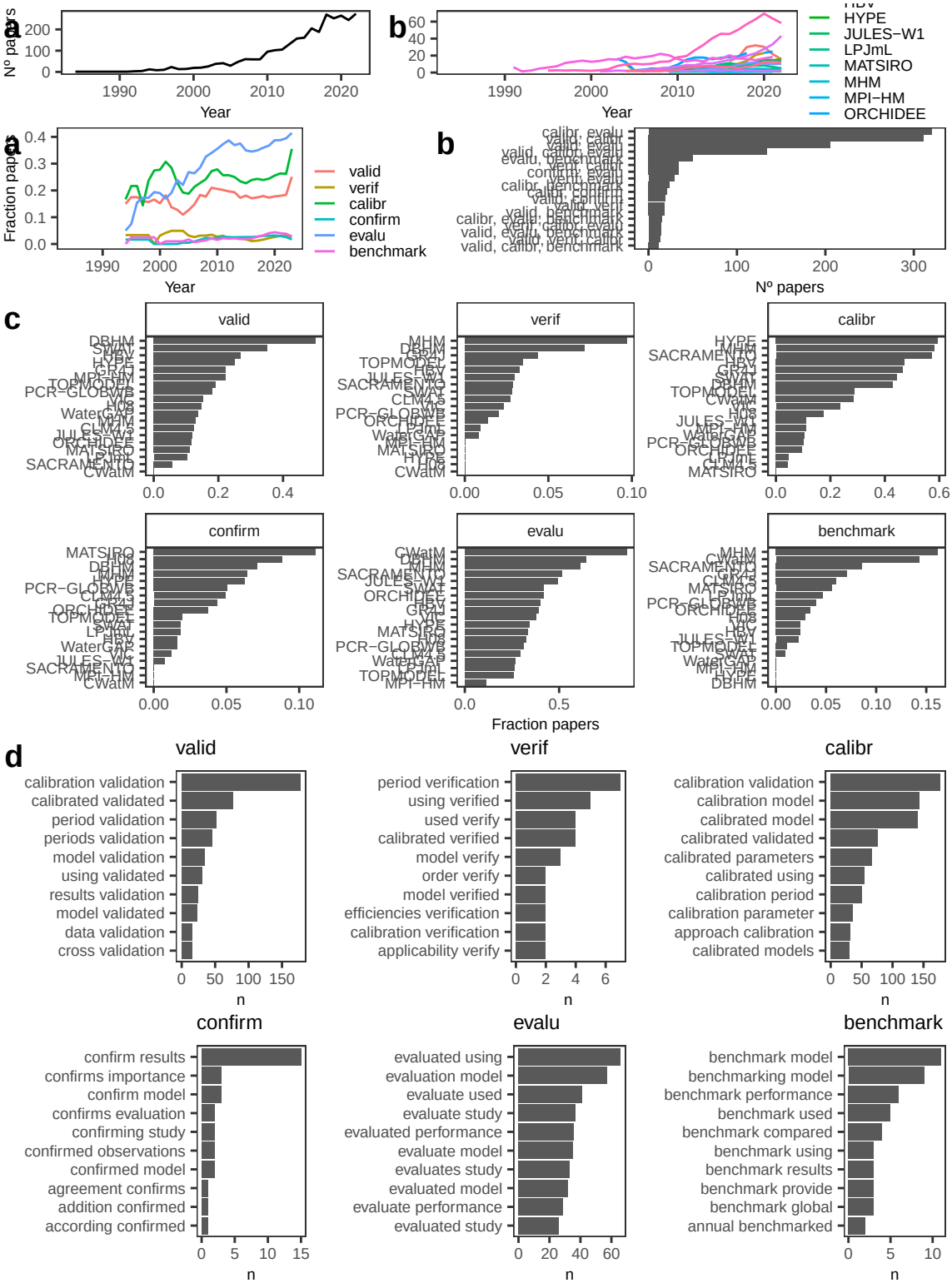



```
# TOKEN ANALYSIS ##################################################################

# Create function ----------------------------------------------------------
tokenize_fun <- function(dt, word, keywords, N.tokens) {

  # Create long dataset
  dt <- melt(dt, measure.vars = keywords)
  output <- dt[variable == word & value == TRUE]

  # Token analysis -----------------------------
  # We count the co-occurences of words without taking into account their order
  # within the n-token
  token.analysis <- output %>%
    unnest_tokens(bigram, abstract.cleaned, token = "ngrams", n = N.tokens) %>%
    separate(bigram, into = c("word1", "word2"), sep = " ") %>%
    data.table() %>%
    .[, `:=`(word1= pmin(word1, word2), word2 = pmax(word1, word2))] %>%
    count(word1, word2, sort = TRUE) %>%
    unite(., col = "bigram", c("word1", "word2"), sep = " ") %>%
    data.table()

  # Vector to retrieve only the bigrams with uncertainti or sensit
  vec <- token.analysis[, str_detect(bigram, word)]

  # Final dataset
  output.dt <- token.analysis[vec]

  # Plot the q0 words most commonly
  # associated with uncertainti and sensit ------
  plot.token <-  output.dt %>%
    .[, sum(n), bigram] %>%
    .[order(-V1)] %>%
    .[, head(.SD, 10)] %>%
    ggplot(., aes(reorder(bigram, V1, sum), V1)) +
    geom_bar(stat = "identity") +
```

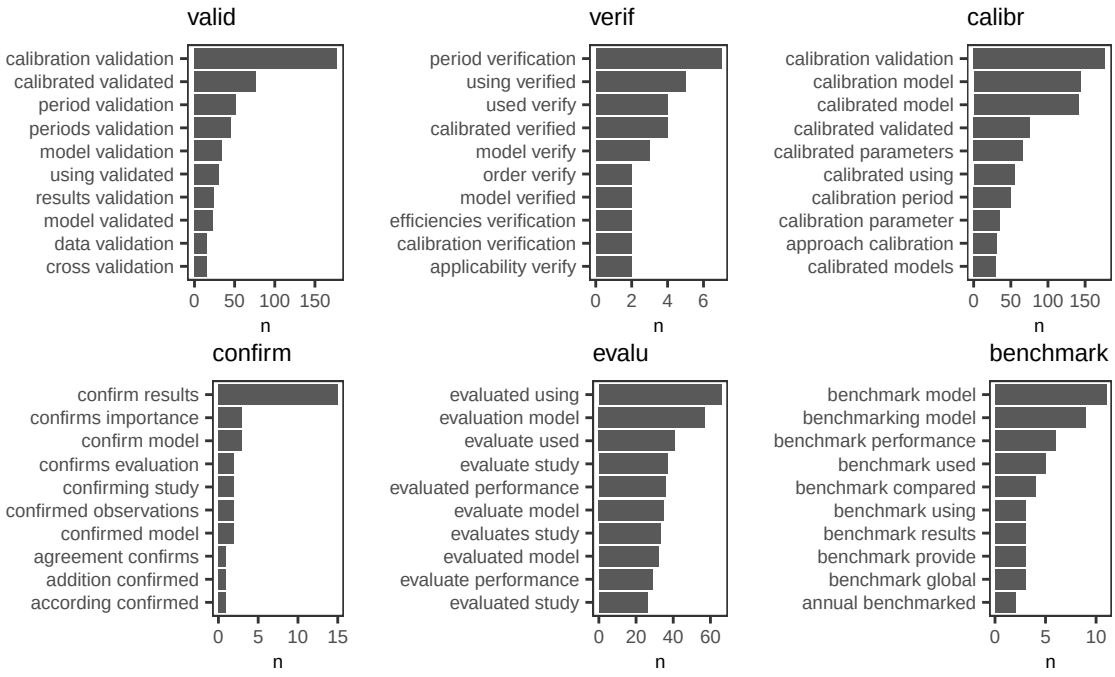
```
    coord_flip() +
    scale_y_continuous(breaks = pretty_breaks(n = 3)) +
    theme_AP() +
    labs(y = "n", x = "") +
    ggtitle(word) +
    theme(legend.position = "none",
          plot.title = element_text(size = 9),
          axis.text.y = element_text(size = 7))

  # Arrange and output -------------------------

  out <- list(output.dt, plot.token)
  names(out) <- c("data", "token")

  return(out)

}
```

```
# RUN TOKEN ANALYSIS ##################################################################

N.tokens <- 2
token.dt <- list()

for (j in keywords.stemmed) {

  token.dt[[j]] <- tokenize_fun(dt = full.dt, word = j,
                                keywords = keywords.stemmed,
                                N.tokens = N.tokens)

}
```

```
# PLOT RESULTS ########################################################################

plot.tokens <- plot_grid(token.dt$valid[[2]], token.dt$verif[[2]], token.dt$calibr[[2]],
                         token.dt$confirm[[2]], token.dt$evalu[[2]], token.dt$benchmark[[2]],
                         ncol = 3)

plot_grid(plot.merged, plot.tokens, ncol = 1, labels = c("", "d"),
          rel_heights = c(0.57, 0.43))
```


a
Nº papers
Year
b
HYPE
JULES−W1
LPJmL
MATSIRO
MHM
MPI−HM
ORCHIDEE
Fraction papers
valid
verif
calibr
confirm
evalu
benchmark
Nº papers
c
Fraction papers
d
n
calibration validation
calibrated validated
period validation
periods validation
model validation
using validated
results validation
model validated
data validation
cross validation
period verification
using verified
used verify
calibrated verified
model verify
order verify
model verified
efficiencies verification
calibration verification
applicability verify
calibration model
calibrated model
calibrated parameters
calibrated using
calibration period
calibration parameter
approach calibration
calibrated models
confirm results
confirms importance
confirm model
confirms evaluation
confirming study
confirmed observations
confirmed model
agreement confirms
addition confirmed
according confirmed
evaluated using
evaluation model
evaluate used
evaluate study
evaluated performance
evaluate model
evaluates study
evaluated model
evaluate performance
evaluated study
benchmark model
benchmarking model
benchmark performance
benchmark used
benchmark compared
benchmark using
benchmark results
benchmark provide
benchmark global
annual benchmarked

```
plot.tokens
```


valid
calibration validation
calibrated validated
period validation
periods validation
model validation
using validated
results validation
model validated
data validation
cross validation
0 50 100 150
n
verif
period verification
using verified
used verify
calibrated verified
model verify
order verify
model verified
efficiencies verification
calibration verification
applicability verify
0 2 4 6
n
calibr
calibration validation
calibration model
calibrated model
calibrated validated
calibrated parameters
calibrated using
calibration period
calibration parameter
approach calibration
calibrated models
0 50 100 150
n
confirm
confirm results
confirms importance
confirm model
confirms evaluation
confirming study
confirmed observations
confirmed model
agreement confirms
addition confirmed
according confirmed
0 5 10 15
n
evalu
evaluated using
evaluation model
evaluate used
evaluate study
evaluated performance
evaluate model
evaluates study
evaluated model
evaluate performance
evaluated study
0 20 40 60
n
benchmark
benchmark model
benchmarking model
benchmark performance
benchmark used
benchmark compared
benchmark using
benchmark results
benchmark provide
benchmark global
annual benchmarked
0 5 10
n

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

sessionInfo()
```

```
## R version 4.3.2 (2023-10-31)
## Platform: aarch64-apple-darwin20 (64-bit)
## Running under: macOS Sonoma 14.2.1
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.3-arm64/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.3-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
##
## time zone: Europe/London
## tzcode source: internal
##
## attached base packages:
## [1] parallel  stats     graphics  grDevices utils     datasets  methods
## [8] base
##
## other attached packages:
##  [1] benchmarkme_1.0.8          tidyquant_1.0.7
##  [3] quantmod_0.4.25            TTR_0.24.3
##  [5] PerformanceAnalytics_2.0.4 xts_0.13.1
##  [7] zoo_1.8-12                 ggrepel_0.9.5
##  [9] LSAfun_0.6.3               rgl_1.1.3
## [11] lsa_0.73.3                 SnowballC_0.7.1
## [13] cowplot_1.1.1              scales_1.3.0
## [15] tidytext_0.4.1             pdftools_3.3.3
## [17] tm_0.7-11                  NLP_0.2-1
## [19] openxlsx_4.2.5.2           lubridate_1.9.2
## [21] forcats_1.0.0              stringr_1.5.1
## [23] dplyr_1.1.4                purrr_1.0.2
## [25] readr_2.1.4                tidyr_1.3.0
## [27] tibble_3.2.1               ggplot2_3.4.4
## [29] tidyverse_2.0.0            data.table_1.14.99
##
## loaded via a namespace (and not attached):
##  [1] tidyselect_1.2.0      filehash_2.4-5        farver_2.1.1
##  [4] fastmap_1.1.1         janeaustenr_1.0.0     digest_0.6.34
##  [7] timechange_0.2.0      lifecycle_1.0.4       qpdf_1.3.2
## [10] tokenizers_0.3.0      magrittr_2.0.3        compiler_4.3.2
## [13] rlang_1.1.3           tools_4.3.2           utf8_1.2.4
## [16] sensobol_1.1.4        yaml_2.3.7            knitr_1.42
## [19] askpass_1.1           labeling_0.4.3        stopwords_2.3
```

```
## [22] htmlwidgets_1.6.2     curl_5.0.0            xml2_1.3.3
## [25] withr_3.0.0           grid_4.3.2            fansi_1.0.6
## [28] colorspace_2.1-0      iterators_1.0.14      tinytex_0.45
## [31] cli_3.6.2             rmarkdown_2.21        generics_0.1.3
## [34] tikzDevice_0.12.4     rstudioapi_0.15.0     httr_1.4.5
## [37] tzdb_0.3.0            base64enc_0.1-3       vctrs_0.6.5
## [40] Matrix_1.6-1.1        jsonlite_1.8.4        slam_0.1-50
## [43] hms_1.1.3             foreach_1.5.2         glue_1.7.0
## [46] benchmarkmeData_1.0.4 codetools_0.2-19      Quandl_2.11.0
## [49] stringi_1.8.3         gtable_0.3.4          quadprog_1.5-8
## [52] munsell_0.5.0         pillar_1.9.0          htmltools_0.5.5
## [55] R6_2.5.1              Rdpack_2.6            doParallel_1.0.17
## [58] evaluate_0.20         lattice_0.21-9        highr_0.10
## [61] rbibutils_2.2.16      Rcpp_1.0.12           zip_2.3.0
## [64] xfun_0.39             pkgconfig_2.0.3
```

```
## 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
```