Package ‘mvrsquared’

February 20, 2020

Type Package

Title Compute the Coefficient of Determination for Vector or Matrix Outcomes

Version 0.0.3

Description Compute the coefficient of determination for outcomes in n-dimensions. May be useful for multidimensional predictions (such as a multinomial model) or calculating goodness of fit from latent variable models such as probabilistic topic models like latent Dirichlet allocation or deterministic topic models like latent semantic analysis. Based on Jones (2019) <arXiv:1911.11061>.

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Encoding UTF-8

URL https://github.com/TommyJones/mvrsquared

BugReports https://github.com/TommyJones/mvrsquared/issues

LazyData true

Imports Matrix, methods, Rcpp (>= 1.0.2)

Suggests dplyr, furrr, knitr, MASS, nnet, parallel, rmarkdown, stats, stringr, testthat, textmineR, tidytext

LinkingTo Rcpp, RcppArmadillo

RoxygenNote 7.0.2

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NeedsCompilation yes

Author Tommy Jones [aut, cre]

Maintainer Tommy Jones <jones.thos.w@gmail.com>

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Calculate R-Squared for univariate or multivariate outcomes.

Usage

calc_rsquared(y, yhat, ybar = NULL, return_ss_only = FALSE)

Arguments

y      The true outcome. This must be a numeric vector, numeric matrix, or coercible to a sparse matrix of class dgCMatrix. See 'Details' below for more information.
yhat   The predicted outcome or a list of two matrices whose dot product makes the predicted outcome. See 'Details' below for more information.
ybar   Numeric scalar or vector; the mean of y. Useful for parallel computation in batches.
return_ss_only Logical. Do you want to forego calculating R-squared and only return the sums of squares?

Details

There is some flexibility in what you can pass as y and yhat. In general, y can be a numeric vector, numeric matrix, a sparse matrix of class dgCMatrix from the Matrix package, or any object that can be coerced into a dgCMatrix.
yhat can be a numeric vector, numeric matrix, or a list of two matrices whose dot product has the same dimensionality as y. If yhat is a list of two matrices you may optionally name them x and w indicating the order of multiplication (x left multiplies w). If unnamed or ambiguously named, then it is assumed that yhat[[1]] left multiplies yhat[[2]].

Value

If return_ss_only = FALSE, calc_rsquared returns a numeric scalar R-squared. If return_ss_only = TRUE, calc_rsquared returns a vector; the first element is the error sum of squares (SSE) and the second element is the total sum of squares (SST). R-squared may then be calculated as 1 - SSE / SST.

Note

Setting return_ss_only to TRUE is useful for parallel or distributed computing for large data sets, particularly when y is a large matrix. However if you do parallel execution you MUST pre-calculate 'ybar' and pass it to the function. If you do not, SST will be calculated based on means of each batch independently. The resulting r-squared will be incorrect.

See example below for parallel computation with future_map from the furr package.
Examples

# standard r-squared with y and yhat as vectors
f <- stats::lm(mpg ~ cyl + disp + hp + wt, data = datasets::mtcars)

y <- f$model$mpg

yhat <- f$fitted.values

calc_rsquared(y = y, yhat = yhat)

# standard r-squared with y as a matrix and yhat containing 'x' and linear coefficients
s <- summary(f)
x <- cbind(1, as.matrix(f$model[, -1]))
w <- matrix(s$coefficients[, 1], ncol = 1)
calc_rsquared(y = matrix(y, ncol = 1), yhat = list(x, w))

# multivariate r-squared with y and yhat as matrices
calc_rsquared(y = cbind(y, y), yhat = cbind(yhat, yhat))

# multivariate r-squared with yhat as a linear reconstruction of two matrices
calc_rsquared(y = cbind(y, y), yhat = list(x, cbind(w, w)))

# multivariate r-squared calculated in parallel

library(furrr)

plan(multiprocess)

batches <- list(list(y = cbind(y[1:16], y[1:16]), yhat = cbind(yhat[1:16], yhat[1:16])),
               list(y = cbind(y[17:32], y[17:32]), yhat = cbind(yhat[17:32], yhat[17:32])))
ybar <- c(mean(y), mean(y))

ss <- future_map(.x = batches,
                 .f = function(ybatch){
                   calc_rsquared(y = ybatch$y, yhat = ybatch$yhat, ybar = ybar, return_ss_only = TRUE)
                 },
                 .options = future_options(scheduling = 2))

sse <- sum(sapply(ss, function(x) x"sse"))

sst <- sum(sapply(ss, function(x) x"sst"))

1 - sse / sst # final r-squared value here
mvrsquared

Description

Compute the Coefficient of Determination for Vector or Matrix Outcomes

Details

Welcome to the mvrsquared package! This package does one thing: calculate the coefficient of determination or "R-squared". However, this implementation is different from what you may be familiar with. In addition to the standard R-squared used frequently in linear regression, `mvrsquared` calculates R-squared for multivariate outcomes. (This is why there is an 'mv' in mvrsquared).

mvrsquared implements R-squared based on a derivation in this paper (https://arxiv.org/abs/1911.11061). It's the same definition of R-squared you're probably familiar with, i.e. 1 - SSE/SST but generalized to n-dimensions.

In the standard case, your outcome and prediction are vectors. In other words, each observation is a single number. This is fine if you are predicting a single variable. But what if you are predicting multiple variables at once? In that case, your outcome and prediction are matrices. This situation occurs frequently in topic modeling or simultaneous equation modeling.
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