### Package ‘loo’

**Type** Package  
**Title** Efficient Leave-One-Out Cross-Validation and WAIC for Bayesian Models  
**Version** 2.8.0  
**Date** 2024-07-03  
**Maintainer** Jonah Gabry <jsg2201@columbia.edu>  
**URL** [https://mc-stan.org/loo/](https://mc-stan.org/loo/), [https://discourse.mc-stan.org](https://discourse.mc-stan.org)  
**BugReports** [https://github.com/stan-dev/loo/issues](https://github.com/stan-dev/loo/issues)  
**Description**  Efficient approximate leave-one-out cross-validation (LOO) for Bayesian models fit using Markov chain Monte Carlo, as described in Vehtari, Gelman, and Gabry (2017) <doi:10.1007/s11222-016-9696-4>. The approximation uses Pareto smoothed importance sampling (PSIS), a new procedure for regularizing importance weights. As a byproduct of the calculations, we also obtain approximate standard errors for estimated predictive errors and for the comparison of predictive errors between models. The package also provides methods for using stacking and other model weighting techniques to average Bayesian predictive distributions.  
**License** GPL (>= 3)  
**LazyData** TRUE  
**Depends** R (>= 3.1.2)  
**Imports** checkmate, matrixStats (>= 0.52), parallel, posterior (>= 1.5.0), stats  
**Suggests** bayesplot (>= 1.7.0), brms (>= 2.10.0), ggplot2, graphics, knitr, rmarkdown, rstan, rstanarm (>= 2.19.0), rstantools, spdep, testthat (>= 2.1.0)  
**VignetteBuilder** knitr  
**Encoding** UTF-8  
**SystemRequirements** pandoc (>= 1.12.3), pandoc-citeproc
RoxygenNote 7.3.1

NeedsCompilation no

Author Aki Vehtari [aut],
Jonah Gabry [cre, aut],
Måns Magnusson [aut],
Yuling Yao [aut],
Paul-Christian Bürkner [aut],
Topi Paananen [aut],
Andrew Gelman [aut],
Ben Goodrich [ctb],
Juho Piironen [ctb],
Bruno Nicenboim [ctb],
Leevi Lindgren [ctb]

Repository CRAN

Date/Publication 2024-07-03 18:50:02 UTC

Contents

loo-package .................................. 3
ap_psis ...................................... 5
compare ..................................... 6
crps .......................................... 7
elpd .......................................... 10
example_loglik_array ...................... 11
extract_log_lik ............................. 12
E_loo ........................................ 13
gpdfit ....................................... 15
importance_sampling ...................... 16
kfold-generic ............................... 17
kfold-helpers ................................ 18
loo .......................................... 19
loo-datasets ................................. 25
loo-glossary ................................ 26
loo_approximate_posterior ............... 28
loo_compare ................................ 31
loo_model_weights ......................... 33
loo_moment_match ......................... 37
loo_moment_match_split .................. 40
loo_predictive_metric .................... 41
loo_subsample .............................. 43
nobs.psis_loo_ss .......................... 47
obs_idx .................................... 47
pareto-k-diagnostic ...................... 48
pointwise .................................. 51
print.loo .................................. 52
psis ........................................ 53
Description

Stan Development Team

This package implements the methods described in Vehtari, Gelman, and Gabry (2017), Vehtari, Simpson, Gelman, Yao, and Gabry (2024), and Yao et al. (2018). To get started see the loo package vignettes, the loo() function for efficient approximate leave-one-out cross-validation (LOO-CV), the psis() function for the Pareto smoothed importance sampling (PSIS) algorithm, or loo_model_weights() for an implementation of Bayesian stacking of predictive distributions from multiple models.

Details

Leave-one-out cross-validation (LOO-CV) and the widely applicable information criterion (WAIC) are methods for estimating pointwise out-of-sample prediction accuracy from a fitted Bayesian model using the log-likelihood evaluated at the posterior simulations of the parameter values. LOO-CV and WAIC have various advantages over simpler estimates of predictive error such as AIC and DIC but are less used in practice because they involve additional computational steps. This package implements the fast and stable computations for approximate LOO-CV laid out in Vehtari, Gelman, and Gabry (2017). From existing posterior simulation draws, we compute LOO-CV using Pareto smoothed importance sampling (PSIS; Vehtari, Simpson, Gelman, Yao, and Gabry, 2024), a new procedure for stabilizing and diagnosing importance weights. As a byproduct of our calculations, we also obtain approximate standard errors for estimated predictive errors and for comparing of predictive errors between two models.

We recommend PSIS-LOO-CV instead of WAIC, because PSIS provides useful diagnostics and effective sample size and Monte Carlo standard error estimates.

Author(s)

Maintainer: Jonah Gabry <jsg2201@columbia.edu>

Authors:

- Aki Vehtari <Aki.Vehtari@aalto.fi>
- Måns Magnusson
- Yuling Yao
- Paul-Christian Bürkner
Other contributors:

- Ben Goodrich [contributor]
- Juho Piironen [contributor]
- Bruno Nicenboim [contributor]
- Leevi Lindgren [contributor]

References


---

**See Also**

Useful links:

- [https://mc-stan.org/loo/](https://mc-stan.org/loo/)
- [https://discourse.mc-stan.org](https://discourse.mc-stan.org)
- Report bugs at [https://github.com/stan-dev/loo/issues](https://github.com/stan-dev/loo/issues)

---

**ap_psis**

**Pareto smoothed importance sampling (PSIS) using approximate posteriors**

**Description**

Pareto smoothed importance sampling (PSIS) using approximate posteriors

**Usage**

```r
ap_psis(log_ratios, log_p, log_g, ...) 
```

```r
## S3 method for class 'array'
ap_psis(log_ratios, log_p, log_g, ..., cores = getOption("mc.cores", 1))
```

```r
## S3 method for class 'matrix'
ap_psis(log_ratios, log_p, log_g, ..., cores = getOption("mc.cores", 1))
```

```r
## Default S3 method:
ap_psis(log_ratios, log_p, log_g, ...)
```

**Arguments**

- `log_ratios` The log-likelihood ratios (ie -log_lik)
- `log_p` The log-posterior (target) evaluated at S samples from the proposal distribution (g). A vector of length S.
- `log_g` The log-density (proposal) evaluated at S samples from the proposal distribution (g). A vector of length S.
- `...` Currently not in use.
The number of cores to use for parallelization. This defaults to the option `mc.cores` which can be set for an entire R session by `options(mc.cores = NUMBER)`. The old option `loo.cores` is now deprecated but will be given precedence over `mc.cores` until `loo.cores` is removed in a future release. **As of version 2.0.0 the default is now 1 core if `mc.cores` is not set**, but we recommend using as many (or close to as many) cores as possible.

- Note for Windows 10 users: it is **strongly recommended** to avoid using the `.Rprofile` file to set `mc.cores` (using the `cores` argument or setting `mc.cores` interactively or in a script is fine).

### Methods (by class)

- **ap_psis(array)**: An $I$ by $C$ by $N$ array, where $I$ is the number of MCMC iterations per chain, $C$ is the number of chains, and $N$ is the number of data points.
- **ap_psis(matrix)**: An $S$ by $N$ matrix, where $S$ is the size of the posterior sample (with all chains merged) and $N$ is the number of data points.
- **ap_psis(default)**: A vector of length $S$ (posterior sample size).

---

### compare

**Model comparison (deprecated, old version)**

### Description

This function is deprecated. Please use the new `loo_compare()` function instead.

### Usage

```r
compare(..., x = list())
```

### Arguments

- `...` At least two objects returned by `loo()` (or `waic()`).
- `x` A list of at least two objects returned by `loo()` (or `waic()`). This argument can be used as an alternative to specifying the objects in `...`.

### Details

When comparing two fitted models, we can estimate the difference in their expected predictive accuracy by the difference in `elpd_loo` or `elpd_waic` (or multiplied by -2, if desired, to be on the deviance scale).

When that difference, `elpd_diff`, is positive then the expected predictive accuracy for the second model is higher. A negative `elpd_diff` favors the first model.

When using `compare()` with more than two models, the values in the `elpd_diff` and `se_diff` columns of the returned matrix are computed by making pairwise comparisons between each model and the model with the best ELPD (i.e., the model in the first row). Although the `elpd_diff`
column is equal to the difference in elpd_loo, do not expect the se_diff column to be equal to the the difference in se_elpd_loo.

To compute the standard error of the difference in ELPD we use a paired estimate to take advantage of the fact that the same set of \(N\) data points was used to fit both models. These calculations should be most useful when \(N\) is large, because then non-normality of the distribution is not such an issue when estimating the uncertainty in these sums. These standard errors, for all their flaws, should give a better sense of uncertainty than what is obtained using the current standard approach of comparing differences of deviances to a Chi-squared distribution, a practice derived for Gaussian linear models or asymptotically, and which only applies to nested models in any case.

Value

A vector or matrix with class ‘compare.loo’ that has its own print method. If exactly two objects are provided in ... or x, then the difference in expected predictive accuracy and the standard error of the difference are returned. If more than two objects are provided then a matrix of summary information is returned (see Details).

References


Examples

```r
## Not run:
loo1 <- loo(log_lik1)
loo2 <- loo(log_lik2)
print(compare(loo1, loo2), digits = 3)
print(compare(x = list(loo1, loo2)))

waic1 <- waic(log_lik1)
waic2 <- waic(log_lik2)
compare(waic1, waic2)

## End(Not run)
```

---

crps

*Continuously ranked probability score*
Description

The \texttt{crps()} and \texttt{scrps()} functions and their \texttt{loo_*()} counterparts can be used to compute the continuously ranked probability score (CRPS) and scaled CRPS (SCRPS) (see Bolin and Wallin, 2022). CRPS is a proper scoring rule, and strictly proper when the first moment of the predictive distribution is finite. Both can be expressed in terms of samples form the predictive distribution. See e.g. Gneiting and Raftery (2007) for a comprehensive discussion on CRPS.

Usage

\begin{verbatim}
  crps(x, ...)
  scrps(x, ...)
  loo_crps(x, ...)
  loo_scrps(x, ...)

  ## S3 method for class 'matrix'
  crps(x, x2, y, ..., permutations = 1)

  ## S3 method for class 'numeric'
  crps(x, x2, y, ..., permutations = 1)

  ## S3 method for class 'matrix'
  loo_crps(
    x,
    x2,
    y,
    log_lik,
    ...,
    permutations = 1,
    r_eff = 1,
    cores = getOption("mc.cores", 1)
  )

  ## S3 method for class 'matrix'
  scrps(x, x2, y, ..., permutations = 1)

  ## S3 method for class 'numeric'
  scrps(x, x2, y, ..., permutations = 1)

  ## S3 method for class 'matrix'
  loo_scrps(
    x,
    x2,
    y,
    log_lik,
    ...
  )
\end{verbatim}
Arguments

\texttt{x} \quad A \ S \ by \ N \ matrix \ (draws \ by \ observations), \ or \ a \ vector \ of \ length \ S \ when \ only \ single \ observation \ is \ provided \ in \ \texttt{y}.

\ldots \quad Passed \ on \ to \ \texttt{E_loo()} \ in \ the \ \texttt{loo_*()} \ version \ of \ these \ functions.

\texttt{x2} \quad Independent \ draws \ from \ the \ same \ distribution \ as \ draws \ in \ \texttt{x}. \ Should \ be \ of \ the \ identical \ dimension.

\texttt{y} \quad A \ vector \ of \ observations \ or \ a \ single \ value.

\texttt{permutations} \quad An \ integer, \ with \ default \ value \ of \ 1, \ specifying \ how \ many \ times \ the \ expected \ value \ of \ |X - X'| (|x - x2|) \ is \ computed. \ The \ row \ order \ of \ \texttt{x2} \ is \ shuffled \ as \ elements \ \texttt{x} \ and \ \texttt{x2} \ are \ typically \ drawn \ given \ the \ same \ values \ of \ parameters. \ This \ happens, \ e.g., \ when \ one \ calls \ \texttt{posterior_predict()} \ twice \ for \ a \ fitted \ \texttt{rstanarm} \ or \ \texttt{brms} \ model. \ Generating \ more \ permutations \ is \ expected \ to \ decrease \ the \ variance \ of \ the \ computed \ expected \ value.

\texttt{log_lik} \quad A \ log-likelihood \ matrix \ the \ same \ size \ as \ \texttt{x}.

\texttt{r_eff} \quad An \ optional \ vector \ of \ relative \ effective \ sample \ size \ estimates \ containing \ one \ element \ per \ observation. \ See \ \texttt{psis()} \ for \ details.

\texttt{cores} \quad The \ number \ of \ cores \ to \ use \ for \ parallelization \ of \ \texttt{[psis()]}. \ See \ \texttt{psis()} \ for \ details.

Details

To compute (S)CRPS, the user needs to provide two sets of draws, \texttt{x} and \texttt{x2}, from the predictive distribution. This is due to the fact that formulas used to compute CRPS involve an expectation of the absolute difference of \texttt{x} and \texttt{x2}, both having the same distribution. See the \texttt{permutations} argument, as well as Gneiting and Raftery (2007) for details.

Value

A list containing two elements: \texttt{estimates} and \texttt{pointwise}. The former reports estimator and standard error and latter the pointwise values.

References


Examples

```r
## Not run:
# An example using rstanarm
library(rstanarm)
data("kidiq")
fit <- stan_glm(kid_score ~ mom_hs + mom_iq, data = kidiq)
ypred1 <- posterior_predict(fit)
ypred2 <- posterior_predict(fit)
crps(ypred1, ypred2, y = fit$y)
loo_crps(ypred1, ypred2, y = fit$y, log_lik = log_lik(fit))
## End(Not run)
```

### elpd

Generic (expected) log-predictive density

#### Description

The `elpd()` methods for arrays and matrices can compute the expected log pointwise predictive density for a new dataset or the log pointwise predictive density of the observed data (an overestimate of the elpd).

#### Usage

```r
elpd(x, ...)
```

#### Arguments

- `x` A log-likelihood array or matrix. The **Methods (by class)** section, below, has detailed descriptions of how to specify the inputs for each method.
- `...` Currently ignored.

#### Details

The `elpd()` function is an S3 generic and methods are provided for 3-D pointwise log-likelihood arrays and matrices.
Methods (by class)

- `elpd(array)`: An I by C by N array, where I is the number of MCMC iterations per chain, C is the number of chains, and N is the number of data points.
- `elpd(matrix)`: An S by N matrix, where S is the size of the posterior sample (with all chains merged) and N is the number of data points.

See Also

The vignette *Holdout validation and K-fold cross-validation of Stan programs with the loo package* for demonstrations of using the `elpd()` methods.

Examples

```r
# Calculate the lpd of the observed data
LLarr <- example_loglik_array()
elpd(LLarr)
```

Description

Example pointwise log-likelihood objects to use in demonstrations and tests. See the **Value** and **Examples** sections below.

Usage

```r
example_loglik_array()
example_loglik_matrix()
```

Value

`example_loglik_array()` returns a 500 (draws) x 2 (chains) x 32 (observations) pointwise log-likelihood array.

`example_loglik_matrix()` returns the same pointwise log-likelihood values as `example_loglik_array()` but reshaped into a 1000 (draws*chains) x 32 (observations) matrix.

Examples

```r
LLarr <- example_loglik_array()
(dim_arr <- dim(LLarr))
LLmat <- example_loglik_matrix()
(dim_mat <- dim(LLmat))

all.equal(dim_mat[1], dim_arr[1] * dim_arr[2])
all.equal(dim_mat[2], dim_arr[3])
```
Description

Convenience function for extracting the pointwise log-likelihood matrix or array from a stanfit object from the rstan package. Note: recent versions of rstan now include a loo() method for stanfit objects that handles this internally.

Usage

extract_log_lik(stanfit, parameter_name = "log_lik", merge_chains = TRUE)

Arguments

- **stanfit** A stanfit object (rstan package).
- **parameter_name** A character string naming the parameter (or generated quantity) in the Stan model corresponding to the log-likelihood.
- **merge_chains** If TRUE (the default), all Markov chains are merged together (i.e., stacked) and a matrix is returned. If FALSE they are kept separate and an array is returned.

Details

Stan does not automatically compute and store the log-likelihood. It is up to the user to incorporate it into the Stan program if it is to be extracted after fitting the model. In a Stan model, the pointwise log likelihood can be coded as a vector in the transformed parameters block (and then summed up in the model block) or it can be coded entirely in the generated quantities block. We recommend using the generated quantities block so that the computations are carried out only once per iteration rather than once per HMC leapfrog step.

For example, the following is the generated quantities block for computing and saving the log-likelihood for a linear regression model with N data points, outcome y, predictor matrix X, coefficients beta, and standard deviation sigma:

```stan
vector[N] log_lik;
for (n in 1:N) log_lik[n] = normal_lpdf(y[n] | X[n,] * beta, sigma);
```

Value

If merge_chains=TRUE, an $S$ by $N$ matrix of (post-warmup) extracted draws, where $S$ is the size of the posterior sample and $N$ is the number of data points. If merge_chains=FALSE, an $I$ by $C$ by $N$ array, where $I \times C = S$. 

```r
all.equal(LLarr[, 1, ], LLmat[1:500, ])
all.equal(LLarr[, 2, ], LLmat[501:1000, ])
```
E_loo

References

---

E_loo Compute weighted expectations

Description
The E_loo() function computes weighted expectations (means, variances, quantiles) using the importance weights obtained from the PSIS smoothing procedure. The expectations estimated by the E_loo() function assume that the PSIS approximation is working well. **A small Pareto k estimate is necessary, but not sufficient, for E_loo() to give reliable estimates.** Additional diagnostic checks for gauging the reliability of the estimates are in development and will be added in a future release.

Usage
E_loo(x, psis_object, ...)

## Default S3 method:
E_loo(
  x,
  psis_object,
  ...,
  type = c("mean", "variance", "sd", "quantile"),
  probs = NULL,
  log_ratios = NULL
)

## S3 method for class 'matrix'
E_loo(
  x,
  psis_object,
  ...,
  type = c("mean", "variance", "sd", "quantile"),
  probs = NULL,
  log_ratios = NULL
)

Arguments

- **x** A numeric vector or matrix.
- **psis_object** An object returned by psis().
- **...** Arguments passed to individual methods.
The type of expectation to compute. The options are "mean", "variance", "sd", and "quantile".

For computing quantiles, a vector of probabilities.

Optionally, a vector or matrix (the same dimensions as x) of raw (not smoothed) log ratios. If working with log-likelihood values, the log ratios are the negative of those values. If log_ratios is specified we are able to compute more accurate Pareto k diagnostics specific to E_loo().

A named list with the following components:

value The result of the computation.

For the matrix method, value is a vector with ncol(x) elements, with one exception: when type="quantile" and multiple values are specified in probs the value component of the returned object is a length(probs) by ncol(x) matrix.

For the default/vector method the value component is scalar, with one exception: when type="quantile" and multiple values are specified in probs the value component is a vector with length(probs) elements.

pareto_k Function-specific diagnostic.

For the matrix method it will be a vector of length ncol(x) containing estimates of the shape parameter k of the generalized Pareto distribution. For the default/vector method, the estimate is a scalar. If log_ratios is not specified when calling E_loo(), the smoothed log-weights are used to estimate Pareto-k’s, which may produce optimistic estimates.

For type="mean", type="var", and type="sd", the returned Pareto-k is usually the maximum of the Pareto-k’s for the left and right tail of hr and the right tail of r, where r is the importance ratio and h = x for type="mean" and h = x^2 for type="var" and type="sd". If h is binary, constant, or not finite, or if type="quantile", the returned Pareto-k is the Pareto-k for the right tail of r.

Examples

```r
if (requireNamespace("rstanarm", quietly = TRUE)) {
  # Use rstanarm package to quickly fit a model and get both a log-likelihood
  # matrix and draws from the posterior predictive distribution
  library("rstanarm")

  # data from help("lm")
  ctl <- c(4.17, 5.58, 5.18, 6.11, 4.50, 4.61, 5.17, 4.53, 5.33, 5.14)
  trt <- c(4.81, 4.17, 4.41, 3.59, 5.87, 3.83, 6.03, 4.89, 4.32, 4.69)
  d <- data.frame(  
    weight = c(ctl, trt),
    group = gl(2, 10, 20, labels = c("Ctl", "Trt"))
  )
  fit <- stan_glm(weight ~ group, data = d, refresh = 0)
  yrep <- posterior_predict(fit)
  dim(yrep)

  log_ratios <- -1 * log_lik(fit)
}
Estimate parameters of the Generalized Pareto distribution

gpdfit

Description

Given a sample \( x \), Estimate the parameters \( k \) and \( \sigma \) of the generalized Pareto distribution (GPD), assuming the location parameter is 0. By default the fit uses a prior for \( k \), which will stabilize estimates for very small sample sizes (and low effective sample sizes in the case of MCMC samples). The weakly informative prior is a Gaussian prior centered at 0.5.

Usage

gpdfit(x, wip = TRUE, min_grid_pts = 30, sort_x = TRUE)

Arguments

- **x**: A numeric vector. The sample from which to estimate the parameters.
- **wip**: Logical indicating whether to adjust \( k \) based on a weakly informative Gaussian prior centered on 0.5. Defaults to TRUE.
- **min_grid_pts**: The minimum number of grid points used in the fitting algorithm. The actual number used is \( \text{min\_grid\_pts} + \text{floor}(\sqrt{\text{length}(x)}) \).
- **sort_x**: If TRUE (the default), the first step in the fitting algorithm is to sort the elements of \( x \). If \( x \) is already sorted in ascending order then sort_x can be set to FALSE to skip the initial sorting step.

Details

Here the parameter \( k \) is the negative of \( k \) in Zhang & Stephens (2009).
importance_sampling

Value
A named list with components k and sigma.

References

See Also
psis(), pareto-k-diagnostic

importance_sampling  A parent class for different importance sampling methods.

Description
A parent class for different importance sampling methods.

Usage
importance_sampling(log_ratios, method, ...)

## S3 method for class 'array'
importance_sampling(
    log_ratios,
    method,
    ..., 
    r_eff = 1,
    cores = getOption("mc.cores", 1)
)

## S3 method for class 'matrix'
importance_sampling(
    log_ratios,
    method,
    ..., 
    r_eff = 1,
    cores = getOption("mc.cores", 1)
)

## Default S3 method:
importance_sampling(log_ratios, method, ..., r_eff = 1)
Arguments

log_ratios An array, matrix, or vector of importance ratios on the log scale (for PSIS-LOO these are negative log-likelihood values). See the Methods (by class) section below for a detailed description of how to specify the inputs for each method.

method The importance sampling method to use. The following methods are implemented:

• "psis": Pareto-Smoothed Importance Sampling (PSIS). Default method.
• "tis": Truncated Importance Sampling (TIS) with truncation at sqrt(S), where S is the number of posterior draws.
• "sis": Standard Importance Sampling (SIS).

... Arguments passed on to the various methods.

r_eff Vector of relative effective sample size estimates containing one element per observation. The values provided should be the relative effective sample sizes of 1/exp(log_ratios) (i.e., 1/ratios). This is related to the relative efficiency of estimating the normalizing term in self-normalizing importance sampling. If r_eff is not provided then the reported PSIS effective sample sizes and Monte Carlo error estimates can be over-optimistic. If the posterior draws are (near) independent then r_eff=1 can be used. r_eff has to be a scalar (same value is used for all observations) or a vector with length equal to the number of observations. The default value is 1. See the relative_eff() helper function for computing r_eff.

cores The number of cores to use for parallelization. This defaults to the option mc.cores which can be set for an entire R session by options(mc.cores = NUMBER). The old option loo.cores is now deprecated but will be given precedence over mc.cores until loo.cores is removed in a future release. As of version 2.0.0 the default is now 1 core if mc.cores is not set, but we recommend using as many (or close to as many) cores as possible.

• Note for Windows 10 users: it is strongly recommended to avoid using the .Rprofile file to set mc.cores (using the cores argument or setting mc.cores interactively or in a script is fine).

Description

For developers of Bayesian modeling packages, loo includes a generic function kfold() so that methods may be defined for K-fold CV without name conflicts between packages. See, for example, the kfold() methods in the rstanarm and brms packages.

The Value section below describes the objects that kfold() methods should return in order to be compatible with loo_compare() and the loo package print methods.
Usage

kfold(x, ...)

is.kfold(x)

Arguments

x
A fitted model object.

... Arguments to pass to specific methods.

Value

For developers defining a kfold() method for a class "foo", the kfold.foo() function should return a list with class c("kfold", "loo") with at least the following named elements:

- "estimates": A 1x2 matrix containing the ELPD estimate and its standard error. The matrix must have row name "elpd_kfold" and column names "Estimate" and "SE".
- "pointwise": A Nx1 matrix with column name "elpd_kfold" containing the pointwise contributions for each data point.

It is important for the object to have at least these classes and components so that it is compatible with other functions like loo_compare() and print() methods.

kfold-split

kfold-split_random(K = 10, N = NULL)

kfold-split_stratified(K = 10, x = NULL)

kfold-split_grouped(K = 10, x = NULL)

Arguments

K The number of folds to use.

N The number of observations in the data.

x A discrete variable of length N with at least K levels (unique values). Will be coerced to a factor.
Details

kfold_split_random() splits the data into K groups of equal size (or roughly equal size).
For a categorical variable x kfold_split_stratified() splits the observations into K groups ensuring that relative category frequencies are approximately preserved.
For a grouping variable x, kfold_split_grouped() places all observations in x from the same group/level together in the same fold. The selection of which groups/levels go into which fold (relevant when there are more groups than folds) is randomized.

Value

An integer vector of length N where each element is an index in 1:K.

Examples

```r
ids <- kfold_split_random(K = 5, N = 20)
print(ids)
table(ids)

x <- sample(c(0, 1), size = 200, replace = TRUE, prob = c(0.05, 0.95))
table(x)
ids <- kfold_split_stratified(K = 5, x = x)
print(ids)
table(ids, x)

grp <- gl(n = 50, k = 15, labels = state.name)
length(grp)
head(table(grp))

ids_10 <- kfold_split_grouped(K = 10, x = grp)
(tab_10 <- table(grp, ids_10))
colSums(tab_10)

ids_9 <- kfold_split_grouped(K = 9, x = grp)
(tab_9 <- table(grp, ids_9))
colSums(tab_9)
```

loo

Efficient approximate leave-one-out cross-validation (LOO)

Description

The loo() methods for arrays, matrices, and functions compute PSIS-LOO CV, efficient approximate leave-one-out (LOO) cross-validation for Bayesian models using Pareto smoothed importance sampling (PSIS). This is an implementation of the methods described in Vehtari, Gelman, and Gabry (2017) and Vehtari, Simpson, Gelman, Yao, and Gabry (2024).

The loo_i() function enables testing log-likelihood functions for use with the loo.function() method.
Usage

```r
loo(x, ...)
```

```r
## S3 method for class 'array'
loo(
  x,
  ..., 
  r_eff = 1,
  save_psis = FALSE,
  cores = getOption("mc.cores", 1),
  is_method = c("psis", "tis", "sis")
)
```

```r
## S3 method for class 'matrix'
loo(
  x,
  ..., 
  r_eff = 1,
  save_psis = FALSE,
  cores = getOption("mc.cores", 1),
  is_method = c("psis", "tis", "sis")
)
```

```r
## S3 method for class `function`
loo(
  x,
  ..., 
  data = NULL,
  draws = NULL,
  r_eff = 1,
  save_psis = FALSE,
  cores = getOption("mc.cores", 1),
  is_method = c("psis", "tis", "sis")
)
```

```r
loo_i(i, llfun, ..., data = NULL, draws = NULL, r_eff = 1, is_method = "psis")
```

```r
is.loo(x)
```

```r
is.psis_loo(x)
```

Arguments

- **x** A log-likelihood array, matrix, or function. The **Methods (by class)** section, below, has detailed descriptions of how to specify the inputs for each method.
- **r_eff** Vector of relative effective sample size estimates for the likelihood (exp(log_lik)) of each observation. This is related to the relative efficiency of estimating the normalizing term in self-normalized importance sampling when using poste-
rior draws obtained with MCMC. If MCMC draws are used and \( r_{\text{eff}} \) is not provided then the reported PSIS effective sample sizes and Monte Carlo error estimates can be over-optimistic. If the posterior draws are (near) independent then \( r_{\text{eff}}=1 \) can be used. \( r_{\text{eff}} \) has to be a scalar (same value is used for all observations) or a vector with length equal to the number of observations. The default value is 1. See the `relative_eff()` helper functions for help computing \( r_{\text{eff}} \).

**save_psis** Should the `psis` object created internally by `loo()` be saved in the returned object? The `loo()` function calls `psis()` internally but by default discards the (potentially large) `psis` object after using it to compute the LOO-CV summaries. Setting `save_psis=TRUE` will add a `psis_object` component to the list returned by `loo`. This is useful if you plan to use the `E_loo()` function to compute weighted expectations after running `loo`. Several functions in the `bayesplot` package also accept `psis` objects.

**cores** The number of cores to use for parallelization. This defaults to the option `mc.cores` which can be set for an entire R session by `options(mc.cores = NUMBER)`. The old option `loo.cores` is now deprecated but will be given precedence over `mc.cores` until `loo.cores` is removed in a future release. **As of version 2.0.0 the default is now 1 core if `mc.cores` is not set**, but we recommend using as many (or close to as many) cores as possible.

• Note for Windows 10 users: it is strongly recommended to avoid using the `.Rprofile` file to set `mc.cores` (using the `cores` argument or setting `mc.cores` interactively or in a script is fine).

**is_method** The importance sampling method to use. The following methods are implemented:

• "psis": Pareto-Smoothed Importance Sampling (PSIS). Default method.
• "tis": Truncated Importance Sampling (TIS) with truncation at \( \sqrt{S} \), where \( S \) is the number of posterior draws.
• "sis": Standard Importance Sampling (SIS).

**data, draws, ...** For the `loo.function()` method and the `loo_i()` function, these are the data, posterior draws, and other arguments to pass to the log-likelihood function. See the **Methods (by class)** section below for details on how to specify these arguments.

**i** For `loo_i()`, an integer in \( 1:N \).

**llfun** For `loo_i()`, the same as `x` for the `loo.function()` method. A log-likelihood function as described in the **Methods (by class)** section.

**Details**

The `loo()` function is an S3 generic and methods are provided for 3-D pointwise log-likelihood arrays, pointwise log-likelihood matrices, and log-likelihood functions. The array and matrix methods are the most convenient, but for models fit to very large datasets the `loo.function()` method is more memory efficient and may be preferable.

**Value**

The `loo()` methods return a named list with class `c("psis_loo", "loo")` and components:
estimates A matrix with two columns (Estimate, SE) and three rows (elpd_loo, p_loo, looic).
This contains point estimates and standard errors of the expected log pointwise predictive
density (elpd_loo), the effective number of parameters (p_loo) and the LOO information
criterion looic (which is just ~2 * elpd_loo, i.e., converted to deviance scale).

pointwise A matrix with five columns (and number of rows equal to the number of observations)
containing the pointwise contributions of the measures (elpd_loo, mcse_elpd_loo, p_loo,
looic, influence_pareto_k). in addition to the three measures in estimates, we also report
pointwise values of the Monte Carlo standard error of elpd_loo (mcse_elpd_loo), and statistics
descrbing the influence of each observation on the posterior distribution (influence_pareto_k).
These are the estimates of the shape parameter k of the generalized Pareto fit to the importance
ratios for each leave-one-out distribution (see the pareto-k-diagnostic page for details).

diagnostics A named list containing two vectors:
  • pareto_k: Importance sampling reliability diagnostics. By default, these are equal to the
    influence_pareto_k in pointwise. Some algorithms can improve importance sampl-
ing reliability and modify these diagnostics. See the pareto-k-diagnostic page for de-
tails.
  • n_eff: PSIS effective sample size estimates.

psis_object This component will be NULL unless the save_psis argument is set to TRUE when
calling loo(). In that case psis_object will be the object of class "psis" that is created
when the loo() function calls psis() internally to do the PSIS procedure.

The loo_i() function returns a named list with components pointwise and diagnostics. These
components have the same structure as the pointwise and diagnostics components of the object
returned by loo() except they contain results for only a single observation.

Methods (by class)
  • loo(array): An I by C by N array, where I is the number of MCMC iterations per chain, C
    is the number of chains, and N is the number of data points.
  • loo(matrix): An S by N matrix, where S is the size of the posterior sample (with all chains
    merged) and N is the number of data points.
  • loo(`function`): A function f() that takes arguments data_i and draws and returns a
    vector containing the log-likelihood for a single observation i evaluated at each posterior
draw. The function should be written such that, for each observation i in 1:N, evaluating
    \[ f(data_i = data[i,, drop=FALSE], draws = draws) \]
results in a vector of length S (size of posterior sample). The log-likelihood function can also
have additional arguments but data_i and draws are required.
If using the function method then the arguments data and draws must also be specified in the
call to loo():
  – data: A data frame or matrix containing the data (e.g. observed outcome and predictors)
    needed to compute the pointwise log-likelihood. For each observation i, the i\text{th} row of
    data will be passed to the data_i argument of the log-likelihood function.
  – draws: An object containing the posterior draws for any parameters needed to compute
    the pointwise log-likelihood. Unlike data, which is indexed by observation, for each
    observation the entire object draws will be passed to the draws argument of the log-
    likelihood function.
The ... can be used if your log-likelihood function takes additional arguments. These arguments are used like the draws argument in that they are recycled for each observation.

Defining loo() methods in a package

Package developers can define loo() methods for fitted models objects. See the example loo.stanfit() method in the Examples section below for an example of defining a method that calls loo.array(). The loo.stanreg() method in the rstanarm package is an example of defining a method that calls loo.function().

References


See Also

- The loo package vignettes for demonstrations.
- The FAQ page on the loo website for answers to frequently asked questions.
- psis() for the underlying Pareto Smoothed Importance Sampling (PSIS) procedure used in the LOO-CV approximation.
- pareto-k-diagnostic for convenience functions for looking at diagnostics.
- loo_compare() for model comparison.

Examples

### Array and matrix methods (using example objects included with loo package)

```r
# Array method
LLarr <- example_loglik_array()
rel_n_eff <- relative_eff(exp(LLarr))
loo(LLarr, r_eff = rel_n_eff, cores = 2)

# Matrix method
LLmat <- example_loglik_matrix()
rel_n_eff <- relative_eff(exp(LLmat), chain_id = rep(1:2, each = 500))
loo(LLmat, r_eff = rel_n_eff, cores = 2)
```

### Using log-likelihood function instead of array or matrix

```r
set.seed(124)
# Simulate data and draw from posterior
N <- 50; K <- 10; S <- 100; a0 <- 3; b0 <- 2
p <- rbeta(1, a0, b0)
y <- rbinom(N, size = K, prob = p)
a <- a0 + sum(y); b <- b0 + N * K - sum(y)
fake_posterior <- as.matrix(rbeta(S, a, b))
```
dim(fake_posterior) # 5 x 1
fake_data <- data.frame(y,K)
dim(fake_data) # N x 2

llfun <- function(data_i, draws) {
  # each time called internally within loo the arguments will be equal to:
  # data_i: ith row of fake_data (fake_data[i,, drop=FALSE])
  # draws: entire fake_posterior matrix
  dbinom(data_i$y, size = data_i$K, prob = draws, log = TRUE)
}

# Use the loo_i function to check that llfun works on a single observation
# before running on all obs. For example, using the 3rd obs in the data:
loo_3 <- loo_i(i = 3, llfun = llfun, data = fake_data, draws = fake_posterior)
print(loo_3$pointwise[, "elpd_loo"])

# Use loo.function method (default r_eff=1 is used as this posterior not obtained via MCMC)
loo_with_fn <- loo(llfun, draws = fake_posterior, data = fake_data)

# If we look at the elpd_loo contribution from the 3rd obs it should be the
# same as what we got above with the loo_i function and i=3:
print(loo_with_fn$pointwise[3, "elpd_loo"])
print(loo_3$pointwise[, "elpd_loo"])

# Check that the loo.matrix method gives same answer as loo.function method
log_lik_matrix <- sapply(1:N, function(i) {
  llfun(data_i = fake_data[i,, drop=FALSE], draws = fake_posterior)
})
loo_with_mat <- loo(log_lik_matrix)
all.equal(loo_with_mat$estimates, loo_with_fn$estimates) # should be TRUE!

### Not run:
#### For package developers: defining loo methods

# An example of a possible loo method for 'stanfit' objects (rstan package).
# A similar method is included in the rstan package.
# In order for users to be able to call loo(stanfit) instead of
# loo.stanfit(stanfit) the NAMESPACE needs to be handled appropriately
# (roxygen2 and devtools packages are good for that).
#
# loo.stanfit <-
# function(x,
#   pars = "log_lik",
#   ...
#   save_psis = FALSE,
#   cores = getOption("mc.cores", 1)) {
#   stopifnot(length(pars) == 1L)
#   LLAarray <- loo::extract_log_lik(stanfit = x,
#                                   parameter_name = pars,
#                                   merge_chains = FALSE)
#   r_eff <- loo::relative_eff(x = exp(LLAarray), cores = cores)
#   loo::loo.array(LLAarray,
#               ...)
```r
r_eff = r_eff,
cores = cores,
save_psis = save_psis)
}
## End(Not run)
```
Description

The pages provides definitions to key terms. Also see the FAQ page on the loo website for answers to frequently asked questions.


**ELPD and elpd_loo**

The ELPD is the theoretical expected log pointwise predictive density for a new dataset (Eq 1 in VGG2017), which can be estimated, e.g., using cross-validation. elpd_loo is the Bayesian LOO estimate of the expected log pointwise predictive density (Eq 4 in VGG2017) and is a sum of N individual pointwise log predictive densities. Probability densities can be smaller or larger than 1, and thus log predictive densities can be negative or positive. For simplicity the ELPD acronym is used also for expected log pointwise predictive probabilities for discrete models. Probabilities are always equal or less than 1, and thus log predictive probabilities are 0 or negative.

**Standard error of elpd_loo**

As elpd_loo is defined as the sum of N independent components (Eq 4 in VGG2017), we can compute the standard error by using the standard deviation of the N components and multiplying by \( \sqrt{N} \) (Eq 23 in VGG2017). This standard error is a coarse description of our uncertainty about the predictive performance for unknown future data. When N is small or there is severe model misspecification, the current SE estimate is overoptimistic and the actual SE can even be twice as large. Even for moderate N, when the SE estimate is an accurate estimate for the scale, it ignores the skewness. When making model comparisons, the SE of the component-wise (pairwise) differences should be used instead (see the se_diff section below and Eq 24 in VGG2017). Sivula et al. (2022) discuss the conditions when the normal approximation used for SE and se_diff is good.

**Monte Carlo SE of elpd_loo**

The Monte Carlo standard error is the estimate for the computational accuracy of MCMC and importance sampling used to compute elpd_loo. Usually this is negligible compared to the standard describing the uncertainty due to finite number of observations (Eq 23 in VGG2017).

**p_loo (effective number of parameters)**

p_loo is the difference between elpd_loo and the non-cross-validated log posterior predictive density. It describes how much more difficult it is to predict future data than the observed data. Asymptotically under certain regularity conditions, p_loo can be interpreted as the effective number of parameters. In well behaving cases p_loo < N and p_loo < p, where p is the total number of parameters in the model. p_loo > N or p_loo > p indicates that the model has very weak predictive capability and may indicate a severe model misspecification. See below for more on interpreting p_loo when there are warnings about high Pareto k diagnostic values.
Pareto $k$ estimates

The Pareto $k$ estimate is a diagnostic for Pareto smoothed importance sampling (PSIS), which is used to compute components of $\text{elpd}_{\text{loo}}$. In importance-sampling LOO the full posterior distribution is used as the proposal distribution. The Pareto $k$ diagnostic estimates how far an individual leave-one-out distribution is from the full distribution. If leaving out an observation changes the posterior too much then importance sampling is not able to give a reliable estimate. Pareto smoothing stabilizes importance sampling and guarantees a finite variance estimate at the cost of some bias.

The diagnostic threshold for Pareto $k$ depends on sample size $S$ (sample size dependent threshold was introduced by Vehtari et al., 2024, and before that fixed thresholds of 0.5 and 0.7 were recommended). For simplicity, loo package uses the nominal sample size $S$ when computing the sample size specific threshold. This provides an optimistic threshold if the effective sample size is less than 2200, but even then if $\text{ESS}/S > 1/2$ the difference is usually negligible. Thinning of MCMC draws can be used to improve the ratio $\text{ESS}/S$.

- If $k < \min(1 - 1/\log_{10}(S), 0.7)$, where $S$ is the sample size, the PSIS estimate and the corresponding Monte Carlo standard error estimate are reliable.
- If $1 - 1/\log_{10}(S) \leq k < 0.7$, the PSIS estimate and the corresponding Monte Carlo standard error estimate are not reliable, but increasing the (effective) sample size $S$ above 2200 may help (this will increase the sample size specific threshold $(1 - 1/\log_{10}(2200)) > 0.7$ and then the bias specific threshold 0.7 dominates).
- If $0.7 \leq k < 1$, the PSIS estimate and the corresponding Monte Carlo standard error have large bias and are not reliable. Increasing the sample size may reduce the variability in the $k$ estimate, which may also result in a lower $k$ estimate.
- If $k \geq 1$, the target distribution is estimated to have non-finite mean. The PSIS estimate and the corresponding Monte Carlo standard error are not well defined. Increasing the sample size may reduce the variability in $k$ estimate, which may also result in a lower $k$ estimate.

Pareto $k$ is also useful as a measure of influence of an observation. Highly influential observations have high $k$ values. Very high $k$ values often indicate model misspecification, outliers or mistakes in data processing. See Section 6 of Gabry et al. (2019) for an example.

Interpreting $p_{\text{loo}}$ when Pareto $k$ is large: If $k > 0.7$ then we can also look at the $p_{\text{loo}}$ estimate for some additional information about the problem:

- If $p_{\text{loo}} < p$ (the total number of parameters in the model), then the model is likely to be misspecified. Posterior predictive checks (PPCs) are then likely to also detect the problem. Try using an overdispersed model, or add more structural information (nonlinearity, mixture model, etc.).
- If $p_{\text{loo}} < p$ and the number of parameters $p$ is relatively large compared to the number of observations (e.g., $p>N/5$), it is likely that the model is so flexible or the population prior so weak that it’s difficult to predict the left out observation (even for the true model). This happens, for example, in the simulated 8 schools (in VGG2017), random effect models with a few observations per random effect, and Gaussian processes and spatial models with short correlation lengths.
- If $p_{\text{loo}} > p$, then the model is likely to be badly misspecified. If the number of parameters $p<<N$, then PPCs are also likely to detect the problem. See the case study at https://avehtari.github.io/modelselection/roaches.html for an example. If $p$ is relatively
large compared to the number of observations, say $p > N/5$ (more accurately we should count number of observations influencing each parameter as in hierarchical models some groups may have few observations and other groups many), it is possible that PPCs won’t detect the problem.

**elpd_diff**

`elpd_diff` is the difference in `elpd_loo` for two models. If more than two models are compared, the difference is computed relative to the model with highest `elpd_loo`.

**se_diff**

The standard error of component-wise differences of `elpd_loo` (Eq 24 in VGG2017) between two models. This SE is smaller than the SE for individual models due to correlation (i.e., if some observations are easier and some more difficult to predict for all models).

**References**


---

**Description**

Efficient approximate leave-one-out cross-validation (LOO) for posterior approximations

**Usage**

```r
loo_approximate_posterior(x, log_p, log_g, ...)
```

```r
## S3 method for class 'array'
loo_approximate_posterior(
  x,
  log_p,
  log_g,
```
...,  
  save_psis = FALSE,  
  cores =getOption("mc.cores", 1)  
)

## S3 method for class 'matrix'
loo_approximate_posterior(  
  x,  
  log_p,  
  log_g,  
  ...,  
  save_psis = FALSE,  
  cores =getOption("mc.cores", 1)  
)

## S3 method for class 'function'
loo_approximate_posterior(  
  x,  
  ...,  
  data = NULL,  
  draws = NULL,  
  log_p = NULL,  
  log_g = NULL,  
  save_psis = FALSE,  
  cores =getOption("mc.cores", 1)  
)

Arguments

x A log-likelihood array, matrix, or function. The Methods (by class) section, below, has detailed descriptions of how to specify the inputs for each method.

log_p The log-posterior (target) evaluated at S samples from the proposal distribution (g). A vector of length S.

log_g The log-density (proposal) evaluated at S samples from the proposal distribution (g). A vector of length S.

save_psis Should the "psis" object created internally by loo_approximate_posterior() be saved in the returned object? See loo() for details.

cores The number of cores to use for parallelization. This defaults to the option mc.cores which can be set for an entire R session by options(mc.cores = NUMBER). The old option loo.cores is now deprecated but will be given precedence over mc.cores until loo.cores is removed in a future release. As of version 2.0.0 the default is now 1 core if mc.cores is not set, but we recommend using as many (or close to as many) cores as possible.

• Note for Windows 10 users: it is strongly recommended to avoid using the .Rprofile file to set mc.cores (using the cores argument or setting mc.cores interactively or in a script is fine).
For the `loo_approximate_posterior` method, these are the data, posterior draws, and other arguments to pass to the log-likelihood function. See the Methods (by class) section below for details on how to specify these arguments.

Details

The `loo_approximate_posterior()` function is an S3 generic and methods are provided for 3-D pointwise log-likelihood arrays, pointwise log-likelihood matrices, and log-likelihood functions. The implementation works for posterior approximations where it is possible to compute the log density for the posterior approximation.

Value

The `loo_approximate_posterior()` methods return a named list with class c("psis_loo_ap", "psis_loo", "loo"). It has the same structure as the objects returned by `loo()` but with the additional slot:

`posterior_approximation` A list with two vectors, `log_p` and `log_g` of the same length containing the posterior density and the approximation density for the individual draws.

Methods (by class)

- `loo_approximate_posterior(array)`: An $I$ by $C$ by $N$ array, where $I$ is the number of MCMC iterations per chain, $C$ is the number of chains, and $N$ is the number of data points.
- `loo_approximate_posterior(matrix)`: An $S$ by $N$ matrix, where $S$ is the size of the posterior sample (with all chains merged) and $N$ is the number of data points.
- `loo_approximate_posterior("function")`: A function $f()$ that takes arguments `data_i` and `draws` and returns a vector containing the log-likelihood for a single observation $i$ evaluated at each posterior draw. The function should be written such that, for each observation $i$ in 1:$N$, evaluating

$$f(data_i = data[i,, drop=FALSE], draws = draws)$$

results in a vector of length $S$ (size of posterior sample). The log-likelihood function can also have additional arguments but `data_i` and `draws` are required.

If using the function method then the arguments `data` and `draws` must also be specified in the call to `loo()`:

- `data`: A data frame or matrix containing the data (e.g. observed outcome and predictors) needed to compute the pointwise log-likelihood. For each observation $i$, the $i$th row of data will be passed to the `data_i` argument of the log-likelihood function.
- `draws`: An object containing the posterior draws for any parameters needed to compute the pointwise log-likelihood. Unlike data, which is indexed by observation, for each observation the entire object `draws` will be passed to the `draws` argument of the log-likelihood function.
- The ... can be used if your log-likelihood function takes additional arguments. These arguments are used like the `draws` argument in that they are recycled for each observation.
**References**


**See Also**

`loo()`, `psis()`, `loo_compare()`

---

### loo_compare

**Model comparison**

**Description**

Compare fitted models based on ELPD.

By default the print method shows only the most important information. Use `print(..., simplify=FALSE)` to print a more detailed summary.

**Usage**

```r
loo_compare(x, ...)
```

```r
## Default S3 method:
loo_compare(x, ...)
```

```r
## S3 method for class 'compare.loo'
print(x, ..., digits = 1, simplify = TRUE)
```

```r
## S3 method for class 'compare.loo_ss'
print(x, ..., digits = 1, simplify = TRUE)
```

**Arguments**

- `x` An object of class "loo" or a list of such objects. If a list is used then the list names will be used as the model names in the output. See Examples.
- `...` Additional objects of class "loo", if not passed in as a single list.
- `digits` For the print method only, the number of digits to use when printing.
- `simplify` For the print method only, should only the essential columns of the summary matrix be printed? The entire matrix is always returned, but by default only the most important columns are printed.
Details

When comparing two fitted models, we can estimate the difference in their expected predictive accuracy by the difference in $\text{elpd}_{\text{loo}}$ or $\text{elpd}_{\text{waic}}$ (or multiplied by $-2$, if desired, to be on the deviance scale).

When using `loo_compare()`, the returned matrix will have one row per model and several columns of estimates. The values in the `$\text{elpd}_\text{diff}$` and `$\text{se}_\text{diff}$` columns of the returned matrix are computed by making pairwise comparisons between each model and the model with the largest ELPD (the model in the first row). For this reason the `$\text{elpd}_\text{diff}$` column will always have the value 0 in the first row (i.e., the difference between the preferred model and itself) and negative values in subsequent rows for the remaining models.

To compute the standard error of the difference in ELPD — which should not be expected to equal the difference of the standard errors — we use a paired estimate to take advantage of the fact that the same set of $N$ data points was used to fit both models. These calculations should be most useful when $N$ is large, because then non-normality of the distribution is not such an issue when estimating the uncertainty in these sums. These standard errors, for all their flaws, should give a better sense of uncertainty than what is obtained using the current standard approach of comparing differences of deviances to a Chi-squared distribution, a practice derived for Gaussian linear models or asymptotically, and which only applies to nested models in any case. Sivula et al. (2022) discuss the conditions when the normal approximation used for SE and `$\text{se}_\text{diff}$` is good.

If more than 11 models are compared, we internally recompute the model differences using the median model by ELPD as the baseline model. We then estimate whether the differences in predictive performance are potentially due to chance as described by McLatchie and Vehtari (2023). This will flag a warning if it is deemed that there is a risk of over-fitting due to the selection process. In that case users are recommended to avoid model selection based on LOO-CV, and instead to favor model averaging/stacking or projection predictive inference.

Value

A matrix with class "compare.loo" that has its own print method. See the Details section.

References


See Also

- The FAQ page on the loo website for answers to frequently asked questions.
**Examples**

```r
# very artificial example, just for demonstration!
LL <- example_loglik_array()
loo1 <- loo(LL)  # should be worst model when compared
loo2 <- loo(LL + 1)  # should be second best model when compared
loo3 <- loo(LL + 2)  # should be best model when compared

comp <- loo_compare(loo1, loo2, loo3)
print(comp, digits = 2)

# show more details with simplify=FALSE
# (will be the same for all models in this artificial example)
print(comp, simplify = FALSE, digits = 3)

# can use a list of objects with custom names
# will use apple, banana, and cherry, as the names in the output
loo_compare(list("apple" = loo1, "banana" = loo2, "cherry" = loo3))

## Not run:
# works for waic (and kfold) too
loo_compare(waic(LL), waic(LL - 10))
## End(Not run)
```

---

**loo_model_weights**

Model averaging/weighting via stacking or pseudo-BMA weighting

**Description**

Model averaging via stacking of predictive distributions, pseudo-BMA weighting or pseudo-BMA+ weighting with the Bayesian bootstrap. See Yao et al. (2018), Vehtari, Gelman, and Gabry (2017), and Vehtari, Simpson, Gelman, Yao, and Gabry (2024) for background.

**Usage**

```r
loo_model_weights(x, ...)
```

## Default S3 method:
```r
loo_model_weights(
  x,
  ...,
  method = c("stacking", "pseudobma"),
  optim_method = "BFGS",
  optim_control = list(),
  BB = TRUE,
  BB_n = 1000,
  alpha = 1,
)```
r_eff_list = NULL,
cores = getOption("mc.cores", 1)
)

stacking_weights(lpd_point, optim_method = "BFGS", optim_control = list())
pseudobma_weights(lpd_point, BB = TRUE, BB_n = 1000, alpha = 1)

Arguments

x
A list of "psis_loo" objects (objects returned by \texttt{loo()}) or pointwise log-
likelihood matrices or, one for each model. If the list elements are named
the names will be used to label the models in the results. Each matrix/object
should have dimensions \(S \times N\), where \(S\) is the size of the posterior sample
(with all chains merged) and \(N\) is the number of data points. If \(x\) is a list of log-
likelihood matrices then \texttt{loo()} is called internally on each matrix. Currently
the \texttt{loo_model_weights()} function is not implemented to be used with results
from K-fold CV, but you can still obtain weights using K-fold CV results by
calling the \texttt{stacking_weights()} function directly.

... Unused, except for the generic to pass arguments to individual methods.

method
Either "stacking" (the default) or "pseudobma", indicating which method to
use for obtaining the weights. "stacking" refers to stacking of predictive distri-
butions and "pseudobma" refers to pseudo-BMA+ weighting (or plain pseudo-
BMA weighting if argument \texttt{BB} is \texttt{FALSE}).

optim_method
If \texttt{method}="stacking", a string passed to the \texttt{method} argument of \texttt{stats::constrOptim()}
to specify the optimization algorithm. The default is \texttt{optim_method="BFGS"},
but other options are available (see \texttt{stats::optim()}).

optim_control
If \texttt{method}="stacking", a list of control parameters for optimization passed to
the \texttt{control} argument of \texttt{stats::constrOptim()}. 

BB
Logical used when \texttt{method}="pseudobma". If \texttt{TRUE} (the default), the Bayesian
bootstrap will be used to adjust the pseudo-BMA weighting, which is called
pseudo-BMA+ weighting. It helps regularize the weight away from 0 and 1, so
as to reduce the variance.

BB_n
For pseudo-BMA+ weighting only, the number of samples to use for the Bayesian
bootstrap. The default is \texttt{BB_n=1000}.

alpha
Positive scalar shape parameter in the Dirichlet distribution used for the Bayesian
bootstrap. The default is \texttt{alpha=1}, which corresponds to a uniform distribution
on the simplex space.

r_eff_list
Optionally, a list of relative effective sample size estimates for the likelihood
(\(\exp(\log_{\text{lik}})\)) of each observation in each model. See \texttt{psis()} and \texttt{relative_eff()}
helper function for computing \(r_{\text{eff}}\). If \(x\) is a list of "psis_loo" objects then
\texttt{r_eff_list} is ignored.

cores
The number of cores to use for parallelization. This defaults to the option
\texttt{mc.cores} which can be set for an entire R session by \texttt{options(mc.cores = NUMBER)}. The old option \texttt{loo.cores} is now deprecated but will be given prece-
dence over \texttt{mc.cores} until \texttt{loo.cores} is removed in a future release. As of
version 2.0.0 the default is now 1 core if mc.cores is not set, but we recommend using as many (or close to as many) cores as possible.

- Note for Windows 10 users: it is strongly recommended to avoid using the .Rprofile file to set mc.cores (using the cores argument or setting mc.cores interactively or in a script is fine).

lpd_point If calling stacking_weights() or pseudobma_weights() directly, a matrix of pointwise leave-one-out (or K-fold) log likelihoods evaluated for different models. It should be a \( N \) by \( K \) matrix where \( N \) is sample size and \( K \) is the number of models. Each column corresponds to one model. These values can be calculated approximately using loo() or by running exact leave-one-out or K-fold cross-validation.

Details

loo_model_weights() is a wrapper around the stacking_weights() and pseudobma_weights() functions that implements stacking, pseudo-BMA, and pseudo-BMA+ weighting for combining multiple predictive distributions. We can use approximate or exact leave-one-out cross-validation (LOO-CV) or K-fold CV to estimate the expected log predictive density (ELPD).

The stacking method (method="stacking"), which is the default for loo_model_weights(), combines all models by maximizing the leave-one-out predictive density of the combination distribution. That is, it finds the optimal linear combining weights for maximizing the leave-one-out log score.

The pseudo-BMA method (method="pseudobma") finds the relative weights proportional to the ELPD of each model. However, when method="pseudobma", the default is to also use the Bayesian bootstrap (BB=TRUE), which corresponds to the pseudo-BMA+ method. The Bayesian bootstrap takes into account the uncertainty of finite data points and regularizes the weights away from the extremes of 0 and 1.

In general, we recommend stacking for averaging predictive distributions, while pseudo-BMA+ can serve as a computationally easier alternative.

Value

A numeric vector containing one weight for each model.

References


See Also

- The loo package vignettes, particularly Bayesian Stacking and Pseudo-BMA weights using the loo package.
• `loo()` for details on leave-one-out ELPD estimation.
• `constrOptim()` for the choice of optimization methods and control-parameters.
• `relative_eff()` for computing $r_{eff}$.

Examples

```r
## Not run:
### Demonstrating usage after fitting models with RStan
library(rstan)

# generate fake data from N(0,1).
N <- 100
y <- rnorm(N, 0, 1)

# Suppose we have three models: N(-1, sigma), N(0.5, sigma) and N(0.6, sigma).
stan_code <- "
data {
  int N;
  vector[N] y;
  real mu_fixed;
}
parameters {
  real<lower=0> sigma;
}
model {
  sigma ~ exponential(1);
  y ~ normal(mu_fixed, sigma);
}
generated quantities {
  vector[N] log_lik;
  for (n in 1:N) log_lik[n] = normal_lpdf(y[n]| mu_fixed, sigma);
}"

mod <- stan_model(model_code = stan_code)
fit1 <- sampling(mod, data=list(N=N, y=y, mu_fixed=-1))
fit2 <- sampling(mod, data=list(N=N, y=y, mu_fixed=0.5))
fit3 <- sampling(mod, data=list(N=N, y=y, mu_fixed=0.6))
model_list <- list(fit1, fit2, fit3)
log_lik_list <- lapply(model_list, extract_log_lik)
# optional but recommended
r_eff_list <- lapply(model_list, function(x) {
  ll_array <- extract_log_lik(x, merge_chains = FALSE)
  relative_eff(exp(ll_array))
})

# stacking method:
wts1 <- loo_model_weights(
  log_lik_list,
  method = "stacking",
  r_eff_list = r_eff_list,
  optim_control = list(reltol=1e-10)
)
Moment matching for efficient approximate leave-one-out cross-validation (LOO)

Description

Moment matching algorithm for updating a loo object when Pareto k estimates are large.

Usage

```r
loo_moment_match(x, ...)
```

## Default S3 method:
loo_moment_match(
  x,
  loo,
  post_draws,
  log_lik_i,
  unconstrain_pars,
  log_prob_upars,
  log_lik_i_upars,
  max_iters = 30L,
  k_threshold = NULL,
  split = TRUE,
  cov = TRUE,
  cores = getOption("mc.cores", 1),
  ...
)

Arguments

x                   A fitted model object.

...                 Further arguments passed to the custom functions documented above.

loo                 A loo object to be modified.

post_draws          A function that takes x as the first argument and returns a matrix of posterior
draws of the model parameters.

log_lik_i           A function that takes x and i and returns a matrix (one column per chain) or a
vector (all chains stacked) of log-likelihood draws of the ith observation based
on the model x. If the draws are obtained using MCMC, the matrix with MCMC
chains separated is preferred.

unconstrain_pars    A function that takes arguments x, pars and returns posterior draws on
the unconstrained space based on the posterior draws on the constrained space
passed via pars.

log_prob_upars       A function that takes arguments x and upars and returns a matrix of log-posterior
density values of the unconstrained posterior draws passed via upars.

log_lik_i_upars      A function that takes arguments x, upars, and i and returns a vector of log-
likelihood draws of the ith observation based on the unconstrained posterior
draws passed via upars.

max_iters            Maximum number of moment matching iterations. Usually this does not need
to be modified. If the maximum number of iterations is reached, there will be a
warning, and increasing max_iters may improve accuracy.

k_threshold          Threshold value for Pareto k values above which the moment matching algo-
                      rithm is used. The default value is 1 - 1 / \log_{10}(S), where S is the sample
                      size.

split                Logical; Indicate whether to do the split transformation or not at the end of
                      moment matching for each LOO fold.
cov
Logical; Indicate whether to match the covariance matrix of the samples or not. If FALSE, only the mean and marginal variances are matched.

cores
The number of cores to use for parallelization. This defaults to the option `mc.cores` which can be set for an entire R session by `options(mc.cores = NUMBER)`. The old option `loo.cores` is now deprecated but will be given precedence over `mc.cores` until `loo.cores` is removed in a future release. **As of version 2.0.0 the default is now 1 core if `mc.cores` is not set**, but we recommend using as many (or close to as many) cores as possible.

- Note for Windows 10 users: it is **strongly recommended** to avoid using the `.Rprofile` file to set `mc.cores` (using the cores argument or setting `mc.cores` interactively or in a script is fine).

Details
The `loo_moment_match()` function is an S3 generic and we provide a default method that takes as arguments user-specified functions `post_draws`, `log_lik_i`, `unconstrain_pars`, `log_prob_upars`, and `log_lik_i_upars`. All of these functions should take `...` as an argument in addition to those specified for each function.

Value
The `loo_moment_match()` methods return an updated `loo` object. The structure of the updated `loo` object is similar, but the method also stores the original Pareto k diagnostic values in the diagnostics field.

Methods (by class)
- `loo_moment_match(default)`: A default method that takes as arguments a user-specified model object `x`, a `loo` object and user-specified functions `post_draws`, `log_lik_i`, `unconstrain_pars`, `log_prob_upars`, and `log_lik_i_upars`.

References

See Also
`loo()`, `loo_moment_match_split()`

Examples
```r
# See the vignette for loo_moment_match()
```
**loo_moment_match_split**

*Split moment matching for efficient approximate leave-one-out cross-validation (LOO)*

**Description**

A function that computes the split moment matching importance sampling loo. Takes in the moment matching total transformation, transforms only half of the draws, and computes a single elpd using multiple importance sampling.

**Usage**

```r
loo_moment_match_split(
  x,  # A fitted model object.
  upars,  # A matrix containing the model parameters in unconstrained space where they can have any real value.
  cov,  # Logical; Indicate whether to match the covariance matrix of the samples or not. If FALSE, only the mean and marginal variances are matched.
  total_shift,  # A vector representing the total shift made by the moment matching algorithm.
  total_scaling,  # A vector representing the total scaling of marginal variance made by the moment matching algorithm.
  total_mapping,  # A vector representing the total covariance transformation made by the moment matching algorithm.
  i,  # Observation index.
  log_prob_upars,  # A function that takes arguments x and upars and returns a matrix of log-posterior density values of the unconstrained posterior draws passed via upars.
  log_lik_i_upars,  # log_lik_i_upars
  r_eff_i,  # cores;
  is_method,  # ...
log lik i upars
A function that takes arguments x, upars, and i and returns a vector of log-
likelihood draws of the ith observation based on the unconstrained posterior
draws passed via upars.

r_eff_i
MCMC relative effective sample size of the ith log likelihood draws.

cores
The number of cores to use for parallelization. This defaults to the option
mc.cores which can be set for an entire R session by options(mc.cores =
NUMBER). The old option loo.cores is now deprecated but will be given prece-
dence over mc.cores until loo.cores is removed in a future release. As of
version 2.0.0 the default is now 1 core if mc.cores is not set, but we recom-
mend using as many (or close to as many) cores as possible.

• Note for Windows 10 users: it is strongly recommended to avoid using
the .Rprofile file to set mc.cores (using the cores argument or setting
mc.cores interactively or in a script is fine).

is_method
The importance sampling method to use. The following methods are imple-
mented:
• "psis": Pareto-Smoothed Importance Sampling (PSIS). Default method.
• "tis": Truncated Importance Sampling (TIS) with truncation at sqrt(S),
where S is the number of posterior draws.
• "sis": Standard Importance Sampling (SIS).

... Further arguments passed to the custom functions documented above.

Value
A list containing the updated log-importance weights and log-likelihood values. Also returns the
updated MCMC effective sample size and the integrand-specific log-importance weights.

References

See Also
loo(), loo_moment_match()
Usage

loo_predictive_metric(x, ...)

## S3 method for class 'matrix'

loo_predictive_metric(
  x,
  y,
  log_lik,
  ...,  
  metric = c("mae", "rmse", "mse", "acc", "balanced_acc"),
  r_eff = 1,
  cores = getOption("mc.cores", 1)
)

Arguments

x A numeric matrix of predictions.

... Additional arguments passed on to E_loo()

y A numeric vector of observations. Length should be equal to the number of rows in x.

log_lik A matrix of pointwise log-likelihoods. Should be of same dimension as x.

metric The type of predictive metric to be used. Currently supported options are "mae", "rmse" and "mse" for regression and for binary classification "acc" and "balanced_acc".

"mae" Mean absolute error.

"mse" Mean squared error.

"rmse" Root mean squared error, given by as the square root of MSE.

"acc" The proportion of predictions indicating the correct outcome.

"balanced_acc" Balanced accuracy is given by the average of true positive and true negative rates.

r_eff A Vector of relative effective sample size estimates containing one element per observation. See psis() for more details.

cores The number of cores to use for parallelization of [psis()]. See psis() for details.

Value

A list with the following components:

estimate Estimate of the given metric.

se Standard error of the estimate.

Examples

if (requireNamespace("rstanarm", quietly = TRUE)) {
  # Use rstanarm package to quickly fit a model and get both a log-likelihood
  # matrix and draws from the posterior predictive distribution
library("rstanarm")

# data from help("lm")
ctl <- c(4.17,5.58,5.18,6.11,4.50,4.61,5.17,4.53,5.33,5.14)
trt <- c(4.81,4.17,4.41,3.59,5.87,3.83,6.03,4.89,4.32,4.69)
d <- data.frame(
  weight = c(ctl, trt),
  group = gl(2, 10, 20, labels = c("Ctl","Trt"))
)
fit <- stan_glm(weight ~ group, data = d, refresh = 0)
ll <- log_lik(fit)
r_eff <- relative_eff(exp(-ll), chain_id = rep(1:4, each = 1000))

mu_pred <- posterior_epred(fit)

mae <- loo_predictive_metric(x = mu_pred, y = d$weight, log_lik = ll,
  pred_error = 'mae', r_eff = r_eff)

mae_90q <- loo_predictive_metric(x = mu_pred, y = d$weight, log_lik = ll,
  pred_error = 'mae', r_eff = r_eff,
  type = 'quantile', probs = 0.9)

---

**loo_subsample**

Efficient approximate leave-one-out cross-validation (LOO) using subsampling, so that less costly and more approximate computation is made for all LOO-fold, and more costly and accurate computations are made only for m<N LOO-folds.

---

**Description**

Efficient approximate leave-one-out cross-validation (LOO) using subsampling, so that less costly and more approximate computation is made for all LOO-fold, and more costly and accurate computations are made only for m<N LOO-folds.

**Usage**

```r
loo_subsample(x, ...)
```

## S3 method for class "function"
loo_subsample(
  x,
  ...,
  data = NULL,
  draws = NULL,
  observations = 400,
  log_p = NULL,
  log_g = NULL,
)
r_eff = 1,
save_psis = FALSE,
cores = getOption("mc.cores", 1),
loo_approximation = "plpd",
loo_approximation_draws = NULL,
estimator = "diff_srs",
llgrad = NULL,
llhess = NULL)

Arguments

- **x**: A function. The Methods (by class) section, below, has detailed descriptions of how to specify the inputs.
- **data, draws, ...**: For `loo_subsample.function()`, these are the data, posterior draws, and other arguments to pass to the log-likelihood function. Note that for some `loo_approximation` s, the draws will be replaced by the posteriors summary statistics to compute loo approximations. See argument `loo_approximation` for details.
- **observations**: The subsample observations to use. The argument can take four (4) types of arguments:
  - NULL to use all observations. The algorithm then just uses standard `loo()` or `loo_approximate_posterior()`.
  - A single integer to specify the number of observations to be subsampled.
  - A vector of integers to provide the indices used to subset the data. These observations need to be subsampled with the same scheme as given by the estimator argument.
  - A `psis_loo_ss` object to use the same observations that were used in a previous call to `loo_subsample()`.
- **log_p, log_g**: Should be supplied only if approximate posterior draws are used. The default (NULL) indicates draws are from "true" posterior (i.e. using MCMC). If not NULL then they should be specified as described in `loo_approximate_posterior()`.
- **r_eff**: Vector of relative effective sample size estimates for the likelihood (exp(log_lik)) of each observation. This is related to the relative efficiency of estimating the normalizing term in self-normalized importance sampling when using posterior draws obtained with MCMC. If MCMC draws are used and r_eff is not provided then the reported PSIS effective sample sizes and Monte Carlo error estimates can be over-optimistic. If the posterior draws are (near) independent then r_eff=1 can be used. r_eff has to be a scalar (same value is used for all observations) or a vector with length equal to the number of observations. The default value is 1. See the `relative_eff()` helper functions for help computing r_eff.
- **save_psis**: Should the "psis" object created internally by `loo_subsample()` be saved in the returned object? See `loo()` for details.
- **cores**: The number of cores to use for parallelization. This defaults to the option `mc.cores` which can be set for an entire R session by `options(mc.cores = NUMBER)`. The old option `loo.cores` is now deprecated but will be given precedence over `mc.cores` until `loo.cores` is removed in a future release. As of
version 2.0.0 the default is now 1 core if mc.cores is not set, but we recommend using as many (or close to as many) cores as possible.

- Note for Windows 10 users: it is strongly recommended to avoid using the .Rprofile file to set mc.cores (using the cores argument or setting mc.cores interactively or in a script is fine).

loo_approximation

What type of approximation of the loo_i’s should be used? The default is "plpd" (the log predictive density using the posterior expectation). There are six different methods implemented to approximate loo_i’s (see the references for more details):

- "plpd": uses the lpd based on point estimates (i.e., \( p(y_i | \hat{\theta}) \)).
- "1lpd": uses the lpd’s (i.e., \( p(y_i | y) \)).
- "tis": uses truncated importance sampling to approximate PSIS-LOO.
- "waic": uses waic (i.e., \( p(y_i | y) - p_{waic} \)).
- "waic_grad_marginal": uses waic approximation using first order delta method and posterior marginal variances to approximate \( p_{waic} \) (i.e. \( p(y_i | \hat{\theta}) - p_{waic_grad_marginal} \)). Requires gradient of likelihood function.
- "waic_grad": uses waic approximation using first order delta method and posterior covariance to approximate \( p_{waic} \) (i.e. \( p(y_i | \hat{\theta}) - p_{waic_grad} \)). Requires gradient of likelihood function.
- "waic_hess": uses waic approximation using second order delta method and posterior covariance to approximate \( p_{waic} \) (i.e. \( p(y_i | \hat{\theta}) - p_{waic_grad} \)). Requires gradient and Hessian of likelihood function.

As point estimates of \( \hat{\theta} \), the posterior expectations of the parameters are used.

loo_approximation_draws

The number of posterior draws used when integrating over the posterior. This is used if loo_approximation is set to "1lpd", "waic", or "tis".

estimator

How should elpd_loo, p_loo and looic be estimated? The default is "diff_srs".

- "diff_srs": uses the difference estimator with simple random sampling without replacement (srs). p_loo is estimated using standard srs. (Magnusson et al., 2020)
- "hh": uses the Hansen-Hurwitz estimator with sampling with replacement proportional to size, where abs of loo_approximation is used as size. (Magnusson et al., 2019)
- "srs": uses simple random sampling and ordinary estimation.

llgrad

The gradient of the log-likelihood. This is only used when loo_approximation is "waic_grad", "waic_grad_marginal", or "waic_hess". The default is NULL.

llhess

The Hessian of the log-likelihood. This is only used with loo_approximation = "waic_hess". The default is NULL.

Details

The loo_subsample() function is an S3 generic and a methods is currently provided for log-likelihood functions. The implementation works for both MCMC and for posterior approximations where it is possible to compute the log density for the approximation.
loo_subsample

Value

loo_subsample() returns a named list with class c("psis_loo_ss", "psis_loo", "loo"). This has the same structure as objects returned by loo() but with the additional slot:

- loo_subsampling: A list with two vectors, log_p and log_g, of the same length containing the posterior density and the approximation density for the individual draws.

Methods (by class)

- loo_subsample(function): A function f() that takes arguments data_i and draws and returns a vector containing the log-likelihood for a single observation i evaluated at each posterior draw. The function should be written such that, for each observation i in 1:N, evaluating

  \[
  f(data_i = data[i,, drop=FALSE], draws = draws)
  \]

  results in a vector of length S (size of posterior sample). The log-likelihood function can also have additional arguments but data_i and draws are required.

  If using the function method then the arguments data and draws must also be specified in the call to loo():

  - data: A data frame or matrix containing the data (e.g. observed outcome and predictors) needed to compute the pointwise log-likelihood. For each observation i, the i-th row of data will be passed to the data_i argument of the log-likelihood function.

  - draws: An object containing the posterior draws for any parameters needed to compute the pointwise log-likelihood. Unlike data, which is indexed by observation, for each observation the entire object draws will be passed to the draws argument of the log-likelihood function.

  - The ... can be used if your log-likelihood function takes additional arguments. These arguments are used like the draws argument in that they are recycled for each observation.

References


See Also

loo(), psis(), loo_compare()
nobs.psis_loo_ss

The number of observations in a psis_loo_ss object.

Description

The number of observations in a psis_loo_ss object.

Usage

## S3 method for class 'psis_loo_ss'
nobs(object, ...)

Arguments

object a psis_loo_ss object.
...
Currently unused.

obs_idx

Get observation indices used in subsampling

Description

Get observation indices used in subsampling

Usage

obs_idx(x, rep = TRUE)

Arguments

x A psis_loo_ss object.
rep If sampling with replacement is used, an observation can have multiple samples and these are then repeated in the returned object if rep=TRUE (e.g., a vector c(1,1,2) indicates that observation 1 has been subsampled two times). If rep=FALSE only the unique indices are returned.

Value

An integer vector.
Diagnostics for Pareto smoothed importance sampling (PSIS)

Description
Print a diagnostic table summarizing the estimated Pareto shape parameters and PSIS effective sample sizes, find the indexes of observations for which the estimated Pareto shape parameter \( k \) is larger than some threshold value, or plot observation indexes vs. diagnostic estimates. The Details section below provides a brief overview of the diagnostics, but we recommend consulting Vehtari, Gelman, and Gabry (2017) and Vehtari, Simpson, Gelman, Yao, and Gabry (2024) for full details.

Usage

- `pareto_k_table(x)`
- `pareto_k_ids(x, threshold = NULL)`
- `pareto_k_values(x)`
- `pareto_k_influence_values(x)`
- `psis_n_eff_values(x)`
- `mcse_loo(x, threshold = NULL)`

## S3 method for class 'psis_loo'
`plot`

```r
x,
diagnostic = c("k", "ESS", "n_eff"),
...,
label_points = FALSE,
main = "PSIS diagnostic plot"
)
```

## S3 method for class 'psis'
`plot`

```r
x,
diagnostic = c("k", "ESS", "n_eff"),
...,
label_points = FALSE,
main = "PSIS diagnostic plot"
)
```

Arguments

- `x` An object created by `loo()` or `psis()`.
threshold

For `pareto_k_ids()`, `threshold` is the minimum `k` value to flag (default is a sample size `S` dependent threshold `1 - 1 / \log_{10}(S)`). For `mcse_loo()`, if any `k` estimates are greater than `threshold` the MCSE estimate is returned as `NA`. See Details for the motivation behind these defaults.

diagnostic

For the `plot` method, which diagnostic should be plotted? The options are "k" for Pareto `k` estimates (the default), or "ESS" or "n_eff" for PSIS effective sample size estimates.

label_points, ...

For the `plot()` method, if `label_points` is `TRUE` the observation numbers corresponding to any values of `k` greater than the diagnostic threshold will be displayed in the plot. Any arguments specified in `...` will be passed to `graphics::text()` and can be used to control the appearance of the labels.

main

For the `plot()` method, a title for the plot.

Details

The reliability and approximate convergence rate of the PSIS-based estimates can be assessed using the estimates for the shape parameter `k` of the generalized Pareto distribution. The diagnostic threshold for Pareto `k` depends on sample size `S` (sample size dependent threshold was introduced by Vehtari et al. (2024), and before that fixed thresholds of 0.5 and 0.7 were recommended). For simplicity, loo package uses the nominal sample size `S` when computing the sample size specific threshold. This provides an optimistic threshold if the effective sample size is less than 2200, but if MCMC-ESS > S/2 the difference is usually negligible. Thinning of MCMC draws can be used to improve the ratio ESS/S.

- If \( k < \min(1 - 1/\log_{10}(S), 0.7) \), where \( S \) is the sample size, the PSIS estimate and the corresponding Monte Carlo standard error estimate are reliable.
- If \( 1 - 1/\log_{10}(S) \leq k < 0.7 \), the PSIS estimate and the corresponding Monte Carlo standard error estimate are not reliable, but increasing the (effective) sample size \( S \) above 2200 may help (this will increase the sample size specific threshold \( (1 - 1/\log_{10}(2200)) > 0.7 \) and then the bias specific threshold 0.7 dominates).
- If \( 0.7 \leq k < 1 \), the PSIS estimate and the corresponding Monte Carlo standard error have large bias and are not reliable. Increasing the sample size may reduce the variability in `k` estimate, which may result in lower `k` estimate, too.
- If \( k \geq 1 \), the target distribution is estimated to have a non-finite mean. The PSIS estimate and the corresponding Monte Carlo standard error are not well defined. Increasing the sample size may reduce the variability in the `k` estimate, which may also result in a lower `k` estimate.

What if the estimated tail shape parameter `k` exceeds the diagnostic threshold?: Importance sampling is likely to work less well if the marginal posterior \( p(\theta^*|y) \) and LOO posterior \( p(\theta^*|y_{-i}) \) are very different, which is more likely to happen with a non-robust model and highly influential observations. If the estimated tail shape parameter `k` exceeds the diagnostic threshold, the user should be warned. (Note: If `k` is greater than the diagnostic threshold then WAIC is also likely to fail, but WAIC lacks as accurate diagnostic.) When using PSIS in the context of approximate LOO-CV, we recommend one of the following actions:

- With some additional computations, it is possible to transform the MCMC draws from the posterior distribution to obtain more reliable importance sampling estimates. This results in a
smaller shape parameter $k$. See `loo_moment_match()` and the vignette *Avoiding model refits in leave-one-out cross-validation with moment matching* for an example of this.

- Sampling from a leave-one-out mixture distribution (see the vignette *Mixture IS leave-one-out cross-validation for high-dimensional Bayesian models*), directly from $p(\theta_i | y_{-i})$ for the problematic observations $i$, or using $K$-fold cross-validation (see the vignette *Holdout validation and K-fold cross-validation of Stan programs with the loo package*) will generally be more stable.

- Using a model that is more robust to anomalous observations will generally make approximate LOO-CV more stable.

**Observation influence statistics:** The estimated shape parameter $k$ for each observation can be used as a measure of the observation’s influence on posterior distribution of the model. These can be obtained with `pareto_k_influence_values()`.

**Effective sample size and error estimates:** In the case that we obtain the samples from the proposal distribution via MCMC the `loo` package also computes estimates for the Monte Carlo error and the effective sample size for importance sampling, which are more accurate for PSIS than for IS and TIS (see Vehtari et al. (2024) for details). However, the PSIS effective sample size estimate will be **over-optimistic when the estimate of $k$ is greater than $\min(1 - 1/\log_{10}(S), 0.7)$**, where $S$ is the sample size.

**Value**

`pareto_k_table()` returns an object of class "pareto_k_table", which is a matrix with columns "Count", "Proportion", and "Min. n_eff", and has its own print method.

`pareto_k_ids()` returns an integer vector indicating which observations have Pareto $k$ estimates above threshold.

`pareto_k_values()` returns a vector of the estimated Pareto $k$ parameters. These represent the reliability of sampling.

`pareto_k_influence_values()` returns a vector of the estimated Pareto $k$ parameters. These represent influence of the observations on the model posterior distribution.

`psis_n_eff_values()` returns a vector of the estimated PSIS effective sample sizes.

`mcse_loo()` returns the Monte Carlo standard error (MCSE) estimate for PSIS-LOO. MCSE will be NA if any Pareto $k$ values are above threshold.

The `plot()` method is called for its side effect and does not return anything. If x is the result of a call to `loo()` or `psis()` then `plot(x, diagnostic)` produces a plot of the estimates of the Pareto shape parameters (diagnostic = "k") or estimates of the PSIS effective sample sizes (diagnostic = "ESS").

**References**


See Also

- `psis()` for the implementation of the PSIS algorithm.
- The FAQ page on the loo website for answers to frequently asked questions.

pointwise

Convenience function for extracting pointwise estimates

Description

Convenience function for extracting pointwise estimates

Usage

```r
pointwise(x, estimate, ...)
```

## S3 method for class 'loo'

```r
pointwise(x, estimate, ...)
```

Arguments

- `x` A loo object, for example one returned by `loo()`, `loo_subsample()`, `loo_approximate_posterior()`, `loo_moment_match()`, etc.
- `estimate` Which pointwise estimate to return. By default all are returned. The objects returned by the different functions (`loo()`, `loo_subsample()`, etc.) have slightly different estimates available. Typically at a minimum the estimates `elpd_loo`, `looic`, `mcse_elpd_loo`, `p_loo`, and `influence_pareto_k` will be available, but there may be others.
- `...` Currently ignored.

Value

A vector of length equal to the number of observations.

Examples

```r
x <- loo(example_loglik_array())
pointwise(x, "elpd_loo")
```
Description

Print methods

Usage

## S3 method for class 'loo'
print(x, digits = 1, ...)

## S3 method for class 'waic'
print(x, digits = 1, ...)

## S3 method for class 'psis_loo'
print(x, digits = 1, plot_k = FALSE, ...)

## S3 method for class 'importance_sampling_loo'
print(x, digits = 1, plot_k = FALSE, ...)

## S3 method for class 'psis_loo_ap'
print(x, digits = 1, plot_k = FALSE, ...)

## S3 method for class 'psis'
print(x, digits = 1, plot_k = FALSE, ...)

## S3 method for class 'importance_sampling'
print(x, digits = 1, plot_k = FALSE, ...)

Arguments

x An object returned by loo(), psis(), or waic().
digits An integer passed to base::round().
... Arguments passed to plot.psis_loo() if plot_k is TRUE.
plot_k Logical. If TRUE the estimates of the Pareto shape parameter \( k \) are plotted. Ignored if \( x \) was generated by waic(). To just plot \( k \) without printing use the plot() method for 'loo' objects.

Value

\( x \), invisibly.

See Also

pareto-k-diagnostic
psis

Pareto smoothed importance sampling (PSIS)

Description

Implementation of Pareto smoothed importance sampling (PSIS), a method for stabilizing importance ratios. The version of PSIS implemented here corresponds to the algorithm presented in Vehtari, Simpson, Gelman, Yao, and Gabry (2024). For PSIS diagnostics see the pareto-k-diagnostic page.

Usage

psis(log_ratios, ...)

## S3 method for class 'array'
psis(log_ratios, ..., r_eff = 1, cores = getOption("mc.cores", 1))

## S3 method for class 'matrix'
psis(log_ratios, ..., r_eff = 1, cores = getOption("mc.cores", 1))

## Default S3 method:
psis(log_ratios, ..., r_eff = 1)

is.psis(x)

is.sis(x)

is.tis(x)

Arguments

log_ratios An array, matrix, or vector of importance ratios on the log scale (for PSIS-LOO these are negative log-likelihood values). See the Methods (by class) section below for a detailed description of how to specify the inputs for each method.

... Arguments passed on to the various methods.

r_eff Vector of relative effective sample size estimates containing one element per observation. The values provided should be the relative effective sample sizes of 1/exp(log_ratios) (i.e., 1/ratios). This is related to the relative efficiency of estimating the normalizing term in self-normalizing importance sampling. If r_eff is not provided then the reported PSIS effective sample sizes and Monte Carlo error estimates can be over-optimistic. If the posterior draws are (near) independent then r_eff=1 can be used. r_eff has to be a scalar (same value is used for all observations) or a vector with length equal to the number of observations. The default value is 1. See the relative_eff() helper function for computing r_eff.
cores

The number of cores to use for parallelization. This defaults to the option `mc.cores` which can be set for an entire R session by `options(mc.cores = NUMBER)`. The old option `loo.cores` is now deprecated but will be given precedence over `mc.cores` until `loo.cores` is removed in a future release. **As of version 2.0.0 the default is now 1 core if `mc.cores` is not set**, but we recommend using as many (or close to as many) cores as possible.

- Note for Windows 10 users: it is **strongly recommended** to avoid using the `.Rprofile` file to set `mc.cores` (using the `cores` argument or setting `mc.cores` interactively or in a script is fine).

For `is.psis()`, an object to check.

**Value**

The `psis()` methods return an object of class "psis", which is a named list with the following components:

- `log_weights` Vector or matrix of smoothed (and truncated) but **unnormalized** log weights. To get normalized weights use the `weights()` method provided for objects of class "psis".

- `diagnostics` A named list containing two vectors:
  - `pareto_k`: Estimates of the shape parameter $k$ of the generalized Pareto distribution. See the [pareto-k-diagnostic page](#) for details.
  - `n_eff`: PSIS effective sample size estimates.

Objects of class "psis" also have the following attributes:

- `norm_const_log` Vector of precomputed values of `colLogSumExps(log_weights)` that are used internally by the weights method to normalize the log weights.
- `tail_len` Vector of tail lengths used for fitting the generalized Pareto distribution.
- `r_eff` If specified, the user’s `r_eff` argument.
- `dims` Integer vector of length 2 containing $S$ (posterior sample size) and $N$ (number of observations).
- `method` Method used for importance sampling, here `psis`.

**Methods (by class)**

- `psis(array)`: An $I$ by $C$ by $N$ array, where $I$ is the number of MCMC iterations per chain, $C$ is the number of chains, and $N$ is the number of data points.
- `psis(matrix)`: An $S$ by $N$ matrix, where $S$ is the size of the posterior sample (with all chains merged) and $N$ is the number of data points.
- `psis(default)`: A vector of length $S$ (posterior sample size).

**References**


See Also

- `loo()` for approximate LOO-CV using PSIS.
- `pareto-k-diagnostic` for PSIS diagnostics.
- The `loo` package vignettes for demonstrations.
- The FAQ page on the `loo` website for answers to frequently asked questions.

Examples

```r
log ratios <- -1 * example_loglik_array()
r_eff <- relative_eff(exp(-log ratios))
psis_result <- psis(log ratios, r_eff = r_eff)
str(psis_result)
plot(psis_result)

# extract smoothed weights
lw <- weights(psis_result)  # default args are log=TRUE, normalize=TRUE
ulw <- weights(psis_result, normalize=FALSE)  # unnormalized log-weights

w <- weights(psis_result, log=FALSE)  # normalized weights (not log-weights)
uw <- weights(psis_result, log=FALSE, normalize = FALSE)  # unnormalized weights
```

---

**psislw**  
Pareto smoothed importance sampling (deprecated, old version)

Description

As of version 2.0.0 this function is deprecated. Please use the `psis()` function for the new PSIS algorithm.

Usage

```r
psislw(
  lw,
  wcp = 0.2,
  wtrunc = 3/4,
  cores = getOption("mc.cores", 1),
  llfun = NULL,
  llargs = NULL,
  ...
)
```
relative_eff()

Convenience function for computing relative efficiencies

Description

relative_eff() computes the the MCMC effective sample size divided by the total sample size.

Arguments

lw A matrix or vector of log weights. For computing LOO, lw = -log_lik, the negative of an S (simulations) by N (data points) pointwise log-likelihood matrix.

wcp The proportion of importance weights to use for the generalized Pareto fit. The \(100*wcp\) from which to estimate the parameters of the generalized Pareto distribution.

wtrunc For truncating very large weights to \(S^{wtrunc}\). Set to zero for no truncation.

cores The number of cores to use for parallelization. This defaults to the option mc.cores which can be set for an entire R session by options(mc.cores = NUMBER), the old option loo.cores is now deprecated but will be given precedence over mc.cores until it is removed. As of version 2.0.0, the default is now 1 core if mc.cores is not set, but we recommend using as many (or close to as many) cores as possible.

llfun, llargs See loo.function().

... Ignored when psislw() is called directly. The ... is only used internally when psislw() is called by the loo() function.

Value

A named list with components lw_smooth (modified log weights) and pareto_k (estimated generalized Pareto shape parameter(s) k).

References


See Also

diagnostic for PSIS diagnostics.
Usage

relative_eff(x, ...)

## Default S3 method:
relative_eff(x, chain_id, ...)

## S3 method for class 'matrix'
relative_eff(x, chain_id, ..., cores = getOption("mc.cores", 1))

## S3 method for class 'array'
relative_eff(x, ..., cores = getOption("mc.cores", 1))

## S3 method for class `function`
relative_eff(x, chain_id, ..., cores = getOption("mc.cores", 1),
    data = NULL,
    draws = NULL)

## S3 method for class 'importance_sampling'
relative_eff(x, ...)

Arguments

x A vector, matrix, 3-D array, or function. See the Methods (by class) section below for details on specifying x, but where "log-likelihood" is mentioned replace it with one of the following depending on the use case:

- For use with the loo() function, the values in x (or generated by x, if a function) should be likelihood values (i.e., exp(log_lik)), not on the log scale.
- For generic use with psis(), the values in x should be the reciprocal of the importance ratios (i.e., exp(-log_ratios)).

chain_id A vector of length NROW(x) containing MCMC chain indexes for each each row of x (if a matrix) or each value in x (if a vector). No chain_id is needed if x is a 3-D array. If there are C chains then valid chain indexes are values in 1:C.

cores The number of cores to use for parallelization.

data, draws, ... Same as for the loo() function method.

Value

A vector of relative effective sample sizes.

Methods (by class)

- relative_eff(default): A vector of length S (posterior sample size).
• `relative_eff(matrix)`: An $S$ by $N$ matrix, where $S$ is the size of the posterior sample (with all chains merged) and $N$ is the number of data points.

• `relative_eff(array)`: An $I$ by $C$ by $N$ array, where $I$ is the number of MCMC iterations per chain, $C$ is the number of chains, and $N$ is the number of data points.

• `relative_eff("function")`: A function $f()$ that takes arguments `data_i` and `draws` and returns a vector containing the log-likelihood for a single observation $i$ evaluated at each posterior draw. The function should be written such that, for each observation $i$ in $1:N$, evaluating

$$f(data_i = data[i, , drop=FALSE], draws = draws)$$

results in a vector of length $S$ (size of posterior sample). The log-likelihood function can also have additional arguments but `data_i` and `draws` are required. If using the function method then the arguments `data` and `draws` must also be specified in the call to `loo()`:

- `data`: A data frame or matrix containing the data (e.g. observed outcome and predictors) needed to compute the pointwise log-likelihood. For each observation $i$, the $i$th row of `data` will be passed to the `data_i` argument of the log-likelihood function.

- `draws`: An object containing the posterior draws for any parameters needed to compute the pointwise log-likelihood. Unlike `data`, which is indexed by observation, for each observation the entire object `draws` will be passed to the `draws` argument of the log-likelihood function.

- `The ... can be used if your log-likelihood function takes additional arguments. These arguments are used like the `draws` argument in that they are recycled for each observation.

• `relative_eff(importance_sampling)`: If `x` is an object of class "psis", `relative_eff()` simply returns the `r_eff` attribute of `x`.

### Examples

```r
LLarr <- example_loglik_array()
LLmat <- example_loglik_matrix()
dim(LLarr)
dim(LLmat)

rel_n_eff_1 <- relative_eff(exp(LLarr))
rel_n_eff_2 <- relative_eff(exp(LLmat), chain_id = rep(1:2, each = 500))
all.equal(rel_n_eff_1, rel_n_eff_2)
```

---

**sis**  
*Standard importance sampling (SIS)*

### Description

Implementation of standard importance sampling (SIS).
sis

Usage

sis(log_ratios, ...)

## S3 method for class 'array'
sis(log_ratios, ..., r_eff = NULL, cores = getOption("mc.cores", 1))

## S3 method for class 'matrix'
sis(log_ratios, ..., r_eff = NULL, cores = getOption("mc.cores", 1))

## Default S3 method:
sis(log_ratios, ..., r_eff = NULL)

Arguments

log_ratios An array, matrix, or vector of importance ratios on the log scale (for Importance
sampling LOO, these are negative log-likelihood values). See the Methods (by
class) section below for a detailed description of how to specify the inputs for
each method.

... Arguments passed on to the various methods.

r_eff Vector of relative effective sample size estimates containing one element per
observation. The values provided should be the relative effective sample sizes of
1/exp(log_ratios) (i.e., 1/ratios). This is related to the relative efficiency of
estimating the normalizing term in self-normalizing importance sampling. See
the relative_eff() helper function for computing r_eff. If using psis with
draws of the log_ratios not obtained from MCMC then the warning message
thrown when not specifying r_eff can be disabled by setting r_eff to NA.

cores The number of cores to use for parallelization. This defaults to the option
mc.cores which can be set for an entire R session by options(mc.cores =
NUMBER). The old option loo.cores is now deprecated but will be given prece-
dence over mc.cores until loo.cores is removed in a future release. As of
version 2.0.0 the default is now 1 core if mc.cores is not set, but we recom-
mend using as many (or close to as many) cores as possible.

• Note for Windows 10 users: it is strongly recommended to avoid using
the .Rprofile file to set mc.cores (using the cores argument or setting
mc.cores interactively or in a script is fine).

Value

The sis() methods return an object of class "sis", which is a named list with the following com-
ponents:

log_weights Vector or matrix of smoothed but unnormalized log weights. To get normalized
weights use the weights() method provided for objects of class sis.
diagnostics A named list containing one vector:
  • pareto_k: Not used in sis, all set to 0.
  • n_eff: effective sample size estimates.
Objects of class "sis" also have the following attributes:

- **norm_const_log**: Vector of precomputed values of `colLogSumExps(log_weights)` that are used internally by the `weights` method to normalize the log weights.
- **r_eff**: If specified, the user's `r_eff` argument.
- **tail_len**: Not used for `sis`.
- **dims**: Integer vector of length 2 containing `S` (posterior sample size) and `N` (number of observations).
- **method**: Method used for importance sampling, here `sis`.

### Methods (by class)

- **sis(array)**: An `I` by `C` by `N` array, where `I` is the number of MCMC iterations per chain, `C` is the number of chains, and `N` is the number of data points.
- **sis(matrix)**: An `S` by `N` matrix, where `S` is the size of the posterior sample (with all chains merged) and `N` is the number of data points.
- **sis(default)**: A vector of length `S` (posterior sample size).

### References


### See Also

- **psis()** for approximate LOO-CV using PSIS.
- **loo()** for approximate LOO-CV.
- **pareto-k-diagnostic** for PSIS diagnostics.

### Examples

```r
log_ratios <- -1 * example_loglik_array()
r_eff <- relative_eff(exp(-log_ratios))
sis_result <- sis(log_ratios, r_eff = r_eff)
str(sis_result)

# extract smoothed weights
lw <- weights(sis_result)  # default args are log=TRUE, normalize=TRUE
ulw <- weights(sis_result, normalize=FALSE)  # unnormalized log-weights

w <- weights(sis_result, log=FALSE)  # normalized weights (not log-weights)
uw <- weights(sis_result, log=FALSE, normalize=FALSE)  # unnormalized weights
```
Truncated importance sampling (TIS)

Description

Implementation of truncated (self-normalized) importance sampling (TIS), truncated at $S^{1/2}$ as recommended by Ionides (2008).

Usage

tis(log_ratios, ...)

## S3 method for class 'array'
tis(log_ratios, ..., r_eff = 1, cores = getOption("mc.cores", 1))

## S3 method for class 'matrix'
tis(log_ratios, ..., r_eff = 1, cores = getOption("mc.cores", 1))

## Default S3 method:
tis(log_ratios, ..., r_eff = 1)

Arguments

- **log_ratios**: An array, matrix, or vector of importance ratios on the log scale (for Importance sampling LOO, these are negative log-likelihood values). See the Methods (by class) section below for a detailed description of how to specify the inputs for each method.
- **...**: Arguments passed on to the various methods.
- **r_eff**: Vector of relative effective sample size estimates containing one element per observation. The values provided should be the relative effective sample sizes of $1/\exp(log\_ratios)$ (i.e., $1/ratios$). This is related to the relative efficiency of estimating the normalizing term in self-normalizing importance sampling. If r_eff is not provided then the reported (T)IS effective sample sizes and Monte Carlo error estimates can be over-optimistic. If the posterior draws are (near) independent then r_eff=1 can be used. r_eff has to be a scalar (same value is used for all observations) or a vector with length equal to the number of observations. The default value is 1. See the relative_eff() helper function for computing r_eff.
- **cores**: The number of cores to use for parallelization. This defaults to the option mc.cores which can be set for an entire R session by options(mc.cores = NUMBER). The old option loo.cores is now deprecated but will be given precedence over mc.cores until loo.cores is removed in a future release. As of version 2.0.0 the default is now 1 core if mc.cores is not set, but we recommend using as many (or close to as many) cores as possible.

- Note for Windows 10 users: it is strongly recommended to avoid using the .Rprofile file to set mc.cores (using the cores argument or setting mc.cores interactively or in a script is fine).
Value

The tis() methods return an object of class "tis", which is a named list with the following components:

log_weights Vector or matrix of smoothed (and truncated) but unnormalized log weights. To get normalized weights use the weights() method provided for objects of class tis.

diagnostics A named list containing one vector:
  • pareto_k: Not used in tis, all set to 0.
  • n_eff: Effective sample size estimates.

Objects of class "tis" also have the following attributes:

norm_const_log Vector of precomputed values of colLogSumExps(log_weights) that are used internally by the weights() method to normalize the log weights.

r_eff If specified, the user’s r_eff argument.

tail_len Not used for tis.

dims Integer vector of length 2 containing S (posterior sample size) and N (number of observations).

Method Method used for importance sampling, here tis.

Methods (by class)

• tis(array): An I by C by N array, where I is the number of MCMC iterations per chain, C is the number of chains, and N is the number of data points.

• tis(matrix): An S by N matrix, where S is the size of the posterior sample (with all chains merged) and N is the number of data points.

• tis(default): A vector of length S (posterior sample size).

References


See Also

• psis() for approximate LOO-CV using PSIS.

• loo() for approximate LOO-CV.

• pareto-k-diagnostic for PSIS diagnostics.

Examples

log_ratios <- -1 * example_loglik_array()
r_eff <- relative_eff(exp(-log_ratios))
tis_result <- tis(log_ratios, r_eff = r_eff)
str(tis_result)

# extract smoothed weights
lw <- weights(tis_result) # default args are log=TRUE, normalize=TRUE
ulw <- weights(tis_result, normalize=FALSE) # unnormalized log-weights
w <- weights(tis_result, log=FALSE) # normalized weights (not log-weights)
uw <- weights(tis_result, log=FALSE, normalize = FALSE) # unnormalized weights

update.psis_loo_ss  

Update psis_loo_ss objects

Description

Update psis_loo_ss objects

Usage

## S3 method for class 'psis_loo_ss'
update(
  object,
  ..., 
  data = NULL, 
  draws = NULL, 
  observations = NULL, 
  r_eff = 1, 
  cores = getOption("mc.cores", 1), 
  loo_approximation = NULL, 
  loo_approximation_draws = NULL, 
  ll_grad = NULL, 
  llhess = NULL,
)

Arguments

object A psis_loo_ss object to update.
... Currently not used.
data, draws See loo_subsample.function().
observations The subsample observations to use. The argument can take four (4) types of arguments:

- NULL to use all observations. The algorithm then just uses standard loo() or loo_approximate_posterior().
- A single integer to specify the number of observations to be subsampled.
- A vector of integers to provide the indices used to subset the data. These observations need to be subsampled with the same scheme as given by the estimator argument.
- A psis_loo_ss object to use the same observations that were used in a previous call to loo_subsample().
**r_eff**

Vector of relative effective sample size estimates for the likelihood (\(\exp(\log_{\text{lik}})\)) of each observation. This is related to the relative efficiency of estimating the normalizing term in self-normalized importance sampling when using posterior draws obtained with MCMC. If MCMC draws are used and \(r_{\text{eff}}\) is not provided then the reported PSIS effective sample sizes and Monte Carlo error estimates can be over-optimistic. If the posterior draws are (near) independent then \(r_{\text{eff}}=1\) can be used. \(r_{\text{eff}}\) has to be a scalar (same value is used for all observations) or a vector with length equal to the number of observations. The default value is 1. See the `relative_eff()` helper functions for help computing \(r_{\text{eff}}\).

**cores**

The number of cores to use for parallelization. This defaults to the option `mc.cores` which can be set for an entire R session by `options(mc.cores = NUMBER)`. The old option `loo.cores` is now deprecated but will be given precedence over `mc.cores` until `loo.cores` is removed in a future release. **As of version 2.0.0 the default is now 1 core if `mc.cores` is not set**, but we recommend using as many (or close to as many) cores as possible.

- Note for Windows 10 users: it is **strongly recommended** to avoid using the `.Rprofile` file to set `mc.cores` (using the `cores` argument or setting `mc.cores` interactively or in a script is fine).

**loo_approximation**

What type of approximation of the \(\text{loo}_i\)'s should be used? The default is "plpd" (the log predictive density using the posterior expectation). There are six different methods implemented to approximate \(\text{loo}_i\)'s (see the references for more details):

- "plpd": uses the lpd based on point estimates (i.e., \(p(y_i|\hat{\theta})\)).
- "lpd": uses the lpd's (i.e., \(p(y_i|y)\)).
- "tis": uses truncated importance sampling to approximate PSIS-LOO.
- "waic": uses waic (i.e., \(p(y_i|\hat{\theta}) - p_{\text{waic}}\)).
- "waic\_grad\_marginal": uses waic approximation using first order delta method and posterior marginal variances to approximate \(p_{\text{waic}}\) (i.e. \(p(y_i|\hat{\theta})-p_{\text{waic\_grad\_marginal}}\)). Requires gradient of likelihood function.
- "waic\_grad": uses waic approximation using first order delta method and posterior covariance to approximate \(p_{\text{waic}}\) (i.e. \(p(y_i|\hat{\theta})-p_{\text{waic\_grad}}\)). Requires gradient of likelihood function.
- "waic\_hess": uses waic approximation using second order delta method and posterior covariance to approximate \(p_{\text{waic}}\) (i.e. \(p(y_i|\hat{\theta})-p_{\text{waic\_hess}}\)). Requires gradient and Hessian of likelihood function.

As point estimates of \(\hat{\theta}\), the posterior expectations of the parameters are used.

**loo_approximation\_draws**

The number of posterior draws used when integrating over the posterior. This is used if `loo_approximation` is set to "lpdf", "waic", or "tis".

**llgrad**

The gradient of the log-likelihood. This is only used when `loo_approximation` is "waic\_grad", "waic\_grad\_marginal", or "waic\_hess". The default is NULL.

**llhess**

The Hessian of the log-likelihood. This is only used with `loo_approximation` = "waic\_hess". The default is NULL.
Details

If observations is updated then if a vector of indices or a psis_loo_ss object is supplied the updated object will have exactly the observations indicated by the vector or psis_loo_ss object. If a single integer is supplied, new observations will be sampled to reach the supplied sample size.

Value

A psis_loo_ss object.

Description

The waic() methods can be used to compute WAIC from the pointwise log-likelihood. However, we recommend LOO-CV using PSIS (as implemented by the loo() function) because PSIS provides useful diagnostics as well as effective sample size and Monte Carlo estimates.

Usage

waic(x, ...)

## S3 method for class 'array'
waic(x, ...)

## S3 method for class 'matrix'
waic(x, ...)

## S3 method for class `function`
waic(x, ..., data = NULL, draws = NULL)

is.waic(x)

Arguments

x A log-likelihood array, matrix, or function. The Methods (by class) section, below, has detailed descriptions of how to specify the inputs for each method.
draws, data, ... For the function method only. See the Methods (by class) section below for details on these arguments.

Value

A named list (of class c("waic", "loo")) with components:
estimates A matrix with two columns ("Estimate", "SE") and three rows ("elpd_waic", "p_waic", "waic"). This contains point estimates and standard errors of the expected log pointwise predictive density (elpd_waic), the effective number of parameters (p_waic) and the information criterion waic (which is just $-2 \times \text{elpd_waic}$, i.e., converted to deviance scale).
pointwise A matrix with three columns (and number of rows equal to the number of observations) containing the pointwise contributions of each of the above measures (elpd_waic, p_waic, waic).

Methods (by class)

- **waic(array)**: An $I$ by $C$ by $N$ array, where $I$ is the number of MCMC iterations per chain, $C$ is the number of chains, and $N$ is the number of data points.

- **waic(matrix)**: An $S$ by $N$ matrix, where $S$ is the size of the posterior sample (with all chains merged) and $N$ is the number of data points.

- **waic(`function`)**: A function $f()$ that takes arguments data_i and draws and returns a vector containing the log-likelihood for a single observation $i$ evaluated at each posterior draw. The function should be written such that, for each observation $i$ in $1:N$, evaluating

  \[
  f(data_i = data[i,, drop=FALSE], draws = draws)
  \]

  results in a vector of length $S$ (size of posterior sample). The log-likelihood function can also have additional arguments but data_i and draws are required.

  If using the function method then the arguments data and draws must also be specified in the call to loo():

  - data: A data frame or matrix containing the data (e.g. observed outcome and predictors) needed to compute the pointwise log-likelihood. For each observation $i$, the $i$th row of data will be passed to the data_i argument of the log-likelihood function.

  - draws: An object containing the posterior draws for any parameters needed to compute the pointwise log-likelihood. Unlike data, which is indexed by observation, for each observation the entire object draws will be passed to the draws argument of the log-likelihood function.

  - The ... can be used if your log-likelihood function takes additional arguments. These arguments are used like the draws argument in that they are recycled for each observation.

References


See Also

- The **loo** package vignettes and Vehtari, Gelman, and Gabry (2017) and Vehtari, Simpson, Gelman, Yao, and Gabry (2024) for more details on why we prefer loo() to waic().

- **loo_compare()** for comparing models on approximate LOO-CV or WAIC.
Examples

```r
### Array and matrix methods
LLarr <- example_loglik_array()
dim(LLarr)

LLmat <- example_loglik_matrix()
dim(LLmat)

waic_arr <- waic(LLarr)
waic_mat <- waic(LLmat)
identical(waic_arr, waic_mat)

## Not run:
log_lik1 <- extract_log_lik(stanfit1)
log_lik2 <- extract_log_lik(stanfit2)
(waic1 <- waic(log_lik1))
(waic2 <- waic(log_lik2))
print(compare(waic1, waic2), digits = 2)

## End(Not run)
```

weights.importance_sampling

*Extract importance sampling weights*

### Description

Extract importance sampling weights

### Usage

```r
## S3 method for class 'importance_sampling'
weights(object, ..., log = TRUE, normalize = TRUE)
```

#### Arguments

- **object**: An object returned by `psis()`, `tis()`, or `sis()`.
- **...**: Ignored.
- **log**: Should the weights be returned on the log scale? Defaults to `TRUE`.
- **normalize**: Should the weights be normalized? Defaults to `TRUE`.

#### Value

The `weights()` method returns an object with the same dimensions as the `log_weights` component of `object`. The `normalize` and `log` arguments control whether the returned weights are normalized and whether or not to return them on the log scale.
Examples

# See the examples at help("psis")
Index

ap_psis, 5
attributes, 54, 60, 62

crps, 7
crps(), 6

Kline (loo-datasets), 25

loo, 19
loo(), 3, 6, 29–31, 34–36, 39, 41, 44, 46, 48, 50–52, 55–57, 60, 62, 65
loo-datasets, 25
loo-glossary, 26
loo-package, 3
loo.function(), 56
loo_approximate_posterior, 28
loo_approximate_posterior(), 44, 51
loo_compare, 31
loo_compare(), 6, 17, 18, 23, 31, 46, 66
loo_crps (crps), 7
loo_i (loo), 19
loo_model_weights, 33
loo_model_weights(), 3
loo_moment_match, 37
loo_moment_match(), 41, 50, 51
loo_moment_match_split, 40
loo_moment_match_split(), 39
loo_predictive_metric, 41
loo_scrps (crps), 7
loo_subsample, 43
loo_subsample(), 51
loo_subsample.function(), 63

mcse_elpd_loo, 22
mcse_loo (pareto-k-diagnostic), 48
milk (loo-datasets), 25

nobs_psis_loo_ss, 47

obs_idx, 47

pareto_k, 13, 14
pareto_k-diagnostic, 16, 22, 23, 48, 52–56, 60, 62
pareto_k_ids (pareto-k-diagnostic), 48

69
pareto_k_influence_values
  (pareto-k-diagnostic), 48
pareto_k_table (pareto-k-diagnostic), 48
pareto_k_values (pareto-k-diagnostic), 48
plot(), 52
plot.loo (pareto-k-diagnostic), 48
plot.psis (pareto-k-diagnostic), 48
plot.psis_loo (pareto-k-diagnostic), 48
plot.psis_loo(), 52
pointwise, 51
print.compare.loo (loo_compare), 31
print.compare.loo_ss (loo_compare), 31
print.importance_sampling (print.loo), 52
print.importance_sampling_loo
  (print.loo), 52
print.loo, 52
print.psis (print.loo), 52
print.psis_loo (print.loo), 52
print.psis_loo_ap (print.loo), 52
print.waic (print.loo), 52
pseudobma_weights (loo_model_weights), 33
PSIS, 13, 19
psis, 53
psis(), 3, 9, 13, 16, 21–23, 31, 34, 42, 46, 48,
  50–52, 55, 57, 60, 62, 67
psis_n_eff_values
  (pareto-k-diagnostic), 48
psislw, 55
relative_eff, 56
relative_eff(), 17, 21, 34, 36, 44, 53, 59,
  61, 64
scrps (crps), 7
se_diff, 32
sis, 58
sis(), 67
stacking_weights (loo_model_weights), 33
stats::constrOptim(), 34
stats::optim(), 34
tis, 61
tis(), 67
update.psis_loo_ss, 63
voice (loo-datasets), 25
voice_loo (loo-datasets), 25
waic, 65
waic(), 6, 52
weights(), 54, 59, 62
weights.importance_sampling, 67