# Package 'projpred'

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**Encoding UTF-8** 

Version 2.9.1

**Title** Projection Predictive Feature Selection

```
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Description Performs projection predictive feature selection for generalized linear
      models (Piironen, Paasiniemi, and Vehtari, 2020, <doi:10.1214/20-EJS1711>)
      with or without multilevel or additive terms (Catalina, Bürkner, and
      Vehtari, 2022, <a href="https://proceedings.mlr.press/v151/catalina22a.html">https://proceedings.mlr.press/v151/catalina22a.html</a>), for
      some ordinal and nominal regression models (Weber, Glass, and Vehtari, 2025,
      <a href="https://doi:10.1007/s00180-024-01506-0">doi:10.1007/s00180-024-01506-0</a>), and for many other regression models
      (using the latent projection by Catalina, Bürkner, and Vehtari, 2021,
      <doi:10.48550/arXiv.2109.04702>, which can also be applied to most of the
      former models). The package is compatible with the 'rstanarm' and 'brms'
      packages, but other reference models can also be used. See the vignettes and
      the documentation for more information and examples.
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URL https://mc-stan.org/projpred/, https://discourse.mc-stan.org
BugReports https://github.com/stan-dev/projpred/issues/
Depends R (>= 3.6.0)
Imports methods, utils, Rcpp, gtools, ggplot2, scales, rstantools (>=
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      abind, MASS, ordinal, nnet, mclogit
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2 Contents

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NeedsCompilation yes
Author Juho Piironen [aut],
Markus Paasiniemi [aut],
Alejandro Catalina [aut],
Frank Weber [aut],
Osvaldo Martin [cre, aut],
Aki Vehtari [aut],
Jonah Gabry [ctb],
Marco Colombo [ctb],
Paul-Christian Bürkner [ctb],
Hamada S. Badr [ctb],
Brian Sullivan [ctb],
Sölvi Rögnvaldsson [ctb],
The LME4 Authors [cph] (see file 'LICENSE' for details),
Yann McLatchie [ctb],
Juho Timonen [ctb]
Maintainer Osvaldo Martin <aloctavodia@gmail.com></aloctavodia@gmail.com>
Repository CRAN

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# Contents

projpred-package
as.matrix.projection
as_draws_matrix.projection
augdat_ilink_binom
augdat_link_binom
break_up_matrix_term
cl_agg
cv-indices
cv_proportions
cv_varsel
df_binom
df_gaussian
extend_family
extra-families
force_search_terms
mesquite
performances
plot.cv_proportions
plot.vsel
pred-projection
predict.refmodel
predictor_terms
print.projection

-package	

proj	pred-package	Pro	ojec	tio	n p	re	dic	tiv	e f	<sup>f</sup> ea	tu	re	se	lec	etic	on													
Index																													7:
	y_wobs_offs			•		•		•	•		•	•	•		•	•	•	•	 •	•	•	•	•	 •	•	•	•	•	/.
	varsel																												
	summary.vsel																												
	suggest_size																												
	solution_terms																												
	run_cvfun																												59
	refmodel-init-get .																												52
	ranking																											. 4	51
	project																											. 4	48
	print.vselsummary																											. 4	4
	print.vsel																											. 4	4
	print.refmodel																											. 4	40

# **Description**

The R package **projpred** performs the projection predictive variable (or "feature") selection for various regression models. We recommend to read the README file (available with enhanced formatting **online**) and the main vignette (topic = "projpred", but also available **online**) before continuing here.

# **Terminology**

Throughout the whole package documentation, we use the term "submodel" for all kinds of candidate models onto which the reference model is projected. For custom reference models, the candidate models don't need to be actual *sub* models of the reference model, but in any case (even for custom reference models), the candidate models are always actual *sub* models of the full formula used by the search procedure. In this regard, it is correct to speak of *sub* models, even in case of a custom reference model.

The following model type abbreviations will be used at multiple places throughout the documentation: GLM (generalized linear model), GLMM (generalized linear multilevel—or "mixed"—model), GAM (generalized additive model), and GAMM (generalized additive multilevel—or "mixed"—model). Note that the term "generalized" includes the Gaussian family as well.

# Draw-wise divergence minimizers

For the projection of the reference model onto a submodel, **projpred** currently relies on the following functions as draw-wise divergence minimizers (in other words, these are the workhorse functions employed by **projpred**'s internal default div\_minimizer functions, see init\_refmodel()):

• Submodel without multilevel or additive terms:

4 projpred-package

For the traditional (or latent) projection (or the augmented-data projection in case of the binomial() or brms::bernoulli() family): An internal C++ function which basically serves the same purpose as lm() for the gaussian() family and glm() for all other families. The returned object inherits from class subfit. Possible tuning parameters for this internal C++ function are: regul (amount of ridge regularization; default: 1e-4), thresh\_conv (convergence threshold; default: 1e-7), qa\_updates\_max (maximum number of quadratic approximation updates; default: 100, but fixed to 1 in case of the Gaussian family with identity link), ls\_iter\_max (maximum number of line search iterations; default: 30, but fixed to 1 in case of the Gaussian family with identity link), normalize (single logical value indicating whether to scale the predictors internally with the returned regression coefficient estimates being back-adjusted appropriately; default: TRUE), beta0\_init (single numeric value giving the starting value for the intercept at centered predictors; default: 0), and beta\_init (numeric vector giving the starting values for the regression coefficients; default: vector of 0s).

- For the augmented-data projection: MASS::polr() (the returned object inherits from class polr) for the brms::cumulative() family or rstanarm::stan\_polr() fits, nnet::multinom() (the returned object inherits from class multinom) for the brms::categorical() family.
- Submodel with multilevel but no additive terms:
  - For the traditional (or latent) projection (or the augmented-data projection in case of the binomial() or brms::bernoulli() family): lme4::lmer() (the returned object inherits from class lmerMod) for the gaussian() family, lme4::glmer() (the returned object inherits from class glmerMod) for all other families.
  - For the augmented-data projection: ordinal::clmm() (the returned object inherits from class clmm) for the brms::cumulative() family, mclogit::mblogit() (the returned object inherits from class mmblogit) for the brms::categorical() family.
- Submodel without multilevel but additive terms: mgcv::gam() (the returned object inherits from class gam).
- Submodel with multilevel and additive terms: gamm4::gamm4() (within **projpred**, the returned object inherits from class gamm4).

#### Verbosity, messages, warnings, errors

Global option projpred. verbose may be used for specifying the value passed to argument verbose of project(), varsel(), and cv\_varsel().

By default, **projpred** catches messages and warnings from the draw-wise divergence minimizers and throws their unique collection after performing all draw-wise divergence minimizations (i.e., draw-wise projections). This can be deactivated by setting global option projpred.warn\_proj\_drawwise to FALSE.

Furthermore, by default, **projpred** checks the convergence of the draw-wise divergence minimizers and throws a warning if any seem to have not converged. This warning is thrown after the warning message from global option projpred.warn\_proj\_drawwise (see above) and can be deactivated by setting global option projpred.check\_convergence to FALSE.

# Parallelization

The projection of the reference model onto a submodel can be run in parallel (across the projected draws). This is powered by the **foreach** package. Thus, any parallel (or sequential) backend compatible with **foreach** can be used, e.g., the backends from packages **doParallel**, **doMPI**, or **doFuture**.

projpred-package 5

Using the global option projpred.parallel\_proj\_trigger, the number of projected draws below which no parallelization is applied (even if a parallel backend is registered) can be modified. Such a "trigger" threshold exists because of the computational overhead of a parallelization which makes the projection parallelization only useful for a sufficiently large number of projected draws. By default, the projection parallelization is turned off, which can also be achieved by supplying Inf (or NULL) to option projpred.parallel\_proj\_trigger. Note that we cannot recommend the projection parallelization on Windows because in our experience, the parallelization overhead is larger there, causing a parallel run to take longer than a sequential run. Also note that the projection parallelization works well for submodels which are GLMs (and hence also for the latent projection if the submodel has no multilevel or additive predictor terms), but for all other types of submodels, the fitted submodel objects are quite big, which—when running in parallel—may lead to excessive memory usage which in turn may crash the R session (on Unix systems, setting an appropriate memory limit via unix::rlimit\_as() may avoid crashing the whole machine). Thus, we currently cannot recommend parallelizing projections onto submodels which are GLMs (in this context, the latent projection onto a submodel without multilevel and without additive terms may be regarded as a projection onto a submodel which is a GLM). However, for cv\_varsel(), there is also a CV parallelization (i.e., a parallelization of projpred's cross-validation) which can be activated via argument parallel (which in turn can be controlled via global option projpred.parallel\_cv).

For the CV parallelization, global option projpred.export\_to\_workers may be set to a character vector of names of objects to export from the global environment to the parallel workers.

During parallelization (either of the projection or the CV), progression updates can be received via the **progressr** package. This only works if the **doFuture** backend is used for parallelization, e.g., via doFuture::registerDoFuture() and future::plan(future::multisession, workers = 4). In that case, the **progressr** package can be used, e.g., by calling progressr::handlers(global = TRUE) before running the projection or the CV in parallel. The **projpred** package also offers the global option projpred.use\_progressr for controlling whether to use the **progressr** package (TRUE or FALSE), but since that global option defaults to requireNamespace("progressr", quietly = TRUE) && interactive() && identical(foreach::getDoParName(), "doFuture"), it usually does not need to be set by the user.

# Multilevel models: "Integrating out" group-level effects

In case of multilevel models, **projpred** offers two global options for "integrating out" group-level effects: projpred.mlvl\_pred\_new and projpred.mlvl\_proj\_ref\_new. When setting projpred.mlvl\_pred\_new to TRUE (default is FALSE), then at prediction time, projpred will treat group levels existing in the training data as new group levels, implying that their group-level effects are drawn randomly from a (multivariate) Gaussian distribution. This concerns both, the reference model and the (i.e., any) submodel. Furthermore, setting projpred.mlvl\_pred\_new to TRUE causes as.matrix.projection() and as\_draws\_matrix.projection() to omit the projected group-level effects (for the group levels from the original dataset). When setting projpred.mlvl\_proj\_ref\_new to TRUE (default is FALSE), then at projection time, the reference model's fitted values (that the submodels fit to) will be computed by treating the group levels from the original dataset as new group levels, implying that their group-level effects will be drawn randomly from a (multivariate) Gaussian distribution (as long as the reference model is a multilevel model, which—for custom reference models—does not need to be the case). This also affects the latent response values for a latent projection correspondingly. Setting projpred.mlvl\_pred\_new to TRUE makes sense, e.g., when the prediction task is such that any group level will be treated as a new one. Typically, setting projpred.mlvl\_proj\_ref\_new to TRUE only makes sense when projpred.mlvl\_pred\_new is already set to TRUE. In that case, the de6 projpred-package

fault of FALSE for projpred.mlvl\_proj\_ref\_new ensures that at projection time, the submodels fit to the best possible fitted values from the reference model, and setting projpred.mlvl\_proj\_ref\_new to TRUE would make sense if the group-level effects should be integrated out completely.

## Memory usage

By setting the global option projpred.run\_gc to TRUE, **projpred** will call gc() at some places (e.g., after each size that the forward search passes through) to free up some memory. These gc() calls are not always necessary to reduce the peak memory usage, but they add runtime (hence the default of FALSE for that global option).

#### Other notes

Global option projpred.digits controls arguments digits of print.vselsummary() and print.vsel().

There are several global options to control arguments of plot.vsel() and plot.cv\_proportions() globally, see section "Usage" of the help pages of these two functions.

Global option projpred.warn\_L1\_interactions may be set to FALSE to deactivate a warning that an L1 search selected an interaction term before all involved lower-order interaction terms (including main-effect terms) were selected (in which case the predictor ranking is automatically modified by **projpred** so that the lower-order interaction terms come before this interaction term).

Most examples are not executed when called via example(). To execute them, their code has to be copied and pasted manually to the console.

#### **Functions**

init\_refmodel(), get\_refmodel() For setting up an object containing information about the reference model, the submodels, and how the projection should be carried out. Explicit calls to
 init\_refmodel() and get\_refmodel() are only rarely needed.

varsel(), cv\_varsel() For running the *search* part and the *evaluation* part for a projection predictive variable selection, possibly with cross-validation (CV).

summary.vsel(), print.vsel(), plot.vsel(), suggest\_size.vsel(), ranking(), cv\_proportions(), plot.cv\_prop
For post-processing the results from varsel() and cv\_varsel().

project() For projecting the reference model onto submodel(s). Typically, this follows the variable selection, but it can also be applied directly (without a variable selection).

as.matrix.projection() and as\_draws\_matrix.projection() For extracting projected parameter draws.

proj\_linpred(), proj\_predict() For making predictions from a submodel (after projecting the reference model onto it).

# Author(s)

Maintainer: Osvaldo Martin <aloctavodia@gmail.com>

Authors:

- Juho Piironen < juho.t.piironen@gmail.com>
- · Markus Paasiniemi

as.matrix.projection 7

- Alejandro Catalina <alecatfel@gmail.com>
- · Frank Weber
- Aki Vehtari

#### Other contributors:

- Jonah Gabry [contributor]
- Marco Colombo [contributor]
- Paul-Christian Bürkner [contributor]
- Hamada S. Badr [contributor]
- Brian Sullivan [contributor]
- Sölvi Rögnvaldsson [contributor]
- The LME4 Authors (see file 'LICENSE' for details) [copyright holder]
- Yann McLatchie [contributor]
- Juho Timonen [contributor]

# See Also

#### Useful links:

```
• https://mc-stan.org/projpred/
```

```
• https://discourse.mc-stan.org
```

• Report bugs at https://github.com/stan-dev/projpred/issues/

as.matrix.projection Extract projected parameter draws and coerce to matrix

# **Description**

This is the as.matrix() method for projection objects (returned by project(), possibly as elements of a list). It extracts the projected parameter draws and returns them as a matrix. In case of different (i.e., nonconstant) weights for the projected draws, see as\_draws\_matrix.projection() for a better solution.

# Usage

```
## S3 method for class 'projection'
as.matrix(x, nm_scheme = NULL, allow_nonconst_wdraws_prj = FALSE, ...)
```

8 as.matrix.projection

## **Arguments**

x An object of class projection (returned by project(), possibly as elements of a list).

nm\_scheme The naming scheme for the columns of the output matrix. Either NULL, "rstanarm",

or "brms", where NULL chooses "rstanarm" or "brms" based on the class of the reference model fit (and uses "rstanarm" if the reference model fit is of an un-

known class).

allow\_nonconst\_wdraws\_prj

A single logical value indicating whether to allow projected draws with different (i.e., nonconstant) weights (TRUE) or not (FALSE). **CAUTION**: Expert use only because if set to TRUE, the weights of the projected draws are stored in an attribute wdraws\_prj and handling this attribute requires special care (e.g., when

subsetting the returned matrix).

... Currently ignored.

#### **Details**

In case of the augmented-data projection for a multilevel submodel of a brms::categorical() reference model, the multilevel parameters (and therefore also their names) slightly differ from those in the **brms** reference model fit (see section "Augmented-data projection" in extend\_family()'s documentation).

## Value

An  $S_{\rm prj} \times Q$  matrix of projected draws, with  $S_{\rm prj}$  denoting the number of projected draws and Q the number of parameters. If allow\_nonconst\_wdraws\_prj is set to TRUE, the weights of the projected draws are stored in an attribute wdraws\_prj. (If allow\_nonconst\_wdraws\_prj is FALSE, projected draws with nonconstant weights cause an error.)

# **Examples**

```
# the projpred::as.matrix.projection() method:
prj_mat <- as.matrix(prj)

# Since the draws have all the same weight here, we can treat them like
# ordinary MCMC draws, e.g., we can summarize them using the `posterior`
# package:
if (requireNamespace("posterior", quietly = TRUE)) {
    print(posterior::summarize_draws(
        posterior::as_draws_matrix(prj_mat),
        "median", "mad", function(x) quantile(x, probs = c(0.025, 0.975))
    ))
}

# Or visualize them using the `bayesplot` package:
if (requireNamespace("bayesplot", quietly = TRUE)) {
    print(bayesplot::mcmc_intervals(prj_mat))
}</pre>
```

as\_draws\_matrix.projection

Extract projected parameter draws and coerce to draws\_matrix (see package posterior)

# **Description**

These are the posterior::as\_draws() and posterior::as\_draws\_matrix() methods for projection objects (returned by project(), possibly as elements of a list). They extract the projected parameter draws and return them as a draws\_matrix. In case of different (i.e., nonconstant) weights for the projected draws, a draws\_matrix allows for a safer handling of these weights (safer in contrast to the matrix returned by as.matrix.projection()), in particular by providing the natural input for posterior::resample\_draws() (see section "Examples" below).

# Usage

```
## S3 method for class 'projection'
as_draws_matrix(x, ...)
## S3 method for class 'projection'
as_draws(x, ...)
```

## Arguments

An object of class projection (returned by project(), possibly as elements of a list).

... Arguments passed to as.matrix.projection(), except for allow\_nonconst\_wdraws\_prj.

## **Details**

In case of the augmented-data projection for a multilevel submodel of a brms::categorical() reference model, the multilevel parameters (and therefore also their names) slightly differ from those in the **brms** reference model fit (see section "Augmented-data projection" in extend\_family()'s documentation).

#### Value

An  $S_{\text{prj}} \times Q$  draws\_matrix (see posterior::draws\_matrix()) of projected draws, with  $S_{\text{prj}}$  denoting the number of projected draws and Q the number of parameters. If the projected draws have nonconstant weights, posterior::weight\_draws() is applied internally.

## **Examples**

```
# Data:
dat_gauss <- data.frame(y = df_gaussian$y, df_gaussian$x)</pre>
# The `stanreg` fit which will be used as the reference model (with small
# values for `chains` and `iter`, but only for technical reasons in this
# example; this is not recommended in general):
fit <- rstanarm::stan_glm(</pre>
 y \sim X1 + X2 + X3 + X4 + X5, family = gaussian(), data = dat_gauss,
 QR = TRUE, chains = 2, iter = 500, refresh = 0, seed = 9876
)
# Projection onto an arbitrary combination of predictor terms (with a small
# value for `nclusters`, but only for illustrative purposes; this is not
# recommended in general):
prj <- project(fit, predictor_terms = c("X1", "X3", "X5"), nclusters = 5,</pre>
               seed = 9182)
# Applying the posterior::as_draws_matrix() generic to the output of
# project() dispatches to the projpred::as_draws_matrix.projection()
# method:
prj_draws <- posterior::as_draws_matrix(prj)</pre>
# Resample the projected draws according to their weights:
set.seed(3456)
prj_draws_resampled <- posterior::resample_draws(prj_draws, ndraws = 1000)</pre>
# The values from the following two objects should be the same (in general,
# this only holds approximately):
print(proportions(table(rownames(prj_draws_resampled))))
print(weights(prj_draws))
# Treat the resampled draws like ordinary draws, e.g., summarize them:
print(posterior::summarize_draws(
 prj_draws_resampled,
  "median", "mad", function(x) quantile(x, probs = c(0.025, 0.975))
))
# Or visualize them using the `bayesplot` package:
```

augdat\_ilink\_binom 11

```
if (requireNamespace("bayesplot", quietly = TRUE)) {
  print(bayesplot::mcmc_intervals(prj_draws_resampled))
}
```

# Description

This is the function which has to be supplied to extend\_family()'s argument augdat\_ilink in case of the augmented-data projection for the binomial() family.

# Usage

```
augdat_ilink_binom(eta_arr, link = "logit")
```

## **Arguments**

eta\_arr An array as described in section "Augmented-data projection" of extend\_family()'s

documentation.

link The same as argument link of binomial().

## Value

An array as described in section "Augmented-data projection" of extend\_family()'s documentation.

augdat\_link\_binom Link function for augmented-data projection with binomial family

# **Description**

This is the function which has to be supplied to extend\_family()'s argument augdat\_link in case of the augmented-data projection for the binomial() family.

## Usage

```
augdat_link_binom(prb_arr, link = "logit")
```

#### **Arguments**

prb\_arr An array as described in section "Augmented-data projection" of extend\_family()'s

documentation.

link The same as argument link of binomial().

12 *cl\_agg* 

# Value

An array as described in section "Augmented-data projection" of extend\_family()'s documentation.

```
break_up_matrix_term Break up matrix terms
```

# **Description**

Sometimes there can be terms in a formula that refer to a matrix instead of a single predictor. This function breaks up the matrix term into individual predictors to handle separately, as that is probably the intention of the user.

# Usage

```
break_up_matrix_term(formula, data)
```

## **Arguments**

formula A formula for a valid model.

data The original data. frame with a matrix as predictor.

## Value

A list containing the expanded formula and the expanded data. frame.

cl\_agg

Weighted averaging within clusters of parameter draws

# **Description**

This function aggregates S parameter draws that have been clustered into  $S_{\rm cl}$  clusters by averaging across the draws that belong to the same cluster. This averaging can be done in a weighted fashion.

# Usage

```
cl_agg(
  draws,
  cl = seq_len(nrow(draws)),
  wdraws = rep(1, nrow(draws)),
  eps_wdraws = 0
)
```

cv-indices 13

# Arguments

cl

draws An  $S \times P$  matrix of parameter draws, with P denoting the number of parameters.

A numeric vector of length S, giving the cluster indices for the draws. The cluster indices need to be values from the set  $\{1, ..., S_{cl}\}$ , except for draws that should be dropped (e.g., by thinning), in which case NA needs to be provided at

the positions of cl corresponding to these draws.

wdraws A numeric vector of length S, giving the weights of the draws. It doesn't matter

whether these are normalized (i.e., sum to 1) or not because internally, these weights are normalized to sum to 1 within each cluster. Draws that should be dropped (e.g., by thinning) can (but must not necessarily) have an NA in wdraws.

eps\_wdraws A positive numeric value (typically small) which will be used to improve numer-

ical stability: The weights of the draws within each cluster are multiplied by 1 – eps\_wdraws. The default of 0 should be fine for most cases; this argument only exists to help in those cases where numerical instabilities occur (which must be detected by the user; this function will not detect numerical instabilities itself).

#### Value

An  $S_{\rm cl} \times P$  matrix of aggregated parameter draws.

## **Examples**

```
set.seed(323)
S <- 100L
P <- 3L
draws <- matrix(rnorm(S * P), nrow = S, ncol = P)</pre>
# Clustering example:
S_cl <- 10L
cl_draws <- sample.int(S_cl, size = S, replace = TRUE)</pre>
draws_cl <- cl_agg(draws, cl = cl_draws)</pre>
# Clustering example with nonconstant `wdraws`:
w_draws <- rgamma(S, shape = 4)</pre>
draws_cl <- cl_agg(draws, cl = cl_draws, wdraws = w_draws)</pre>
# Thinning example (implying constant `wdraws`):
S_th <- 50L
idxs_thin <- round(seq(1, S, length.out = S_th))
th_draws <- rep(NA, S)
th_draws[idxs_thin] <- seq_len(S_th)</pre>
draws_th <- cl_agg(draws, cl = th_draws)</pre>
```

14 cv-indices

## **Description**

These are helper functions to create cross-validation (CV) folds, i.e., to split up the indices from 1 to n into K subsets ("folds") for K-fold CV. These functions are potentially useful when creating the input for arguments cvfits and cvfun of init\_refmodel() (or argument cvfits of cv\_varsel.refmodel()). Function cvfolds() is deprecated; please use cv\_folds() instead (apart from the name, they are the same). The return value of cv\_folds() and cv\_ids() is different, see below for details.

# Usage

```
cv_folds(n, K, seed = NA)
cvfolds(n, K, seed = NA)
cv_ids(n, K, out = c("foldwise", "indices"), seed = NA)
```

# **Arguments**

n	Number of observations.
K	Number of folds. Must be at least 2 and not exceed n.
seed	Pseudorandom number generation (PRNG) seed by which the same results can be obtained again if needed. Passed to argument seed of set.seed(), but can also be NA to not call set, seed() at all. If not NA, then the PRNG state is reset

also be NA to not call set.seed() at all. If not NA, then the PRNG state is reset (to the state before calling cv\_folds() or cv\_ids()) upon exiting cv\_folds()

Format of the output, either "foldwise" or "indices". See below for details. out

## Value

cv\_folds() returns a vector of length n such that each element is an integer between 1 and K denoting which fold the corresponding data point belongs to. The return value of cv\_ids() depends on the out argument. If out = "foldwise", the return value is a list with K elements, each being a list with elements tr and ts giving the training and test indices, respectively, for the corresponding fold. If out = "indices", the return value is a list with elements tr and ts each being a list with K elements giving the training and test indices, respectively, for each fold.

## **Examples**

```
n <- 100
set.seed(1234)
y <- rnorm(n)
cv \leftarrow cv_ids(n, K = 5)
# Mean within the test set of each fold:
cvmeans <- sapply(cv, function(fold) mean(y[fold$ts]))</pre>
```

cv\_proportions 15

cv_proportions	Ranking proportions from fold-wise predictor rankings
	3 F - F

# **Description**

Calculates the ranking proportions from the fold-wise predictor rankings in a cross-validation (CV) with fold-wise searches. For a given predictor x and a given submodel size j, the ranking proportion is the proportion of CV folds which have predictor x at position j of their predictor ranking. While these ranking proportions are helpful for investigating variability in the predictor ranking, they can also be *cumulated* across submodel sizes. The cumulated ranking proportions are more helpful when it comes to model selection.

# Usage

```
cv_proportions(object, ...)
## S3 method for class 'ranking'
cv_proportions(object, cumulate = FALSE, ...)
## S3 method for class 'vsel'
cv_proportions(object, ...)
```

# **Arguments**

object	For cv_proportions.ranking(): an object of class ranking (returned by ranking()). For cv_proportions.vsel(): an object of class vsel (returned by varsel()) or cv_varsel()) that ranking() will be applied to internally before then calling cv_proportions.ranking().
•••	For cv_proportions.vsel(): arguments passed to ranking.vsel() and cv_proportions.ranking(). For cv_proportions.ranking(): currently ignored.
cumulate	A single logical value indicating whether the ranking proportions should be cumulated across increasing submodel sizes (TRUE) or not (FALSE).

## Value

A numeric matrix containing the ranking proportions. This matrix has nterms\_max rows and nterms\_max columns, with nterms\_max as specified in the (possibly implicit) ranking() call. The rows correspond to the submodel sizes and the columns to the predictor terms (sorted according to the full-data predictor ranking). If cumulate is FALSE, then the returned matrix is of class cv\_proportions. If cumulate is TRUE, then the returned matrix is of classes cv\_proportions\_cumul and cv\_proportions (in this order).

Note that if cumulate is FALSE, then the values in the returned matrix only need to sum to 1 (column-wise and row-wise) if nterms\_max (see above) is equal to the full model size. Likewise, if cumulate is TRUE, then the value 1 only needs to occur in each column of the returned matrix if nterms\_max is equal to the full model size.

The cv\_proportions() function is only applicable if the ranking object includes fold-wise predictor rankings (i.e., if it is based on a vsel object created by cv\_varsel() with validate\_search = TRUE). If the ranking object contains only a full-data predictor ranking (i.e., if it is based on a vsel object created by varsel() or by cv\_varsel(), but the latter with validate\_search = FALSE), then an error is thrown because in that case, there are no fold-wise predictor rankings from which to calculate ranking proportions.

#### See Also

```
plot.cv_proportions()
```

## **Examples**

```
# For an example, see `?plot.cv_proportions`.
```

cv\_varsel

Run search and performance evaluation with cross-validation

## **Description**

Run the *search* part and the *evaluation* part for a projection predictive variable selection. The search part determines the predictor ranking (also known as solution path), i.e., the best submodel for each submodel size (number of predictor terms). The evaluation part determines the predictive performance of the submodels along the predictor ranking. In contrast to varsel(), cv\_varsel() performs a cross-validation (CV) by running the search part with the training data of each CV fold separately (an exception is explained in section "Note" below) and by running the evaluation part on the corresponding test set of each CV fold. A special method is cv\_varsel.vsel() because it re-uses the search results from an earlier cv\_varsel() (or varsel()) run, as illustrated in the main vignette.

## Usage

```
cv_varsel(object, ...)
## Default S3 method:
cv_varsel(object, ...)

## S3 method for class 'vsel'
cv_varsel(
  object,
  cv_method = object$cv_method %||% "L00",
  nloo = object$nloo,
  K = object$K %||% if (!inherits(object, "datafit")) 5 else 10,
  cvfits = object$cvfits,
  validate_search = object$validate_search %||% TRUE,
  ...
```

```
)
## S3 method for class 'refmodel'
cv_varsel(
  object,
 method = "forward",
  cv_method = if (!inherits(object, "datafit")) "L00" else "kfold",
  ndraws = NULL,
  nclusters = 20.
  ndraws_pred = 400,
  nclusters_pred = NULL,
  refit_prj = !inherits(object, "datafit"),
  nterms_max = NULL,
  penalty = NULL,
  verbose = getOption("projpred.verbose", as.integer(interactive())),
  nloo = if (cv_method == "LOO") object$nobs else NULL,
 K = if (!inherits(object, "datafit")) 5 else 10,
  cvfits = object$cvfits,
  search_control = NULL,
  lambda_min_ratio = 1e-05,
  nlambda = 150,
  thresh = 1e-06,
  validate_search = TRUE,
  seed = NA,
  search_terms = NULL,
  search_out = NULL,
  parallel = getOption("projpred.parallel_cv", FALSE),
)
```

## **Arguments**

object An object of class refmodel (returned by get\_refmodel() or init\_refmodel()) or an object that can be passed to argument object of get\_refmodel().

For cv\_varsel.default(): Arguments passed to get\_refmodel() as well as to cv\_varsel.refmodel(). For cv\_varsel.vsel(): Arguments passed to cv\_varsel.refmodel(). For cv\_varsel.refmodel(): Arguments passed to the divergence minimizer (see argument div\_minimizer of init\_refmodel() as well as section "Draw-wise divergence minimizers" of projpred-package) when refitting the submodels for the performance evaluation (if refit\_prj is

TRUE).

The CV method, either "L00" or "kfold". In the "L00" case, a Pareto-smoothed importance sampling leave-one-out CV (PSIS-LOO CV) is performed, which avoids refitting the reference model nloo times (in contrast to a standard LOO-CV). In the "kfold" case, a *K*-fold CV is performed. See also section "Note" below.

Only relevant if cv\_method = "LOO" and validate\_search = TRUE. If nloo > 0 is smaller than the number of all observations, full LOO-CV (i.e., PSIS-LOO CV

nloo

cv\_method

> with validate\_search = TRUE and with nloo = n where n denotes the number of all observations) is approximated by subsampled LOO-CV, i.e., by combining the fast (i.e., validate\_search = FALSE) LOO result for the selected models and nloo leave-one-out searches using the difference estimator with simple random sampling (SRS) without replacement (WOR) (Magnusson et al., 2020). Smaller nloo values lead to faster computation, but higher uncertainty in the evaluation part. If NULL, all observations are used (as by default). Note that performance statistic "auc" (see argument stats of summary.vsel() and plot.vsel()) is not supported in case of subsampled LOO-CV. Furthermore, option "best" for argument baseline of summary.vsel() and plot.vsel() is not supported in case of subsampled LOO-CV.

Κ

Only relevant if cv\_method = "kfold" and if cvfits is NULL (which is the case for reference model objects created by get\_refmodel.stanreg() or brms::get\_refmodel.brmsfit()) Number of folds in K-fold CV.

cvfits

Only relevant if cv\_method = "kfold". The same as argument cvfits of init\_refmodel(), but repeated here so that output from run\_cvfun() can be inserted here straightforwardly.

validate\_search

A single logical value indicating whether to cross-validate also the search part, i.e., whether to run the search separately for each CV fold (TRUE) or not (FALSE). With FALSE, the computation is faster, but the predictive performance estimates of the selected submodels are optimistically biased. However, these fast biased estimates can be useful to obtain initial information on the usefulness of projection predictive variable selection.

method

The method for the search part. Possible options are "forward" for forward search and "L1" for L1 search. See also section "Details" below.

ndraws

Number of posterior draws used in the search part. Ignored if nclusters is not NULL or in case of L1 search (because L1 search always uses a single cluster). If both (nclusters and ndraws) are NULL, the number of posterior draws from the reference model is used for ndraws. See also section "Details" below.

nclusters

Number of clusters of posterior draws used in the search part. Ignored in case of L1 search (because L1 search always uses a single cluster). For the meaning of NULL, see argument ndraws. See also section "Details" below.

ndraws\_pred

Only relevant if refit\_prj is TRUE. Number of posterior draws used in the evaluation part. Ignored if nclusters\_pred is not NULL. If both (nclusters\_pred and ndraws\_pred) are NULL, the number of posterior draws from the reference model is used for ndraws\_pred. See also section "Details" below.

nclusters\_pred

Only relevant if refit\_prj is TRUE. Number of clusters of posterior draws used in the evaluation part. For the meaning of NULL, see argument ndraws\_pred. See also section "Details" below.

refit\_prj

For the evaluation part, should the projections onto the submodels along the predictor ranking be performed again using ndraws\_pred draws or nclusters\_pred clusters (TRUE) or should their projections from the search part, which used ndraws draws or nclusters clusters, be re-used (FALSE)?

nterms\_max

Maximum submodel size (number of predictor terms) up to which the search is continued. If NULL, then min(19, D) is used where D is the number of terms

> in the reference model (or in search\_terms, if supplied). Note that nterms\_max does not count the intercept, so use nterms\_max = 0 for the intercept-only model. (Correspondingly, D above does not count the intercept.)

penalty

Only relevant for L1 search. A numeric vector determining the relative penalties or costs for the predictors. A value of 0 means that those predictors have no cost and will therefore be selected first, whereas Inf means those predictors will never be selected. If NULL, then 1 is used for each predictor.

verbose

A single integer value from the set  $\{0, 1, 2, 3, 4\}$  (for varse1(), 3 and 4 have the same effect), indicating how much information (if any) to print out during the computations. Higher values indicate that more information should be printed, 0 deactivates the verbose mode. Internally, argument verbose is coerced to integer via as.integer(), so technically, a single logical value or a single numeric value work as well.

search\_control A list of "control" arguments (i.e., tuning parameters) for the search. In case of forward search, these arguments are passed to the divergence minimizer (see argument div\_minimizer of init\_refmodel() as well as section "Draw-wise divergence minimizers" of projpred-package). In case of forward search, NULL causes . . . to be used not only for the performance evaluation, but also for the search. In case of L1 search, possible arguments are:

- lambda\_min\_ratio: Ratio between the smallest and largest lambda in the L1-penalized search (default: 1e-5). This parameter essentially determines how long the search is carried out, i.e., how large submodels are explored. No need to change this unless the program gives a warning about this.
- nlambda: Number of values in the lambda grid for L1-penalized search (default: 150). No need to change this unless the program gives a warning about this.
- thresh: Convergence threshold when computing the L1 path (default: 1e-6). Usually, there is no need to change this.

lambda\_min\_ratio

Deprecated (please use search\_control instead). Only relevant for L1 search. Ratio between the smallest and largest lambda in the L1-penalized search. This parameter essentially determines how long the search is carried out, i.e., how large submodels are explored. No need to change this unless the program gives a warning about this.

nlambda

Deprecated (please use search\_control instead). Only relevant for L1 search. Number of values in the lambda grid for L1-penalized search. No need to change this unless the program gives a warning about this.

thresh

Deprecated (please use search\_control instead). Only relevant for L1 search. Convergence threshold when computing the L1 path. Usually, there is no need to change this.

seed

Pseudorandom number generation (PRNG) seed by which the same results can be obtained again if needed. Passed to argument seed of set.seed(), but can also be NA to not call set.seed() at all. If not NA, then the PRNG state is reset (to the state before calling cv\_varsel()) upon exiting cv\_varsel(). Here, seed is used for clustering the reference model's posterior draws (if !is.null(nclusters) or !is.null(nclusters\_pred)), for subsampling PSIS-LOO CV folds (if nloo

is smaller than the number of observations), for sampling the folds in K-fold CV, and for drawing new group-level effects when predicting from a multilevel submodel (however, not yet in case of a GAMM).

search\_terms Only relevant for forward search. A custom character vector of predictor term

blocks to consider for the search. Section "Details" below describes more precisely what "predictor term block" means. The intercept ("1") is always included internally via union(), so there's no difference between including it explicitly or omitting it. The default search\_terms considers all the terms in the

reference model's formula.

search\_out Intended for internal use.

parallel A single logical value indicating whether to run costly parts of the CV in par-

allel (TRUE) or not (FALSE). See also section "Note" below as well as section

"Parallelization" in projpred-package.

#### **Details**

Arguments ndraws, nclusters, nclusters\_pred, and ndraws\_pred are automatically truncated at the number of posterior draws in the reference model (which is 1 for datafits). Using less draws or clusters in ndraws, nclusters, nclusters\_pred, or ndraws\_pred than posterior draws in the reference model may result in slightly inaccurate projection performance. Increasing these arguments affects the computation time linearly.

For argument method, there are some restrictions: For a reference model with multilevel or additive formula terms or a reference model set up for the augmented-data projection, only the forward search is available. Furthermore, argument search\_terms requires a forward search to take effect.

L1 search is faster than forward search, but forward search may be more accurate. Furthermore, forward search may find a sparser model with comparable performance to that found by L1 search, but it may also overfit when more predictors are added. This overfit can be detected by running search validation (see cv\_varsel()).

An L1 search may select an interaction term before all involved lower-order interaction terms (including main-effect terms) have been selected. In **projpred** versions > 2.6.0, the resulting predictor ranking is automatically modified so that the lower-order interaction terms come before this interaction term, but if this is conceptually undesired, choose the forward search instead.

The elements of the search\_terms character vector don't need to be individual predictor terms. Instead, they can be building blocks consisting of several predictor terms connected by the + symbol. To understand how these building blocks work, it is important to know how **projpred**'s forward search works: It starts with an empty vector chosen which will later contain already selected predictor terms. Then, the search iterates over model sizes  $j \in \{0, ..., J\}$  (with J denoting the maximum submodel size, not counting the intercept). The candidate models at model size j are constructed from those elements from search\_terms which yield model size j when combined with the chosen predictor terms. Note that sometimes, there may be no candidate models for model size j. Also note that internally, search\_terms is expanded to include the intercept ("1"), so the first step of the search (model size 0) always consists of the intercept-only model as the only candidate.

As a search\_terms example, consider a reference model with formula  $y \sim x1 + x2 + x3$ . Then, to ensure that x1 is always included in the candidate models, specify search\_terms = c("x1", "x1 + x2", "x1 + x3", "x1 + x2 + x3") (or, in a simpler way that leads to the same results, search\_terms = c("x1", "x1 + x2", "x1 + x3"), for which helper function force\_search\_terms() exists). This

search would start with  $y \sim 1$  as the only candidate at model size 0. At model size 1,  $y \sim x1$  would be the only candidate. At model size 2,  $y \sim x1 + x2$  and  $y \sim x1 + x3$  would be the two candidates. At the last model size of 3,  $y \sim x1 + x2 + x3$  would be the only candidate. As another example, to exclude x1 from the search, specify search\_terms = c("x2", "x3", "x2 + x3") (or, in a simpler way that leads to the same results, search\_terms = c("x2", "x3")).

#### Value

An object of class vsel. The elements of this object are not meant to be accessed directly but instead via helper functions (see the main vignette and projpred-package).

#### Note

If validate\_search is FALSE, the search is not included in the CV so that only a single full-data search is run. If the number of observations is large, the fast PSIS-LOO CV along the full-data search path is likely to be accurate. If the number of observations is small or moderate, the fast PSIS-LOO CV along the full-data search path is likely to have optimistic bias in the middle of the search path. This result can be used to guide further actions and the optimistic bias can be greatly reduced by using validate\_search = TRUE.

PSIS uses the Pareto- $\hat{k}$  diagnostic to assess the reliability of PSIS-LOO CV. Global option projpred.warn\_psis (default TRUE) controls whether the Pareto- $\hat{k}$  diagnostics may result in warnings. See loo::loo-glossary for how to interpret the Pareto- $\hat{k}$  values and the warning thresholds. **projpred** does not support the usually recommended moment-matching (see loo::loo\_moment\_match() and brms::loo\_moment\_match()), mixture importance sampling (vignette("loo2-mixis", package="loo")), or reloo-ing (brms::reloo()). If the reference model PSIS-LOO CV Pareto- $\hat{k}$  values are good, but there are high Pareto- $\hat{k}$  values for the projected models, you can try increasing the number of draws used for the PSIS-LOO CV (ndraws in case of refit\_prj = FALSE; ndraws\_pred in case of refit\_prj = TRUE). If increasing the number of draws does not help and if the reference model PSIS-LOO CV Pareto- $\hat{k}$  values are high, and the reference model PSIS-LOO CV results change substantially when using moment-matching, mixture importance sampling, or reloo-ing, we recommend to use K-fold CV within projpred.

For PSIS-LOO CV, **projpred** calls loo::psis() (or, exceptionally, loo::sis(), see below) with  $r_eff = NA$ . This is only a problem if there was extreme autocorrelation between the MCMC iterations when the reference model was built. In those cases however, the reference model should not have been used anyway, so we don't expect **projpred**'s  $r_eff = NA$  to be a problem.

PSIS cannot be used if the number of draws or clusters is too small. In such cases, **projpred** resorts to standard importance sampling (SIS) and shows a message about this. Throughout the documentation, the term "PSIS" is used even though in fact, **projpred** resorts to SIS in these special cases. If SIS is used, check that the reference model PSIS-LOO CV Pareto- $\hat{k}$  values are good.

With parallel = TRUE, costly parts of **projpred**'s CV can be run in parallel. Costly parts are the fold-wise searches and performance evaluations in case of validate\_search = TRUE. (Note that in case of K-fold CV, the K reference model refits are not affected by argument parallel; only **projpred**'s CV is affected.) The parallelization is powered by the **foreach** package. Thus, any parallel (or sequential) backend compatible with **foreach** can be used, e.g., the backends from packages **doParallel**, **doMPI**, or **doFuture**. For GLMs, this CV parallelization should work reliably, but for other models (such as GLMMs), it may lead to excessive memory usage which in turn may crash the R session (on Unix systems, setting an appropriate memory limit via unix::rlimit\_as() may avoid crashing the whole machine). However, the problem of excessive memory usage is less

pronounced for the CV parallelization than for the projection parallelization described in projectpackage. In that regard, the CV parallelization is recommended over the projection parallelization.

#### References

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Vehtari, Aki, Daniel Simpson, Andrew Gelman, Yuling Yao, and Jonah Gabry. 2024. "Pareto Smoothed Importance Sampling." *Journal of Machine Learning Research*, 25 (72):1–58. https://jmlr.org/papers/v25/19-556.html.

## See Also

```
varsel()
```

## **Examples**

df\_binom 23

df\_binom

Binomial toy example

# **Description**

Binomial toy example

# Usage

df\_binom

#### **Format**

A simulated classification dataset containing 100 observations.

- y response, 0 or 1.
- **x** predictors, 30 in total.

## **Source**

https://web.stanford.edu/~hastie/glmnet/glmnetData/BNExample.RData

df\_gaussian

Gaussian toy example

# Description

Gaussian toy example

# Usage

df\_gaussian

# **Format**

A simulated regression dataset containing 100 observations.

- y response, real-valued.
- x predictors, 20 in total. Mean and SD are approximately 0 and 1, respectively.

# Source

https://web.stanford.edu/~hastie/glmnet/glmnetData/QSExample.RData

extend\_family

Extend a family

### **Description**

This function adds some internally required elements to an object of class family (see, e.g., family()). It is called internally by init\_refmodel(), so you will rarely need to call it yourself.

## Usage

```
extend_family(
  family,
  latent = FALSE,
  latent_y_unqs = NULL,
  latent_ilink = NULL,
  latent_ll_oscale = NULL,
  latent_ppd_oscale = NULL,
  augdat_y_unqs = NULL,
  augdat_link = NULL,
  augdat_ilink = NULL,
  augdat_args_link = list(),
  augdat_args_ilink = list(),
  ...
)
```

## Arguments

family

An object of class family.

latent

A single logical value indicating whether to use the latent projection (TRUE) or not (FALSE). Note that setting latent = TRUE causes all arguments starting with augdat\_ to be ignored.

latent\_y\_unqs

Only relevant for a latent projection where the original response space has finite support (i.e., the original response values may be regarded as categories), in which case this needs to be the character vector of unique response values (which will be assigned to family\$cats internally) or may be left at NULL (so that **projpred** will try to infer it from family\$cats). See also section "Latent projection" below.

latent\_ilink

Only relevant for the latent projection, in which case this needs to be the inverse-link function. If the original response family was the binomial() or the poisson() family, then latent\_ilink can be NULL, in which case an internal default will be used. Can also be NULL in all other cases, but then an internal default based on family\$linkinv will be used which might not work for all families. See also section "Latent projection" below.

latent\_ll\_oscale

Only relevant for the latent projection, in which case this needs to be the function computing response-scale (not latent-scale) log-likelihood values. If !is.null(family\$cats)

(after taking latent\_y\_unqs into account) or if the original response family was the binomial() or the poisson() family, then latent\_ll\_oscale can be NULL, in which case an internal default will be used. Can also be NULL in all other cases, but then downstream functions will have limited functionality (a message thrown by extend\_family() will state what exactly won't be available). See also section "Latent projection" below.

#### latent\_ppd\_oscale

Only relevant for the latent projection, in which case this needs to be the function sampling response values given latent predictors that have been transformed to response scale using latent\_ilink. If !is.null(family\$cats) (after taking latent\_y\_unqs into account) or if the original response family was the binomial() or the poisson() family, then latent\_ppd\_oscale can be NULL, in which case an internal default will be used. Can also be NULL in all other cases, but then downstream functions will have limited functionality (a message thrown by extend\_family() will state what exactly won't be available). See also section "Latent projection" below. Note that although this function has the abbreviation "PPD" in its name (which stands for "posterior predictive distribution"), projpred currently only uses it in proj\_predict(), i.e., for sampling from what would better be termed posterior-projection predictive distribution (PPPD).

augdat\_y\_unqs

Only relevant for augmented-data projection, in which case this needs to be the character vector of unique response values (which will be assigned to family\$cats internally) or may be left at NULL if family\$cats is already non-NULL. See also section "Augmented-data projection" below.

augdat\_link

Only relevant for augmented-data projection, in which case this needs to be the link function. Use NULL for the traditional projection. See also section "Augmented-data projection" below.

augdat\_ilink

Only relevant for augmented-data projection, in which case this needs to be the inverse-link function. Use NULL for the traditional projection. See also section "Augmented-data projection" below.

augdat\_args\_link

Only relevant for augmented-data projection, in which case this may be a named list of arguments to pass to the function supplied to augdat\_link.

augdat\_args\_ilink

Only relevant for augmented-data projection, in which case this may be a named list of arguments to pass to the function supplied to augdat\_ilink.

Ignored (exists only to swallow up further arguments which might be passed to this function).

## **Details**

In the following, N,  $C_{\rm cat}$ ,  $C_{\rm lat}$ ,  $S_{\rm ref}$ , and  $S_{\rm prj}$  from help topic refmodel-init-get are used. Note that N does not necessarily denote the number of original observations; it can also refer to new observations. Furthermore, let S denote either  $S_{\rm ref}$  or  $S_{\rm prj}$ , whichever is appropriate in the context where it is used.

#### Value

The family object extended in the way needed by **projpred**.

#### **Augmented-data projection**

As their first input, the functions supplied to arguments augdat\_link and augdat\_ilink have to accept:

- For augdat\_link: an  $S \times N \times C_{\text{cat}}$  array containing the probabilities for the response categories. The order of the response categories is the same as in family\$cats (see argument augdat\_y\_unqs).
- For augdat\_ilink: an  $S \times N \times C_{\mathrm{lat}}$  array containing the linear predictors.

The return value of these functions needs to be:

- For augdat\_link: an  $S \times N \times C_{\mathrm{lat}}$  array containing the linear predictors.
- For augdat\_ilink: an  $S \times N \times C_{\text{cat}}$  array containing the probabilities for the response categories. The order of the response categories has to be the same as in family\$cats (see argument augdat\_y\_unqs).

For the augmented-data projection, the response vector resulting from extract\_model\_data (see init\_refmodel()) is coerced to a factor (using as.factor()) at multiple places throughout this package. Inside of init\_refmodel(), the levels of this factor have to be identical to family\$cats (after applying extend\_family() inside of init\_refmodel()). Everywhere else, these levels have to be a subset of <refmodel>\$family\$cats (where <refmodel> is an object resulting from init\_refmodel()). See argument augdat\_y\_unqs for how to control family\$cats.

For ordinal **brms** families, be aware that the submodels (onto which the reference model is projected) currently have the following restrictions:

- The discrimination parameter disc is not supported (i.e., it is a constant with value 1).
- The thresholds are "flexible" (see brms::brmsfamily()).
- The thresholds do not vary across the levels of a factor-like variable (see argument gr of brms::resp\_thres()).
- The "probit\_approx" link is replaced by "probit".

For the brms::categorical() family, be aware that:

- For multilevel submodels, the group-level effects are allowed to be correlated between different response categories.
- For multilevel submodels, **mclogit** versions < 0.9.4 may throw the error 'a' (<number> x 1) must be square. Updating **mclogit** to a version >= 0.9.4 should fix this.

## Latent projection

The function supplied to argument latent\_ilink needs to have the prototype

```
latent_ilink(lpreds, cl_ref, wdraws_ref = rep(1, length(cl_ref)))
```

where:

- 1preds accepts an  $S \times N$  matrix containing the linear predictors.
- cl\_ref accepts a numeric vector of length  $S_{ref}$ , containing **projpred**'s internal cluster indices for these draws.

• wdraws\_ref accepts a numeric vector of length  $S_{\rm ref}$ , containing weights for these draws. These weights should be treated as not being normalized (i.e., they don't necessarily sum to 1).

The return value of latent\_ilink needs to contain the linear predictors transformed to the original response space, with the following structure:

- If is.null(family\$cats) (after taking latent\_y\_unqs into account): an  $S \times N$  matrix.
- If !is.null(family\$cats) (after taking latent\_y\_unqs into account): an  $S \times N \times C_{\text{cat}}$  array. In that case, latent\_ilink needs to return *probabilities* (for the response categories given in family\$cats, after taking latent\_y\_unqs into account).

The function supplied to argument latent\_ll\_oscale needs to have the prototype

#### where:

- ilpreds accepts the return value from latent\_ilink.
- dis accepts a vector of length S containing dispersion parameter draws.
- ullet y\_oscale accepts a vector of length N containing response values on the original response scale.
- ullet wobs accepts a numeric vector of length N containing observation weights.
- cl\_ref accepts the same input as argument cl\_ref of latent\_ilink.
- wdraws\_ref accepts the same input as argument wdraws\_ref of latent\_ilink.

The return value of latent\_ll\_oscale needs to be an  $S \times N$  matrix containing the response-scale (not latent-scale) log-likelihood values for the N observations from its inputs.

The function supplied to argument latent\_ppd\_oscale needs to have the prototype

#### where:

- ilpreds\_resamp accepts the return value from latent\_ilink, but possibly with resampled (clustered) draws (see argument nresample\_clusters of proj\_predict()).
- dis\_resamp accepts a vector of length dim(ilpreds\_resamp)[1] containing dispersion parameter draws, possibly resampled (in the same way as the draws in ilpreds\_resamp, see also argument idxs\_prjdraws).
- $\bullet$  wobs accepts a numeric vector of length N containing observation weights.
- cl\_ref accepts the same input as argument cl\_ref of latent\_ilink.

28 extra-families

- wdraws\_ref accepts the same input as argument wdraws\_ref of latent\_ilink.
- idxs\_prjdraws accepts a numeric vector of length dim(ilpreds\_resamp)[1] containing the resampled indices of the projected draws (i.e., these indices are values from the set {1, ..., dim(ilpreds)[1]} where ilpreds denotes the return value of latent\_ilink).

The return value of latent\_ppd\_oscale needs to be a dim(ilpreds\_resamp)[1]  $\times N$  matrix containing the response-scale (not latent-scale) draws from the posterior(-projection) predictive distributions for the N observations from its inputs.

If the bodies of these three functions involve parameter draws from the reference model which have not been projected (e.g., for latent\_ilink, the thresholds in an ordinal model), cl\_agg() is provided as a helper function for aggregating these reference model draws in the same way as the draws have been aggregated for the first argument of these functions (e.g., lpreds in case of latent\_ilink).

In fact, the weights passed to argument wdraws\_ref are nonconstant only in case of cv\_varsel() with cv\_method = "LOO" and validate\_search = TRUE. In that case, the weights passed to this argument are the PSIS-LOO CV weights for one observation. Note that although argument wdraws\_ref has the suffix \_ref, wdraws\_ref does not necessarily obtain weights for the *initial* reference model's posterior draws: In case of cv\_varsel() with cv\_method = "kfold", these weights may refer to one of the K reference model refits (but in that case, they are constant anyway).

If family\$cats is not NULL (after taking latent\_y\_unqs into account), then the response vector resulting from extract\_model\_data (see init\_refmodel()) is coerced to a factor (using as.factor()) at multiple places throughout this package. Inside of init\_refmodel(), the levels of this factor have to be identical to family\$cats (after applying extend\_family() inside of init\_refmodel()). Everywhere else, these levels have to be a subset of <refmodel>\$family\$cats (where <refmodel> is an object resulting from init\_refmodel()).

extra-families

Extra family objects

# **Description**

Family objects not in the set of default family objects.

## Usage

```
Student_t(link = "identity", nu = 3)
```

#### **Arguments**

link Name of the link function. In contrast to the default family objects, this has to

be a character string here.

nu Degrees of freedom for the Student-*t* distribution.

## Value

A family object analogous to those described in family.

force\_search\_terms 29

#### Note

Support for the Student\_t() family is still experimental.

force\_search\_terms

Force search terms

# **Description**

A helper function to construct the input for argument search\_terms of varsel() or cv\_varsel() if certain predictor terms should be forced to be selected first whereas other predictor terms are optional (i.e., they are subject to the variable selection, but only after the inclusion of the "forced" terms).

## Usage

```
force_search_terms(forced_terms, optional_terms)
```

# **Arguments**

forced\_terms A character vector of predictor terms that should be selected first.

optional\_terms A character vector of predictor terms that should be subject to the variable selection after the inclusion of the "forced" terms.

## Value

A character vector that may be used as input for argument search\_terms of varsel() or cv\_varsel().

## See Also

```
varsel(), cv_varsel()
```

# **Examples**

```
# Data:
dat_gauss <- data.frame(y = df_gaussian$y, df_gaussian$x)

# The `stanreg` fit which will be used as the reference model (with small
# values for `chains` and `iter`, but only for technical reasons in this
# example; this is not recommended in general):
fit <- rstanarm::stan_glm(
    y ~ X1 + X2 + X3 + X4 + X5, family = gaussian(), data = dat_gauss,
    QR = TRUE, chains = 2, iter = 500, refresh = 0, seed = 9876
)

# We will force X1 and X2 to be selected first:
search_terms_forced <- force_search_terms(
    forced_terms = paste0("X", 1:2),
    optional_terms = paste0("X", 3:5)</pre>
```

30 mesquite

mesquite

Mesquite data set

## **Description**

The mesquite bushes yields dataset from Gelman and Hill (2006) (https://sites.stat.columbia.edu/gelman/arm/).

## Usage

mesquite

## **Format**

The response variable is the total weight (in grams) of photosynthetic material as derived from actual harvesting of the bush. The predictor variables are:

**diam1** diameter of the canopy (the leafy area of the bush) in meters, measured along the longer axis of the bush.

**diam2** canopy diameter measured along the shorter axis.

canopy height height of the canopy.

total height total height of the bush.

**density** plant unit density (# of primary stems per plant unit).

**group** group of measurements (0 for the first group, 1 for the second group).

#### Source

https://sites.stat.columbia.edu/gelman/arm/examples/mesquite/mesquite.dat

#### References

Gelman, Andrew, and Jennifer Hill. 2006. *Data Analysis Using Regression and Multilevel/Hierarchical Models*. Cambridge, UK: Cambridge University Press. doi:10.1017/CBO9780511790942.

performances 31

performances

Predictive performance results

# **Description**

Retrieves the predictive performance summaries after running varsel() or cv\_varsel(). These summaries are computed by summary.vsel(), so the main method of performances() is performances.vselsummary() (objects of class vselsummary are returned by summary.vsel()). As a shortcut method, performances.vsel() is provided as well (objects of class vsel are returned by varsel() and cv\_varsel()). For a graphical representation, see plot.vsel().

## Usage

```
performances(object, ...)
## S3 method for class 'vselsummary'
performances(object, ...)
## S3 method for class 'vsel'
performances(object, ...)
```

#### **Arguments**

object

The object from which to retrieve the predictive performance results. Possible classes may be inferred from the names of the corresponding methods (see also

the description).

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For performances.vsel(): arguments passed to summary.vsel(). For performances.vselsummary() currently ignored.

Value

An object of class performances which is a list with the following elements:

- submodels: The predictive performance results for the submodels, as a data. frame.
- reference\_model: The predictive performance results for the reference model, as a named vector.

# **Examples**

```
# Data:
dat_gauss <- data.frame(y = df_gaussian$y, df_gaussian$x)

# The `stanreg` fit which will be used as the reference model (with small
# values for `chains` and `iter`, but only for technical reasons in this
# example; this is not recommended in general):
fit <- rstanarm::stan_glm(
    y ~ X1 + X2 + X3 + X4 + X5, family = gaussian(), data = dat_gauss,
    QR = TRUE, chains = 2, iter = 500, refresh = 0, seed = 9876</pre>
```

32 plot.cv\_proportions

plot.cv\_proportions

Plot ranking proportions from fold-wise predictor rankings

# **Description**

Plots the ranking proportions (see cv\_proportions()) from the fold-wise predictor rankings in a cross-validation with fold-wise searches. This is a visualization of the *transposed* matrix returned by cv\_proportions(). The proportions printed as text inside of the colored tiles are rounded to whole percentage points (the plotted proportions themselves are not rounded).

## Usage

```
## S3 method for class 'cv_proportions'
plot(
    x,
    text_angle = getOption("projpred.plot_cv_proportions_text_angle", NULL),
    ...
)

## S3 method for class 'ranking'
plot(x, ...)
```

## **Arguments**

x For plot.cv\_proportions(): an object of class cv\_proportions (returned by cv\_proportions(), possibly with cumulate = TRUE). For plot.ranking(): an object of class ranking (returned by ranking()) that cv\_proportions() will be applied to internally before then calling plot.cv\_proportions().

text\_angle Passed to argument angle of ggplot2::element\_text() for the y-axis tick labels. In case of long predictor names, text\_angle = 45 might be helpful (for example).

For plot.ranking(): arguments passed to cv\_proportions.ranking() and plot.cv\_proportions(). For plot.cv\_proportions(): currently ignored.

## Value

A **ggplot2** plotting object (of class gg and ggplot).

## Author(s)

Idea and original code by Aki Vehtari. Slight modifications of the original code by Frank Weber, Yann McLatchie, and Sölvi Rögnvaldsson. Final implementation in **projpred** by Frank Weber.

# **Examples**

```
# Data:
dat_gauss <- data.frame(y = df_gaussian$y, df_gaussian$x)</pre>
# The `stanreg` fit which will be used as the reference model (with small
# values for `chains` and `iter`, but only for technical reasons in this
# example; this is not recommended in general):
fit <- rstanarm::stan_glm(</pre>
 y \sim X1 + X2 + X3 + X4 + X5, family = gaussian(), data = dat_gauss,
 QR = TRUE, chains = 2, iter = 1000, refresh = 0, seed = 9876
# Run cv_varsel() (with L1 search and small values for `K`, `nterms_max`, and
# `nclusters_pred`, but only for the sake of speed in this example; this is
# not recommended in general):
cvvs <- cv_varsel(fit, method = "L1", cv_method = "kfold", K = 2,</pre>
                  nterms_max = 3, nclusters_pred = 10, seed = 5555)
# Extract predictor rankings:
rk <- ranking(cvvs)
# Compute ranking proportions:
pr_rk <- cv_proportions(rk)</pre>
# Visualize the ranking proportions:
gg_pr_rk <- plot(pr_rk)</pre>
print(gg_pr_rk)
# Since the object returned by plot.cv_proportions() is a standard ggplot2
# plotting object, you can modify the plot easily, e.g., to remove the
print(gg_pr_rk + ggplot2::theme(legend.position = "none"))
```

plot.vsel

Plot predictive performance

# Description

This is the plot() method for vsel objects (returned by varsel()) or cv\_varsel()). It visualizes the predictive performance of the reference model (possibly also that of some other "baseline" model) and that of the submodels along the full-data predictor ranking. Basic information about the (CV) variability in the ranking of the predictors is included as well (if available; inferred from cv\_proportions()). For a tabular representation, see summary.vsel() and performances().

#### **Usage**

```
## S3 method for class 'vsel'
plot(
  х,
  nterms_max = NULL,
  stats = "elpd",
  deltas = FALSE,
  alpha = 2 * pnorm(-1),
  baseline = if (!inherits(x$refmodel, "datafit")) "ref" else "best",
  thres_elpd = NA,
  resp_oscale = TRUE,
  point_size = getOption("projpred.plot_vsel_point_size", 3),
  bar_thickness = getOption("projpred.plot_vsel_bar_thickness", 1),
 ranking_nterms_max = getOption("projpred.plot_vsel_ranking_nterms_max", NULL),
 ranking_abbreviate = getOption("projpred.plot_vsel_ranking_abbreviate", FALSE),
 ranking_abbreviate_args = getOption("projpred.plot_vsel_ranking_abbreviate_args",
    list()),
  ranking_repel = getOption("projpred.plot_vsel_ranking_repel", NULL),
 ranking_repel_args = getOption("projpred.plot_vsel_ranking_repel_args", list()),
 ranking_colored = getOption("projpred.plot_vsel_ranking_colored", FALSE),
 show_cv_proportions = getOption("projpred.plot_vsel_show_cv_proportions", FALSE),
  cumulate = FALSE,
  text_angle = getOption("projpred.plot_vsel_text_angle", 45),
 size_position = getOption("projpred.plot_vsel_size_position", "primary_x_top"),
)
```

## **Arguments**

x An object of class vsel (returned by varsel() or cv\_varsel()).

nterms\_max

Maximum submodel size (number of predictor terms) for which the performance statistics are calculated. Using NULL is effectively the same as length(ranking(object)\$fulldata). Note that nterms\_max does not count the intercept, so use nterms\_max = 0 for the intercept-only model. For plot.vsel(), nterms\_max must be at least 1.

stats

One or more character strings determining which performance statistics (i.e., utilities or losses) to estimate based on the observations in the evaluation (or "test") set (in case of cross-validation, these are all observations because they are partitioned into multiple test sets; in case of varsel() with d\_test = NULL, these are again all observations because the test set is the same as the training set). Available statistics are:

- "elpd": expected log (pointwise) predictive density (for a new dataset)
  (ELPD). Estimated by the sum of the observation-specific log predictive
  density values (with each of these predictive density values being a—possibly
  weighted—average across the parameter draws). For the corresponding uncertainty interval, a normal approximation is used.
- "mlpd": mean log predictive density (MLPD), that is, the ELPD divided by the number of observations. For the corresponding uncertainty interval, a

normal approximation is used.

- "gmpd": geometric mean predictive density (GMPD), that is, exp() of the MLPD. The GMPD is especially helpful for discrete response families (because there, the GMPD is bounded by zero and one). For the corresponding standard error, the delta method is used. The corresponding uncertainty interval type is "exponentiated normal approximation" because the uncertainty interval bounds are the exponentiated uncertainty interval bounds of the MLPD.
- "mse": mean squared error (only available in the situations mentioned in section "Details" below). For the corresponding uncertainty interval, a lognormal approximation is used if deltas is FALSE and a normal approximation is used if deltas is TRUE (or "mixed", in case of plot.vsel()).
- "rmse": root mean squared error (only available in the situations mentioned in section "Details" below). For the corresponding standard error, the delta method is used. For the corresponding uncertainty interval, a log-normal approximation is used if deltas is FALSE and a normal approximation is used if deltas is TRUE (or "mixed", in case of plot.vsel()).
- "R2": R-squared, i.e., coefficient of determination (only available in the situations mentioned in section "Details" below). For the corresponding standard error, the delta method is used. For the corresponding uncertainty interval, a normal approximation is used.
- "acc" (or its alias, "pctcorr"): classification accuracy (only available in
  the situations mentioned in section "Details" below). By "classification accuracy", we mean the proportion of correctly classified observations. For
  this, the response category ("class") with highest probability (the probabilities are model-based) is taken as the prediction ("classification") for an
  observation. For the corresponding uncertainty interval, a normal approximation is used.
- "auc": area under the ROC curve (only available in the situations mentioned in section "Details" below). For the corresponding standard error and lower and upper uncertainty interval bounds, bootstrapping is used. Not supported in case of subsampled LOO-CV (see argument nloo of cv\_varsel()).

deltas

May be set to FALSE, TRUE, or "mixed". If FALSE, the submodel performance statistics are plotted on their actual scale and the uncertainty bars match this scale. If TRUE, the submodel statistics are plotted relatively to the baseline model (see argument baseline) and the uncertainty bars match this scale. For the GMPD, the term "relatively" refers to the *ratio* vs. the baseline model (i.e., the submodel statistic divided by the baseline model statistic). For all other stats, "relatively" refers to the *difference* from the baseline model (i.e., the submodel statistic minus the baseline model statistic). If set to "mixed", the deltas = FALSE point estimates are combined with the uncertainty bars from the deltas = TRUE plot.

alpha

A number determining the (nominal) coverage 1 – alpha of the uncertainty intervals. For example, in case of a normal-approximation uncertainty interval, alpha = 2 \* pnorm(-1) corresponds to a uncertainty interval stretching by one standard error on either side of the point estimate.

baseline For summary.vsel(): Only relevant if deltas is TRUE. For plot.vsel(): Al-

ways relevant. Either "ref" or "best", indicating whether the baseline is the reference model or the best submodel found (in terms of stats[1]), respectively. In case of subsampled LOO-CV, baseline = "best" is not supported.

thres\_elpd Only relevant if any(stats %in% c("elpd", "mlpd", "gmpd")). The thresh-

old for the ELPD difference (taking the submodel's ELPD minus the baseline model's ELPD) above which the submodel's ELPD is considered to be close enough to the baseline model's ELPD. An equivalent rule is applied in case of the MLPD and the GMPD. See suggest\_size() for a formalization. Supplying

NA deactivates this.

resp\_oscale Only relevant for the latent projection. A single logical value indicating whether

to calculate the performance statistics on the original response scale (TRUE) or

on latent scale (FALSE).

point\_size Passed to argument size of ggplot2::geom\_point() and controls the size of

the points.

bar\_thickness Passed to argument linewidth of ggplot2::geom\_linerange() and controls

the thickness of the uncertainty bars.

ranking\_nterms\_max

Maximum submodel size (number of predictor terms) for which the predictor names and the corresponding ranking proportions are added on the x-axis. Using NULL is effectively the same as using nterms\_max. Using NA causes the predictor names and the corresponding ranking proportions to be omitted, which requires size\_position = "primary\_x\_bottom". Note that ranking\_nterms\_max does not count the intercept, so ranking\_nterms\_max = 1 corresponds to the submodel consisting of the first (non-intercept) predictor term.

ranking\_abbreviate

A single logical value indicating whether the predictor names in the full-data predictor ranking should be abbreviated by abbreviate() (TRUE) or not (FALSE). See also argument ranking\_abbreviate\_args and section "Value".

ranking\_abbreviate\_args

A list of arguments (except for names.arg) to be passed to abbreviate() in case of ranking\_abbreviate = TRUE.

ranking\_repel Either NULL, "text", or "label". By NULL, the full-data predictor ranking and

the corresponding ranking proportions are placed below the x-axis. By "text" or "label", they are placed within the plotting area, using ggrepel::geom\_text\_repel()

or ggrepel::geom\_label\_repel(), respectively. See also argument ranking\_repel\_args.

ranking\_repel\_args

A list of arguments (except for mapping) to be passed to ggrepel::geom\_text\_repel() or ggrepel::geom\_label\_repel() in case of ranking\_repel = "text" or ranking\_repel = "label", respectively.

ranking\_colored

A single logical value indicating whether the points and the uncertainty bars should be gradient-colored according to the CV ranking proportions (TRUE, currently only works if show\_cv\_proportions is TRUE as well) or not (FALSE). The CV ranking proportions may be cumulated (see argument cumulate). Note that the point and the uncertainty bar at submodel size 0 (i.e., at the intercept-only

plot.vsel 37

model) are always colored in gray because the intercept is forced to be selected before any predictors are selected (in other words, the reason is that for submodel size 0, the question of variability across CV folds is not appropriate in the first place).

show\_cv\_proportions

text\_angle

A single logical value indicating whether the CV ranking proportions (see cv\_proportions()) should be displayed (TRUE) or not (FALSE).

cumulate Passed to argument cumulate of cv\_proportions(). Affects the ranking pro-

portions given on the x-axis (below the full-data predictor ranking).

Passed to argument angle of ggplot2::element\_text() for the x-axis tick labels. Note that the default of argument angle in ggplot2::element\_text() is NULL (which implies no rotation) whereas we use a default of text\_angle = 45 here. If text\_angle > 0 (< 0), the x-axis text is automatically right-aligned (left-aligned). If -90 < text\_angle && text\_angle < 90 && text\_angle != 0, the x-axis text is also top-aligned. When controlling text\_angle via global option projpred.plot\_vsel\_text\_angle, keep in mind that a global option set to NULL is treated like an unset global option, so options(projpred.plot\_vsel\_text\_angle)

= NULL) would result in text\_angle = 45, not text\_angle = 0.

size\_position A single character string specifying the position of the submodel sizes. Either "primary\_x\_bottom" for including them in the x-axis tick labels, "primary\_x\_top" for putting them above the x-axis (the current default), or "secondary\_x" for

putting them into a secondary x-axis. Currently, "primary\_x\_top" and "secondary\_x" may not be combined with ranking\_nterms\_max = NA (i.e., only "primary\_x\_bottom"

works with ranking\_nterms\_max = NA).

Arguments passed to the internal function which is used for bootstrapping (if applicable; see argument stats). Currently, relevant arguments are B (the number of bootstrap samples, defaulting to 2000) and seed (see set.seed(), but defaulting to NA so that set.seed() is not called within that function at all).

#### **Details**

The stats options "mse", "rmse", and "R2" are only available for:

- the traditional projection,
- the latent projection with resp\_oscale = FALSE,
- the latent projection with resp\_oscale = TRUE in combination with <refmodel>\$family\$cats being NULL.

The stats option "acc" (= "pctcorr") is only available for:

- the binomial() family in case of the traditional projection,
- all families in case of the augmented-data projection,
- the binomial() family (on the original response scale) in case of the latent projection with resp\_oscale = TRUE in combination with <refmodel>\$family\$cats being NULL,
- all families (on the original response scale) in case of the latent projection with resp\_oscale = TRUE in combination with <refmodel>\$family\$cats being not NULL.

38 plot.vsel

The stats option "auc" is only available for:

- the binomial() family in case of the traditional projection,
- the binomial() family (on the original response scale) in case of the latent projection with resp\_oscale = TRUE in combination with <refmodel>\$family\$cats being NULL.

Note that the stats option "auc" is not supported in case of subsampled LOO-CV (see argument nloo of cv\_varsel()).

#### Value

A **ggplot2** plotting object (of class gg and ggplot). If ranking\_abbreviate is TRUE, the output of abbreviate() is stored in an attribute called projpred\_ranking\_abbreviated (to allow the abbreviations to be easily mapped back to the original predictor names).

#### **Horizontal lines**

As long as the reference model's performance is computable, it is always shown in the plot as a dashed red horizontal line. If baseline = "best", the baseline model's performance is shown as a dotted black horizontal line. If !is.na(thres\_elpd) and any(stats %in% c("elpd", "mlpd", "gmpd")), the value supplied to thres\_elpd (which is automatically adapted internally in case of the MLPD or the GMPD or deltas = FALSE or deltas = "mixed") is shown as a dot-dashed gray horizontal line for the reference model and, if baseline = "best", as a long-dashed green horizontal line for the baseline model.

## **Examples**

pred-projection

Predictions from a submodel (after projection)

# Description

After the projection of the reference model onto a submodel, the linear predictors (for the original or a new dataset) based on that submodel can be calculated by proj\_linpred(). These linear predictors can also be transformed to response scale and averaged across the projected parameter draws. Furthermore, proj\_linpred() returns the corresponding log predictive density values if the (original or new) dataset contains response values. The proj\_predict() function draws from the predictive distributions (there is one such distribution for each observation from the original or new dataset) of the submodel that the reference model has been projected onto. If the projection has not been performed yet, both functions call project() internally to perform the projection. Both functions can also handle multiple submodels at once (for objects of class vsel or objects returned by a project() call to an object of class vsel; see project()).

## Usage

```
proj_linpred(
  object,
  newdata = NULL,
  offsetnew = NULL,
 weightsnew = NULL,
  filter_nterms = NULL,
  transform = FALSE,
  integrated = FALSE,
  allow_nonconst_wdraws_prj = return_draws_matrix,
  return_draws_matrix = FALSE,
  .seed = NA,
)
proj_predict(
  object,
  newdata = NULL,
 offsetnew = NULL,
 weightsnew = NULL,
  filter_nterms = NULL,
  nresample_clusters = 1000.
  return_draws_matrix = FALSE,
  .seed = NA,
  resp_oscale = TRUE,
)
```

## **Arguments**

object An object returned by project() or an object that can be passed to argument

object of project().

newdata Passed to argument newdata of the reference model's extract\_model\_data

function (see init\_refmodel()). Provides the predictor (and possibly also the response) data for the new (or old) observations. May also be NULL for using the

original dataset. If not NULL, any NAs will trigger an error.

offsetnew Passed to argument orhs of the reference model's extract\_model\_data func-

tion (see init\_refmodel()). Used to get the offsets for the new (or old) obser-

vations.

weightsnew Passed to argument wrhs of the reference model's extract\_model\_data func-

tion (see init\_refmodel()). Used to get the weights for the new (or old) ob-

servations.

filter\_nterms Only applies if object is an object returned by project(). In that case, filter\_nterms

can be used to filter object for only those elements (submodels) with a number of predictor terms in filter\_nterms. Therefore, needs to be a numeric vector

or NULL. If NULL, use all submodels.

transform For proj\_linpred() only. A single logical value indicating whether the linear

predictor should be transformed to response scale using the inverse-link function (TRUE) or not (FALSE). In case of the latent projection, argument transform is similar in spirit to argument resp\_oscale from other functions and affects the scale of both output elements pred and 1pd (see sections "Details" and "Value"

below).

integrated For proj\_linpred() only. A single logical value indicating whether the output

should be averaged across the projected posterior draws (TRUE) or not (FALSE).

allow\_nonconst\_wdraws\_prj

Only relevant for proj\_linpred() and only if integrated is FALSE. A single logical value indicating whether to allow projected draws with different (i.e., nonconstant) weights (TRUE) or not (FALSE). If return\_draws\_matrix is TRUE, allow\_nonconst\_wdraws\_prj is internally set to TRUE as well. **CAUTION**: Expert use only because if set to TRUE, the weights of the projected draws are stored in attributes wdraws\_prj and handling these attributes requires special

care (e.g., when subsetting the returned matrices).

return\_draws\_matrix

A single logical value indicating whether to return an object (in case of proj\_predict())

or objects (in case of proj\_linpred()) of class draws\_matrix (see posterior::draws\_matrix()).

In case of proj\_linpred() and projected draws with nonconstant weights (as well as integrated being FALSE), posterior::weight\_draws() is applied in-

ternally.

. seed Pseudorandom number generation (PRNG) seed by which the same results can

be obtained again if needed. Passed to argument seed of set.seed(), but can also be NA to not call set.seed() at all. If not NA, then the PRNG state is reset (to the state before calling proj\_linpred() or proj\_predict()) upon exiting proj\_linpred() or proj\_predict(). Here, .seed is used for drawing new

group-level effects in case of a multilevel submodel (however, not yet in case of

a GAMM) and for drawing from the predictive distributions of the submodel(s) in case of proj\_predict(). If a clustered projection was performed, then in proj\_predict(), .seed is also used for drawing from the set of projected clusters of posterior draws (see argument nresample\_clusters). If project() is called internally with seed = NA (or with seed being a lazily evaluated expression that uses the PRNG), then .seed also affects the PRNG usage there.

Arguments passed to project() if object is not already an object returned by project().

nresample\_clusters

For proj\_predict() with clustered projection (and nonconstant weights for the projected draws) only. Number of draws to return from the predictive distributions of the submodel(s). Not to be confused with argument nclusters of project(): nresample\_clusters gives the number of draws (*with* replacement) from the set of clustered posterior draws after projection (with this set being determined by argument nclusters of project()).

Only relevant for the latent projection. A single logical value indicating whether to draw from the posterior-projection predictive distributions on the original response scale (TRUE) or on latent scale (FALSE).

#### Details

Currently, proj\_predict() ignores observation weights that are not equal to 1. A corresponding warning is thrown if this is the case.

In case of the latent projection and transform = FALSE:

- Output element pred contains the linear predictors without any modifications that may be due to the original response distribution (e.g., for a brms::cumulative() model, the ordered thresholds are not taken into account).
- Output element 1pd contains the *latent* log predictive density values, i.e., those corresponding to the latent Gaussian distribution. If newdata is not NULL, this requires the latent response values to be supplied in a column called .<response\_name> of newdata where <response\_name> needs to be replaced by the name of the original response variable (if <response\_name> contained parentheses, these have been stripped off by init\_refmodel(); see the left-hand side of formula(<refmodel>)). For technical reasons, the existence of column <response\_name> in newdata is another requirement (even though .<response\_name> is actually used).

# Value

In the following,  $S_{\rm prj}$ , N,  $C_{\rm cat}$ , and  $C_{\rm lat}$  from help topic refmodel-init-get are used. (For proj\_linpred() with integrated = TRUE, we have  $S_{\rm prj}=1$ .) Furthermore, let C denote either  $C_{\rm cat}$  (if transform = TRUE) or  $C_{\rm lat}$  (if transform = FALSE). Then, if the prediction is done for one submodel only (i.e., length(nterms) == 1 || !is.null(predictor\_terms) in the explicit or implicit call to project(), see argument object):

- proj\_linpred() returns a list with the following elements:
  - Element pred contains the actual predictions, i.e., the linear predictors, possibly transformed to response scale (depending on argument transform).

Element 1pd is non-NULL only if newdata is NULL or if newdata contains response values
in the corresponding column. In that case, it contains the log predictive density values
(conditional on each of the projected parameter draws if integrated = FALSE and averaged across the projected parameter draws if integrated = TRUE).

In case of (i) the traditional projection, (ii) the latent projection with transform = FALSE, or (iii) the latent projection with transform = TRUE and <refmodel>\$family\$cats (where <refmodel> is an object resulting from init\_refmodel(); see also extend\_family()'s argument latent\_y\_unqs) being NULL, both elements are  $S_{\mathrm{prj}} \times N$  matrices (converted to a possibly weighted—draws\_matrix if argument return\_draws\_matrix is TRUE, see the description of this argument). In case of (i) the augmented-data projection or (ii) the latent projection with transform = TRUE and <refmodel>\$family\$cats being not NULL, pred is an  $S_{
m prj} imes N imes C$  array (if argument return\_draws\_matrix is TRUE, this array is "compressed" to an  $S_{\text{prj}} \times (N \cdot C)$  matrix—with the columns consisting of C blocks of N rows—and then converted to a—possibly weighted—draws\_matrix) and 1pd is an  $S_{pri} \times N$  matrix (converted to a—possibly weighted—draws\_matrix if argument return\_draws\_matrix is TRUE). If return\_draws\_matrix is FALSE and allow\_nonconst\_wdraws\_prj is TRUE and integrated is FALSE and the projected draws have nonconstant weights, then both list elements have the weights of these draws stored in an attribute wdraws\_prj. (If return\_draws\_matrix, allow\_nonconst\_wdraws\_prj, and integrated are all FALSE, then projected draws with nonconstant weights cause an error.)

• proj\_predict() returns an  $S_{\rm prj} \times N$  matrix of predictions where  $S_{\rm prj}$  denotes nresample\_clusters in case of clustered projection (or, more generally, in case of projected draws with nonconstant weights). If argument return\_draws\_matrix is TRUE, the returned matrix is converted to a draws\_matrix (see posterior::draws\_matrix()). In case of (i) the augmented-data projection or (ii) the latent projection with resp\_oscale = TRUE and <refmodel>\$family\$cats being not NULL, the returned matrix (or draws\_matrix) has an attribute called cats (the character vector of response categories) and the values of the matrix (or draws\_matrix) are the predicted indices of the response categories (these indices refer to the order of the response categories from attribute cats).

If the prediction is done for more than one submodel, the output from above is returned for each submodel, giving a named list with one element for each submodel (the names of this list being the numbers of predictor terms of the submodels when counting the intercept, too).

## **Examples**

```
# Data:
dat_gauss <- data.frame(y = df_gaussian$y, df_gaussian$x)

# The `stanreg` fit which will be used as the reference model (with small
# values for `chains` and `iter`, but only for technical reasons in this
# example; this is not recommended in general):
fit <- rstanarm::stan_glm(
   y ~ X1 + X2 + X3 + X4 + X5, family = gaussian(), data = dat_gauss,
   QR = TRUE, chains = 2, iter = 500, refresh = 0, seed = 9876
)

# Projection onto an arbitrary combination of predictor terms (with a small
# value for `ndraws`, but only for the sake of speed in this example; this
# is not recommended in general):</pre>
```

predict.refmodel 43

predict.refmodel

Predictions or log posterior predictive densities from a reference model

## **Description**

This is the predict() method for refmodel objects (returned by get\_refmodel()) or init\_refmodel()). It offers three types of output which are all based on the reference model and new (or old) observations: Either the linear predictor on link scale, the linear predictor transformed to response scale, or the log posterior predictive density.

## Usage

```
## $3 method for class 'refmodel'
predict(
  object,
  newdata = NULL,
  ynew = NULL,
  offsetnew = NULL,
  weightsnew = NULL,
  type = "response",
  ...
)
```

# Arguments

object

An object of class refmodel (returned by get\_refmodel()) or init\_refmodel()).

newdata

Passed to argument newdata of the reference model's extract\_model\_data function (see init\_refmodel()). Provides the predictor (and possibly also the response) data for the new (or old) observations. May also be NULL for using the original dataset. If not NULL, any NAs will trigger an error.

ynew

If not NULL, then this needs to be a vector of new (or old) response values. See also section "Value" below. In case of (i) the augmented-data projection or (ii) the latent projection with type = "response" and object\$family\$cats being not NULL, ynew is internally coerced to a factor (using as.factor()). The levels of this factor have to be a subset of object\$family\$cats (see extend\_family()'s arguments augdat\_y\_unqs and latent\_y\_unqs, respectively).

44 predict.refmodel

offsetnew Passed to argument orhs of the reference model's extract\_model\_data func-

tion (see init\_refmodel()). Used to get the offsets for the new (or old) obser-

vations.

weightsnew Passed to argument wrhs of the reference model's extract\_model\_data func-

tion (see init\_refmodel()). Used to get the weights for the new (or old) ob-

servations.

type Usually only relevant if is.null(ynew), but for the latent projection, this also

affects the !is.null(ynew) case (see below). The scale on which the predictions are returned, either "link" or "response" (see predict.glm() but note that predict.refmodel() does not adhere to the typical R convention of a default prediction on link scale). For both scales, the predictions are averaged across the posterior draws. In case of the latent projection, argument type is similar in spirit to argument resp\_oscale from other functions: If (i) is.null(ynew), then argument type affects the predictions as described above. In that case, note that type = "link" yields the linear predictors without any modifications that may be due to the original response distribution (e.g., for a brms::cumulative() model, the ordered thresholds are not taken into account). If (ii) !is.null(ynew), then argument type also affects the scale of the log posterior predictive densities (type = "response" for the original response scale,

... Currently ignored.

#### **Details**

Argument weightsnew is only relevant if !is.null(ynew).

In case of a multilevel reference model, group-level effects for new group levels are drawn randomly from a (multivariate) Gaussian distribution. When setting projpred.mlvl\_pred\_new to TRUE, all group levels from newdata (even those that already exist in the original dataset) are treated as new group levels (if is.null(newdata), all group levels from the original dataset are considered as new group levels in that case).

type = "link" for the latent Gaussian scale).

#### Value

In the following, N,  $C_{\rm cat}$ , and  $C_{\rm lat}$  from help topic refmodel-init-get are used. Furthermore, let C denote either  $C_{\rm cat}$  (if type = "response") or  $C_{\rm lat}$  (if type = "link"). Then, if is null (ynew), the returned object contains the reference model's predictions (with the scale depending on argument type) as:

- a length-N vector in case of (i) the traditional projection, (ii) the latent projection with type = "link", or (iii) the latent projection with type = "response" and object\$family\$cats being NULL;
- an  $N \times C$  matrix in case of (i) the augmented-data projection or (ii) the latent projection with type = "response" and object\$family\$cats being not NULL.

If !is.null(ynew), the returned object is a length-N vector of log posterior predictive densities evaluated at ynew.

predictor\_terms 45

predictor\_terms

Predictor terms used in a project() run

# **Description**

For a projection object (returned by project(), possibly as elements of a list), this function extracts the combination of predictor terms onto which the projection was performed.

## Usage

```
predictor_terms(object, ...)
## S3 method for class 'projection'
predictor_terms(object, ...)
```

# **Arguments**

object An object of class projection (returned by project(), possibly as elements of a list) from which to retrieve the predictor terms.

... Currently ignored.

# Value

A character vector of predictor terms.

# **Examples**

46 print.refmodel

print.projection

Print information about project() output

## **Description**

This is the print() method for objects of class projection. This method mainly exists to avoid cluttering the console when printing such objects accidentally.

## Usage

```
## S3 method for class 'projection'
print(x, ...)
```

# **Arguments**

x An object of class projection (returned by project(), possibly as elements of a list).

... Currently ignored.

#### Value

The input object x (invisible).

print.refmodel

Print information about a reference model object

# Description

This is the print() method for reference model objects (objects of class refmodel). This method mainly exists to avoid cluttering the console when printing such objects accidentally.

## Usage

```
## S3 method for class 'refmodel'
print(x, ...)
```

# Arguments

x An object of class refmodel (returned by get\_refmodel()) or init\_refmodel()).

... Currently ignored.

#### Value

The input object x (invisible).

print.vsel 47

print.vsel

Print results (summary) of a varsel() or cv\_varsel() run

## **Description**

This is the print() method for vsel objects (returned by varsel() or cv\_varsel()). It displays a summary of a varsel() or cv\_varsel() run by first calling summary.vsel() and then print.vselsummary().

# Usage

```
## S3 method for class 'vsel'
print(x, digits = getOption("projpred.digits", 2), ...)
```

# Arguments

```
x An object of class vsel (returned by varsel() or cv_varsel()).

digits Passed to argument digits of print.vselsummary().

... Arguments passed to summary.vsel().
```

## Value

The output of summary.vsel() (invisible).

print.vselsummary

Print summary of a varsel() or cv\_varsel() run

# **Description**

This is the print() method for summary objects created by summary.vsel(). It displays a summary of the results from a varsel() or cv\_varsel() run.

## Usage

```
## S3 method for class 'vselsummary'
print(x, digits = getOption("projpred.digits", 2), ...)
```

# Arguments

X	An object of class vselsummary.
digits	Passed to print.data.frame() (for the table containing the submodel performance evaluation results) and print.default() (for the vector containing the reference model performance evaluation results).
	Arguments passed to print.data.frame() (for the table containing the submodel performance evaluation results) and print.default() (for the vector containing the reference model performance evaluation results).

48 project

#### **Details**

In the submodel predictive performance table printed at (or towards) the bottom, column ranking\_fulldata contains the full-data predictor ranking and column cv\_proportions\_diag contains the main diagonal of the matrix returned by cv\_proportions() (with cumulate as set in the summary.vsel() call that created x). To retrieve the fold-wise predictor rankings, use the ranking() function, possibly followed by cv\_proportions() for computing the ranking proportions (which can be visualized by plot.cv\_proportions()).

## Value

The output of summary.vsel() (invisible).

project

Projection onto submodel(s)

# Description

Project the posterior of the reference model onto the parameter space of a single submodel consisting of a specific combination of predictor terms or (after variable selection) onto the parameter space of a single or multiple submodels of specific sizes.

## Usage

```
project(
  object,
  nterms = NULL,
  solution_terms = predictor_terms,
  predictor_terms = NULL,
  refit_prj = TRUE,
  ndraws = 400,
  nclusters = NULL,
  seed = NA,
  verbose = getOption("projpred.verbose", as.integer(interactive())),
  ...
)
```

#### **Arguments**

object

An object which can be used as input to get\_refmodel() (in particular, objects of class refmodel).

nterms

Only relevant if object is of class vsel (returned by varsel()) or cv\_varsel()). Ignored if !is.null(predictor\_terms). Number of terms for the submodel (the corresponding combination of predictor terms is taken from object). If a numeric vector, then the projection is performed for each element of this vector. If NULL (and is.null(predictor\_terms)), then the value suggested by suggest\_size() is taken (with default arguments for suggest\_size(), implying that this suggested size is based on the ELPD). Note that nterms does not count the intercept, so use nterms = 0 for the intercept-only model.

49 project

solution\_terms Deprecated. Please use argument predictor\_terms instead. predictor\_terms

> If not NULL, then this needs to be a character vector of predictor terms for the submodel onto which the projection will be performed. Argument nterms is ignored in that case. For an object which is not of class vsel, predictor\_terms

must not be NULL.

A single logical value indicating whether to fit the submodels (again) (TRUE) refit\_prj

> or—if object is of class vsel—to re-use the submodel fits from the full-data search that was run when creating object (FALSE). For an object which is not of class vsel, refit\_prj must be TRUE. See also section "Details" below.

Only relevant if refit\_prj is TRUE. Number of posterior draws to be projected. ndraws

Ignored if nclusters is not NULL or if the reference model is of class datafit (in which case one cluster is used). If both (nclusters and ndraws) are NULL, the number of posterior draws from the reference model is used for ndraws. See

also section "Details" below.

nclusters Only relevant if refit\_prj is TRUE. Number of clusters of posterior draws to

> be projected. Ignored if the reference model is of class datafit (in which case one cluster is used). For the meaning of NULL, see argument ndraws. See also

section "Details" below.

seed Pseudorandom number generation (PRNG) seed by which the same results can

> be obtained again if needed. Passed to argument seed of set.seed(), but can also be NA to not call set.seed() at all. If not NA, then the PRNG state is reset (to the state before calling project()) upon exiting project(). Here, seed is used for clustering the reference model's posterior draws (if !is.null(nclusters)) and for drawing new group-level effects when predicting from a multilevel sub-

model (however, not yet in case of a GAMM) and having global option projpred.mlvl\_pred\_new

set to TRUE. (Such a prediction takes place when calculating output elements dis

and ce.)

A single integer value from the set  $\{0,1,2\}$  (if !is.null(predictor\_terms), verbose

1 and 2 have the same effect), indicating how much information (if any) to print out during the computations. Higher values indicate that more information should be printed, 0 deactivates the verbose mode. Internally, argument verbose is coerced to integer via as.integer(), so technically, a single logical

value or a single numeric value work as well.

Arguments passed to get\_refmodel() (if get\_refmodel() is actually used; see argument object) as well as to the divergence minimizer (if refit\_prj is

TRUE).

#### **Details**

Arguments ndraws and nclusters are automatically truncated at the number of posterior draws in the reference model (which is 1 for datafits). Using less draws or clusters in ndraws or nclusters than posterior draws in the reference model may result in slightly inaccurate projection performance. Increasing these arguments affects the computation time linearly.

If refit\_prj = FALSE (which is only possible if object is of class vsel), project() retrieves the submodel fits from the full-data search that was run when creating object. Usually, the search

50 project

relies on a rather coarse clustering or thinning of the reference model's posterior draws (by default, varsel() and cv\_varsel() use nclusters = 20). Consequently, project() with refit\_prj = FALSE then inherits this coarse clustering or thinning.

#### Value

If the projection is performed onto a single submodel (i.e., length(nterms) == 1 || !is.null(predictor\_terms)), an object of class projection which is a list containing the following elements:

dis Projected draws for the dispersion parameter.

ce The cross-entropy part of the Kullback-Leibler (KL) divergence from the reference model to the submodel. For some families, this is not the actual cross-entropy, but a reduced one where terms which would cancel out when calculating the KL divergence have been dropped. In case of the Gaussian family, that reduced cross-entropy is further modified, yielding merely a proxy.

wdraws\_prj Weights for the projected draws.

predictor\_terms A character vector of the submodel's predictor terms.

- outdmin A list containing the submodel fits (one fit per projected draw). This is the same as the return value of the div\_minimizer function (see init\_refmodel()), except if project() was used with an object of class vsel based on an L1 search as well as with refit\_prj = FALSE, in which case this is the output from an internal *L1-penalized* divergence minimizer.
- cl\_ref A numeric vector of length equal to the number of posterior draws in the reference model, containing the cluster indices of these draws.
- wdraws\_ref A numeric vector of length equal to the number of posterior draws in the reference model, giving the weights of these draws. These weights should be treated as not being normalized (i.e., they don't necessarily sum to 1).
- const\_wdraws\_prj A single logical value indicating whether the projected draws have constant weights (TRUE) or not (FALSE).

refmodel The reference model object.

If the projection is performed onto more than one submodel, the output from above is returned for each submodel, giving a list with one element for each submodel.

The elements of an object of class projection are not meant to be accessed directly but instead via helper functions (see the main vignette and projpred-package; see also as\_draws\_matrix.projection(), argument return\_draws\_matrix of proj\_linpred(), and argument nresample\_clusters of proj\_predict() for the intended use of the weights stored in element wdraws\_prj).

# **Examples**

```
# Data:
dat_gauss <- data.frame(y = df_gaussian$y, df_gaussian$x)

# The `stanreg` fit which will be used as the reference model (with small
# values for `chains` and `iter`, but only for technical reasons in this
# example; this is not recommended in general):
fit <- rstanarm::stan_glm(
    y ~ X1 + X2 + X3 + X4 + X5, family = gaussian(), data = dat_gauss,
    QR = TRUE, chains = 2, iter = 500, refresh = 0, seed = 9876</pre>
```

ranking 51

ranking

Predictor ranking(s)

## Description

Extracts the *predictor ranking(s)* from an object of class vsel (returned by varsel()) or cv\_varsel()). A predictor ranking is simply a character vector of predictor terms ranked by predictive relevance (with the most relevant term first). In any case, objects of class vsel contain the predictor ranking based on the *full-data* search. If an object of class vsel is based on a cross-validation (CV) with fold-wise searches (i.e., if it was created by cv\_varsel() with validate\_search = TRUE), then it also contains *fold-wise* predictor rankings.

## Usage

```
ranking(object, ...)
## S3 method for class 'vsel'
ranking(object, nterms_max = NULL, ...)
```

## **Arguments**

object The object from which to retrieve the predictor ranking(s). Possible classes may be inferred from the names of the corresponding methods (see also the description).

... Currently ignored.

Maximum submodel size (number of predictor terms) for the predictor ranking(s), i.e., the submodel size at which to cut off the predictor ranking(s). Using NULL is effectively the same as setting nterms\_max to the full model size, i.e.,

this means to not cut off the predictor ranking(s) at all. Note that nterms\_max does not count the intercept, so nterms\_max = 1 corresponds to the submodel consisting of the first (non-intercept) predictor term.

#### Value

An object of class ranking which is a list with the following elements:

- fulldata: The predictor ranking from the full-data search.
- foldwise: The predictor rankings from the fold-wise searches in the form of a character matrix (only available if object is based on a CV with fold-wise searches, otherwise element foldwise is NULL). The rows of this matrix correspond to the CV folds and the columns to the submodel sizes. Each row contains the predictor ranking from the search of that CV fold.

#### See Also

```
cv_proportions()
```

## **Examples**

```
# For an example, see `?plot.cv_proportions`.
```

refmodel-init-get

Reference model and more general information

# **Description**

Function get\_refmodel() is a generic function whose methods usually call init\_refmodel() which is the underlying workhorse (and may also be used directly without a call to get\_refmodel()).

Both, get\_refmodel() and init\_refmodel(), create an object containing information needed for the projection predictive variable selection, namely about the reference model, the submodels, and how the projection should be carried out. For the sake of simplicity, the documentation may refer to the resulting object also as "reference model" or "reference model object", even though it also contains information about the submodels and the projection.

A "typical" reference model object is created by get\_refmodel.stanreg() and brms::get\_refmodel.brmsfit(), either implicitly by a call to a top-level function such as project(), varsel(), and cv\_varsel() or explicitly by a call to get\_refmodel(). All non-"typical" reference model objects will be called "custom" reference model objects.

Some arguments are for K-fold cross-validation (K-fold CV) only; see cv\_varsel() for the use of K-fold CV in **projpred**.

## Usage

```
get_refmodel(object, ...)
## S3 method for class 'refmodel'
get_refmodel(object, ...)
## S3 method for class 'vsel'
get_refmodel(object, ...)
## S3 method for class 'projection'
get_refmodel(object, ...)
## Default S3 method:
get_refmodel(object, family = NULL, ...)
## S3 method for class 'stanreg'
get_refmodel(object, latent = FALSE, dis = NULL, ...)
init_refmodel(
  object,
  data,
  formula,
  family,
  ref_predfun = NULL,
  div_minimizer = NULL,
  proj_predfun = NULL,
  extract_model_data = NULL,
  cvfun = NULL,
  cvfits = NULL,
  dis = NULL,
  cvrefbuilder = NULL,
  called_from_cvrefbuilder = FALSE,
)
```

# Arguments

object

For init\_refmodel(), an object that the functions from arguments extract\_model\_data and ref\_predfun can be applied to, with a NULL object being treated specially (see section "Value" below). For get\_refmodel.default(), an object that function family() can be applied to in order to retrieve the family (if argument family is NULL), additionally to the properties required for init\_refmodel(). For non-default methods of get\_refmodel(), an object of the corresponding class.

. . .

For get\_refmodel.default() and get\_refmodel.stanreg(): arguments passed to init\_refmodel(). For the get\_refmodel() generic: arguments passed to the appropriate method. For init\_refmodel(): arguments passed to extend\_family() (apart from family).

family

An object of class family representing the observation model (i.e., the distributional family for the response) of the submodels. (However, the link and the inverse-link function of this family are also used for quantities like predictions and fitted values related to the reference model.) May be NULL for get\_refmodel.default() in which case the family is retrieved from object. For custom reference models, family does not have to coincide with the family of the reference model (if the reference model possesses a formal family at all). In typical reference models, however, these families do coincide. Furthermore, the latent projection is an exception where family is not the family of the submodels (in that case, the family of the submodels is the gaussian() family).

latent

A single logical value indicating whether to use the latent projection (TRUE) or not (FALSE). Note that setting latent = TRUE causes all arguments starting with augdat\_ to be ignored.

dis

A vector of posterior draws for the reference model's dispersion parameter or more precisely—the posterior values for the reference model's parameter-conditional predictive variance (assuming that this variance is the same for all observations). May be NULL if the submodels have no dispersion parameter or if the submodels do have a dispersion parameter, but object is NULL (in which case 0 is used for dis). Note that for the gaussian() family, dis is the standard deviation, not the variance.

data

A data. frame containing the data to use for the projection predictive variable selection. Any contrasts attributes of the dataset's columns are silently removed. For custom reference models, the columns of data do not necessarily have to coincide with those of the dataset used for fitting the reference model, but keep in mind that a row-subset of data is used for argument newdata of  $ref_predfun during K-fold CV.$ 

formula

The full formula to use for the search procedure. For custom reference models, this does not necessarily coincide with the reference model's formula. For general information about formulas in R, see formula. For information about possible right-hand side (i.e., predictor) terms in formula here, see the main vignette and section "Formula terms" below. For multilevel formulas, see also package **lme4** (in particular, functions lme4::lmer() and lme4::glmer()). For additive formulas, see also packages **mgcv** (in particular, function mgcv::gam()) and **gamm4** (in particular, function gamm4::gamm4()).

ref\_predfun

Prediction function for the linear predictor of the reference model, including offsets (if existing). See also section "Arguments ref\_predfun, proj\_predfun, and div\_minimizer" below. If object is NULL, ref\_predfun is ignored and an internal default is used instead.

div\_minimizer

A function for minimizing the Kullback-Leibler (KL) divergence from the reference model to a submodel (i.e., for performing the projection of the reference model onto a submodel). The output of div\_minimizer is used, e.g., by proj\_predfun's argument fits. See also section "Arguments ref\_predfun, proj\_predfun, and div\_minimizer" below.

proj\_predfun

Prediction function for the linear predictor of a submodel onto which the reference model is projected. See also section "Arguments ref\_predfun, proj\_predfun, and div\_minimizer" below.

extract\_model\_data

A function for fetching some variables (response, observation weights, offsets) from the original dataset (supplied to argument data) or from a new dataset. May be NULL for using an internal default that essentially corresponds to y\_wobs\_offs(). See also section "Argument extract\_model\_data" below.

cvfun

For K-fold CV only. A function that, given a fold indices vector, fits the reference model separately for each fold and returns the K model fits as a list. If object is NULL, cvfun may be NULL for using an internal default. Only one of cvfits and cvfun needs to be provided (for K-fold CV). Note that cvfits takes precedence over cvfun, i.e., if both are provided, cvfits is used.

cvfits

For K-fold CV only. A list containing the K reference model refits from which reference model objects are created. This list needs to have an attribute called folds, consisting of an integer vector giving the fold indices (one fold index per observation). Only one of cvfits and cvfun needs to be provided (for K-fold CV). Note that cvfits takes precedence over cvfun, i.e., if both are provided, cvfits is used.

cvrefbuilder

For K-fold CV only. A function that, given a reference model fit for fold  $k \in \{1,...,K\}$ , returns an object of the same type as  $\mathtt{init\_refmodel}()$  does. The reference model fit for fold k is the k-th element of the return value of  $\mathtt{cvfun}$  or the k-th element of the list supplied to  $\mathtt{cvfits}$  (either here in  $\mathtt{init\_refmodel}()$  or in  $\mathtt{cv\_varsel.refmodel}()$ ), extended by elements  $\mathtt{omitted}$  (containing the indices of the left-out observations in that fold) and  $\mathtt{projpred\_k}$  (containing the integer k) if that k-th element is a list itself (otherwise,  $\mathtt{omitted}$  and  $\mathtt{projpred\_k}$  are appended as attributes). Argument  $\mathtt{cvrefbuilder}$  may be NULL for using an internal default:  $\mathtt{get\_refmodel}()$  if object is not NULL and a function calling  $\mathtt{init\_refmodel}()$  appropriately (with the assumption  $\mathtt{dis} = \emptyset$ ) if object is NULL.

## called\_from\_cvrefbuilder

A single logical value indicating whether <code>init\_refmodel()</code> is called from a <code>cvrefbuilder</code> function (TRUE) or not (FALSE). Currently, TRUE only causes some warnings to be suppressed (warnings which don't need to be thrown for each of the K reference model objects because it is sufficient to throw them for the original reference model object only). This argument is mainly for internal use, but may also be helpful for users with a custom <code>cvrefbuilder</code> function.

#### Value

An object that can be passed to all the functions that take the reference model fit as the first argument, such as varsel(), cv\_varsel(), project(), proj\_linpred(), and proj\_predict(). Usually, the returned object is of class refmodel. However, if object is NULL, the returned object is of class datafit as well as of class refmodel (with datafit being first). Objects of class datafit are handled differently at several places throughout this package.

The elements of the returned object are not meant to be accessed directly but instead via downstream functions (see the functions mentioned above as well as predict.refmodel()).

## Formula terms

Although bad practice (in general), a reference model lacking an intercept can be used within **projected**. However, it will always be projected onto submodels which *include* an intercept. The reason is that even if the true intercept in the reference model is zero, this does not need to hold for the submodels.

In multilevel (group-level) terms, function calls on the right-hand side of the | character (e.g., (1 | gr(group\_variable)), which is possible in **brms**) are currently not allowed in **projpred**.

For additive models (still an experimental feature), only mgcv::s() and mgcv::t2() are currently supported as smooth terms. Furthermore, these need to be called without any arguments apart from the predictor names (symbols). For example, for smoothing the effect of a predictor x, only s(x) or t2(x) are allowed. As another example, for smoothing the joint effect of two predictors x and z, only s(x, z) or t2(x, z) are allowed (and analogously for higher-order joint effects, e.g., of three predictors). Note that all smooth terms need to be included in formula (there is no random argument as in rstanarm::stan\_gamm4(), for example).

## Arguments ref\_predfun, proj\_predfun, and div\_minimizer

Arguments ref\_predfun, proj\_predfun, and div\_minimizer may be NULL for using an internal default (see projpred-package for the functions used by the default divergence minimizers). Otherwise, let N denote the number of observations (in case of CV, these may be reduced to each fold),  $S_{\rm ref}$  the number of posterior draws for the reference model's parameters, and  $S_{\rm prj}$  the number of draws for the parameters of a submodel that the reference model has been projected onto (short: the number of projected draws). For the augmented-data projection, let  $C_{\rm cat}$  denote the number of response categories,  $C_{\rm lat}$  the number of latent response categories (which typically equals  $C_{\rm cat}-1$ ), and define  $N_{\rm augcat}:=N\cdot C_{\rm cat}$  as well as  $N_{\rm auglat}:=N\cdot C_{\rm lat}$ . Then the functions supplied to these arguments need to have the following prototypes:

- ref\_predfun: ref\_predfun(fit, newdata = NULL) where:
  - fit accepts the reference model fit as given in argument object (but possibly refitted to a subset of the observations, as done in K-fold CV).
  - newdata accepts either NULL (for using the original dataset, typically stored in fit) or data for new observations (at least in the form of a data.frame).
- proj\_predfun: proj\_predfun(fits, newdata) where:
  - fits accepts a list of length  $S_{\rm prj}$  containing this number of submodel fits. This list is the same as that returned by project() in its output element outdmin (which in turn is the same as the return value of div\_minimizer, except if project() was used with an object of class vsel based on an L1 search as well as with refit\_prj = FALSE).
  - newdata accepts data for new observations (at least in the form of a data. frame).
- div\_minimizer does not need to have a specific prototype, but it needs to be able to be called with the following arguments:
  - formula accepts either a standard formula with a single response (if  $S_{\rm prj}=1$  or in case of the augmented-data projection) or a formula with  $S_{\rm prj}>1$  response variables cbind()-ed on the left-hand side in which case the projection has to be performed for each of the response variables separately.
  - data accepts a data. frame to be used for the projection. In case of the traditional or the latent projection, this dataset has N rows. In case of the augmented-data projection, this dataset has  $N_{\rm augcat}$  rows.

- family accepts an object of class family.
- weights accepts either observation weights (at least in the form of a numeric vector) or NULL (for using a vector of ones as weights).
- projpred\_var accepts an  $N \times S_{\rm prj}$  matrix of predictive variances (necessary for **projpred**'s internal GLM fitter) in case of the traditional or the latent projection and an  $N_{\rm augcat} \times S_{\rm prj}$  matrix (containing only NAs) in case of the augmented-data projection.
- projpred\_ws\_aug accepts an  $N \times S_{\rm prj}$  matrix of expected values for the response in case of the traditional or the latent projection and an  $N_{\rm augcat} \times S_{\rm prj}$  matrix of probabilities for the response categories in case of the augmented-data projection.
- . . . accepts further arguments specified by the user (or by **projpred**).

The return value of these functions needs to be:

- ref\_predfun: for the traditional or the latent projection, an  $N \times S_{\rm ref}$  matrix; for the augmented-data projection, an  $S_{\rm ref} \times N \times C_{\rm lat}$  array (the only exception is the augmented-data projection for the binomial() family in which case ref\_predfun needs to return an  $N \times S_{\rm ref}$  matrix just like for the traditional projection because the array is constructed by an internal wrapper function).
- proj\_predfun: for the traditional or the latent projection, an  $N \times S_{\rm prj}$  matrix; for the augmented-data projection, an  $N \times C_{\rm lat} \times S_{\rm prj}$  array.
- div\_minimizer: a list of length  $S_{\rm prj}$  containing this number of submodel fits.

#### Argument extract\_model\_data

The function supplied to argument extract\_model\_data needs to have the prototype

where:

- object accepts the reference model fit as given in argument object (but possibly refitted to a subset of the observations, as done in *K*-fold CV).
- newdata accepts data for new observations (at least in the form of a data.frame).
- wrhs accepts at least (i) a right-hand side formula consisting only of the variable in newdata containing the observation weights or (ii) NULL for using the observation weights corresponding to newdata (typically, the observation weights are stored in a column of newdata; if the model was fitted without observation weights, a vector of ones should be used).
- orhs accepts at least (i) a right-hand side formula consisting only of the variable in newdata containing the offsets or (ii) NULL for using the offsets corresponding to newdata (typically, the offsets are stored in a column of newdata; if the model was fitted without offsets, a vector of zeros should be used).
- extract\_y accepts a single logical value indicating whether output element y (see below) shall be NULL (TRUE) or not (FALSE).

The return value of extract\_model\_data needs to be a list with elements y, weights, and offset, each being a numeric vector containing the data for the response, the observation weights,

and the offsets, respectively. An exception is that y may also be NULL (depending on argument extract\_y), a non-numeric vector, or a factor.

The weights and offsets returned by extract\_model\_data will be assumed to hold for the reference model as well as for the submodels.

Above, arguments wrhs and orhs were assumed to have defaults of NULL. It should be possible to use defaults other than NULL, but we strongly recommend to use NULL. If defaults other than NULL are used, they need to imply the behaviors described at items "(ii)" (see the descriptions of wrhs and orhs).

## Augmented-data projection

If a custom reference model for an augmented-data projection is needed, see also extend\_family().

For the augmented-data projection, the response vector resulting from extract\_model\_data is internally coerced to a factor (using as.factor()). The levels of this factor have to be identical to family\$cats (after applying extend\_family() internally; see extend\_family()'s argument augdat\_y\_unqs).

Note that response-specific offsets (i.e., one length-N offset vector per response category) are not supported by **projpred** yet. So far, only offsets which are the same across all response categories are supported. This is why in case of the brms::categorical() family, offsets are currently not supported at all.

Currently, object = NULL (i.e., a datafit; see section "Value") is not supported in case of the augmented-data projection.

# Latent projection

If a custom reference model for a latent projection is needed, see also extend\_family().

For the latent projection, family\$cats (after applying extend\_family() internally; see extend\_family()'s argument latent\_y\_unqs) currently must not be NULL if the original (i.e., non-latent) response is a factor. Conversely, if family\$cats (after applying extend\_family()) is non-NULL, the response vector resulting from extract\_model\_data is internally coerced to a factor (using as.factor()). The levels of this factor have to be identical to that non-NULL element family\$cats.

Currently, object = NULL (i.e., a datafit; see section "Value") is not supported in case of the latent projection.

## **Examples**

```
# Data:
dat_gauss <- data.frame(y = df_gaussian$y, df_gaussian$x)

# The `stanreg` fit which will be used as the reference model (with small
# values for `chains` and `iter`, but only for technical reasons in this
# example; this is not recommended in general):
fit <- rstanarm::stan_glm(
    y ~ X1 + X2 + X3 + X4 + X5, family = gaussian(), data = dat_gauss,
    QR = TRUE, chains = 2, iter = 500, refresh = 0, seed = 9876
)

# Define the reference model object explicitly:</pre>
```

run\_cvfun 59

```
ref <- get_refmodel(fit)</pre>
print(class(ref)) # gives `"refmodel"`
# Now see, for example, `?varsel`, `?cv_varsel`, and `?project` for
# possible post-processing functions. Most of the post-processing functions
# call get_refmodel() internally at the beginning, so you will rarely need
# to call get_refmodel() yourself.
# A custom reference model object which may be used in a variable selection
# where the candidate predictors are not a subset of those used for the
# reference model's predictions:
ref_cust <- init_refmodel(</pre>
 fit,
 data = dat_gauss,
 formula = y \sim X6 + X7,
 family = gaussian(),
 cvfun = function(folds) {
   kfold(
      fit, K = max(folds), save_fits = TRUE, folds = folds, cores = 1
   )$fits[, "fit"]
 },
 dis = as.matrix(fit)[, "sigma"],
 cvrefbuilder = function(cvfit) {
    init_refmodel(cvfit,
                  data = dat_gauss[-cvfit$omitted, , drop = FALSE],
                  formula = y \sim X6 + X7,
                  family = gaussian(),
                  dis = as.matrix(cvfit)[, "sigma"],
                  called_from_cvrefbuilder = TRUE)
 }
)
# Now, the post-processing functions mentioned above (for example,
# varsel(), cv_varsel(), and project()) may be applied to `ref_cust`.
```

run\_cvfun

Create cvfits from cvfun

## **Description**

A helper function that can be used to create input for cv\_varsel.refmodel()'s argument cvfits by running first cv\_folds() and then the reference model object's cvfun (see init\_refmodel()). This is helpful if K-fold CV is run multiple times based on the same K reference model refits.

# Usage

```
run_cvfun(object, ...)
## Default S3 method:
run_cvfun(object, ...)
```

run\_cvfun

```
## S3 method for class 'refmodel'
run_cvfun(
  object,
  K = if (!inherits(object, "datafit")) 5 else 10,
  folds = NULL,
  seed = NA,
   ...
)
```

## **Arguments**

object	An object of class refmodel (returned by get_refmodel() or init_refmodel()) or an object that can be passed to argument object of get_refmodel().
• • •	For run_cvfun.default(): Arguments passed to get_refmodel(). For run_cvfun.refmodel(): Currently ignored.
К	Number of folds. Must be at least 2 and not exceed the number of observations. Ignored if folds is not NULL.
folds	Either NULL for determining the CV folds automatically via cv_folds() (using argument K) or a numeric (in fact, integer) vector giving the fold index for each observation. In the latter case, argument K is ignored.
seed	Pseudorandom number generation (PRNG) seed by which the same results can be obtained again if needed. Passed to argument seed of set.seed(), but can also be NA to not call set.seed() at all. If not NA, then the PRNG state is reset (to the state before calling run_cvfun()) upon exiting run_cvfun().

# Value

An object that can be used as input for cv\_varsel.refmodel()'s argument cvfits.

# **Examples**

```
# Data:
dat_gauss <- data.frame(y = df_gaussian$y, df_gaussian$x)</pre>
# The `stanreg` fit which will be used as the reference model (with small
# values for `chains` and `iter`, but only for technical reasons in this
# example; this is not recommended in general):
fit <- rstanarm::stan_glm(</pre>
  y \sim X1 + X2 + X3 + X4 + X5, family = gaussian(), data = dat_gauss,
  QR = TRUE, chains = 2, iter = 500, refresh = 0, seed = 9876
)
# Define the reference model object explicitly (not really necessary here
# because the get_refmodel() call is quite fast in this example, but in
# general, this approach is faster than defining the reference model object
# multiple times implicitly):
ref <- get_refmodel(fit)</pre>
# Run the reference model object's `cvfun` (with a small value for `K`, but
# only for the sake of speed in this example; this is not recommended in
```

solution\_terms 61

```
# general):
cv_fits <- run_cvfun(ref, K = 2, seed = 184)
# Run cv_varsel() (with L1 search and small values for `nterms_max` and
# `nclusters_pred`, but only for the sake of speed in this example; this is
# not recommended in general) and use `cv_fits` there:
cvvs_L1 <- cv_varsel(ref, method = "L1", cv_method = "kfold",</pre>
                     cvfits = cv_fits, nterms_max = 3, nclusters_pred = 10,
                     seed = 5555)
# Now see, for example, `?print.vsel`, `?plot.vsel`, `?suggest_size.vsel`,
# and `?ranking` for possible post-processing functions.
# The purpose of run_cvfun() is to create an object that can be used in
# multiple cv_varsel() calls, e.g., to check the sensitivity to the search
# method (L1 or forward):
cvvs_fw <- cv_varsel(ref, method = "forward", cv_method = "kfold",</pre>
                     cvfits = cv_fits, nterms_max = 3, nclusters = 5,
                     nclusters_pred = 10, seed = 5555)
# Stratified K-fold CV is straightforward:
n_strat <- 3L
set.seed(692)
# Some example strata:
strat_fac <- sample(paste0("lvl", seq_len(n_strat)), size = nrow(dat_gauss),</pre>
                    replace = TRUE,
                    prob = diff(c(0, pnorm(seq_len(n_strat - 1L) - 0.5), 1)))
table(strat_fac)
# Use loo::kfold_split_stratified() to create the folds vector:
folds_strat <- loo::kfold_split_stratified(K = 2, x = strat_fac)</pre>
table(folds_strat, strat_fac)
# Call run_cvfun(), but this time with argument `folds` instead of `K` (here,
# specifying argument `seed` would not be necessary because of the set.seed()
# call above, but we specify it nonetheless for the sake of generality):
cv_fits_strat <- run_cvfun(ref, folds = folds_strat, seed = 391)</pre>
# Now use `cv_fits_strat` analogously to `cv_fits` from above.
```

solution\_terms

Retrieve the full-data solution path from a varsel() or cv\_varsel() run or the predictor combination from a project() run

# Description

The solution\_terms.vsel() method retrieves the solution path from a full-data search (vsel objects are returned by varsel() or cv\_varsel()). The solution\_terms.projection() method retrieves the predictor combination onto which a projection was performed (projection objects are returned by project(), possibly as elements of a list). Both methods (and hence also the solution\_terms() generic) are deprecated and will be removed in a future release. Please use ranking() instead of solution\_terms.vsel() (ranking()'s output element fulldata contains the full-data predictor ranking that is extracted by solution\_terms.vsel(); ranking()'s output

62 suggest\_size

element foldwise contains the fold-wise predictor rankings—if available—which were previously not accessible via a built-in function) and predictor\_terms() instead of solution\_terms.projection().

# Usage

```
solution_terms(object, ...)
## S3 method for class 'vsel'
solution_terms(object, ...)
## S3 method for class 'projection'
solution_terms(object, ...)
```

## **Arguments**

object The object from which to retrieve the predictor terms. Possible classes may be inferred from the names of the corresponding methods (see also the description).

... Currently ignored.

#### Value

A character vector of predictor terms.

suggest\_size

Suggest submodel size

# **Description**

This function can suggest an appropriate submodel size based on a decision rule described in section "Details" below. Note that this decision is quite heuristic and should be interpreted with caution. It is recommended to examine the results via plot.vsel(), cv\_proportions(), plot.cv\_proportions(), and/or summary.vsel() and to make the final decision based on what is most appropriate for the problem at hand.

# Usage

```
suggest_size(object, ...)
## S3 method for class 'vsel'
suggest_size(
  object,
  stat = "elpd",
  pct = 0,
  type = "upper",
  thres_elpd = NA,
  warnings = TRUE,
  ...
)
```

suggest\_size 63

#### **Arguments**

object	An object of class vsel (returned by varsel() or cv_varsel()).
	Arguments passed to summary.vsel(), except for object, stats (which is set to stat), type, and deltas (which is set to TRUE). See section "Details" below for some important arguments which may be passed here.
stat	Performance statistic (i.e., utility or loss) used for the decision. See argument stats of summary.vsel() and plot.vsel() for possible choices.
pct	A number giving the proportion ( <i>not</i> percents) of the <i>relative</i> null model utility one is willing to sacrifice. See section "Details" below for more information.
type	Either "upper" or "lower" determining whether the decision is based on the upper or lower uncertainty interval bound, respectively. See section "Details" below for more information.
thres_elpd	Only relevant if stat %in% c("elpd", "mlpd", "gmpd")). The threshold for the ELPD difference (taking the submodel's ELPD minus the baseline model's ELPD) above which the submodel's ELPD is considered to be close enough to the baseline model's ELPD. An equivalent rule is applied in case of the MLPD and the GMPD. See section "Details" for a formalization. Supplying NA deactivates this.
warnings	Mainly for internal use. A single logical value indicating whether to throw warnings if automatic suggestion fails. Usually there is no reason to set this to FALSE.

## **Details**

In general (beware of special cases below), the suggested model size is the smallest model size  $j \in \{0,1,...,\text{nterms\_max}\}$  for which either the lower or upper bound (depending on argument type) of the uncertainty interval (with nominal coverage 1 – alpha; see argument alpha of summary.vsel()) for  $U_j - U_{\text{base}}$  (with  $U_j$  denoting the j-th submodel's true utility and  $U_{\text{base}}$  denoting the baseline model's true utility) falls above (or is equal to)

$$pct \cdot (u_0 - u_{base})$$

where  $u_0$  denotes the null model's estimated utility and  $u_{\text{base}}$  the baseline model's estimated utility. The baseline model is either the reference model or the best submodel found (see argument baseline of summary.vsel()).

In doing so, loss statistics like the root mean squared error (RMSE) and the mean squared error (MSE) are converted to utilities by multiplying them by -1, so a call such as suggest\_size(object, stat = "rmse", type = "upper") finds the smallest model size whose upper uncertainty interval bound for the *negative* RMSE or MSE exceeds (or is equal to) the cutoff (or, equivalently, has the lower uncertainty interval bound for the RMSE or MSE below—or equal to—the cutoff). This is done to make the interpretation of argument type the same regardless of argument stat.

For the geometric mean predictive density (GMPD), the decision rule above is applied on  $\log()$  scale. In other words, if the true GMPD is denoted by  $U_j^*$  for the j-th submodel and  $U_{\rm base}^*$  for the baseline model (so that  $U_j$  and  $U_{\rm base}$  from above are given by  $U_j = \log(U_j^*)$  and  $U_{\rm base} = \log(U_{\rm base}^*)$ ), then  $\operatorname{suggest\_size}()$  yields the smallest model size whose lower or upper (depending on argument type) uncertainty interval bound for  $\frac{U_j^*}{U_{\rm base}^*}$  exceeds (or is equal to)

$$\left(\frac{u_0^*}{u_{\mathrm{base}}^*}\right)^{\mathrm{pct}}$$

64 suggest\_size

where  $u_0^*$  denotes the null model's estimated GMPD and  $u_{\text{base}}^*$  the baseline model's estimated GMPD.

If !is.na(thres\_elpd) and stat = "elpd", the decision rule above is extended: The suggested model size is then the smallest model size j fulfilling the rule above  $or\ u_j - u_{\rm base} > {\rm thres\_elpd}$ . Correspondingly, in case of stat = "mlpd" (and !is.na(thres\_elpd)), the suggested model size is the smallest model size j fulfilling the rule above  $or\ u_j - u_{\rm base} > \frac{{\rm thres\_elpd}}{N}$  with N denoting the number of observations. Correspondingly, in case of stat = "gmpd" (and !is.na(thres\_elpd)), the suggested model size is the smallest model size j fulfilling the rule above  $or\ \frac{u_j^*}{u_{\rm base}^*} > \exp(\frac{{\rm thres\_elpd}}{N})$ .

For example (disregarding the special extensions in case of !is.na(thres\_elpd) with stat %in% c("elpd", "mlpd", "gmpd")), alpha = 2 \* pnorm(-1), pct = 0, and type = "upper" means that we select the smallest model size for which the upper bound of the 1 - 2 \* pnorm(-1) (approximately 68.3 %) uncertainty interval for  $U_j - U_{\text{base}}$  ( $\frac{U_j^*}{U_{\text{base}}^*}$  in case of the GMPD) exceeds (or is equal to) zero (one in case of the GMPD), that is (if stat is a performance statistic for which a normal-approximation uncertainty interval is used, see argument stats of summary.vsel() and plot.vsel()), for which the submodel's utility estimate is at most one standard error smaller than the baseline model's utility estimate (with that standard error referring to the utility difference).

Apart from the two summary.vsel() arguments mentioned above (alpha and baseline), resp\_oscale is another important summary.vsel() argument that may be passed via . . . .

#### Value

A single numeric value, giving the suggested submodel size (or NA if the suggestion failed).

The intercept is not counted by suggest\_size(), so a suggested size of zero stands for the interceptonly model.

## **Examples**

summary.vsel 65

summary.vsel

Summary of a varsel() or cv\_varsel() run

## **Description**

This is the summary() method for vsel objects (returned by varsel() or cv\_varsel()). Apart from some general information about the varsel() or cv\_varsel() run, it shows the full-data predictor ranking, basic information about the (CV) variability in the ranking of the predictors (if available; inferred from cv\_proportions()), and estimates for user-specified predictive performance statistics. For a graphical representation, see plot.vsel(). For extracting the predictive performance results printed at the bottom of the output created by this summary() method, see performances().

# Usage

```
## S3 method for class 'vsel'
summary(
  object,
  nterms_max = NULL,
  stats = "elpd",
  type = c("mean", "se", "diff", "diff.se"),
  deltas = FALSE,
  alpha = 2 * pnorm(-1),
  baseline = if (!inherits(object$refmodel, "datafit")) "ref" else "best",
  resp_oscale = TRUE,
  cumulate = FALSE,
  ...
)
```

#### **Arguments**

object

An object of class vsel (returned by varsel() or cv\_varsel()).

nterms\_max

Maximum submodel size (number of predictor terms) for which the performance statistics are calculated. Using NULL is effectively the same as length(ranking(object)\$fulldata). Note that nterms\_max does not count the intercept, so use nterms\_max = 0 for the intercept-only model. For plot.vsel(), nterms\_max must be at least 1.

stats

One or more character strings determining which performance statistics (i.e., utilities or losses) to estimate based on the observations in the evaluation (or "test") set (in case of cross-validation, these are all observations because they are partitioned into multiple test sets; in case of varsel() with d\_test = NULL, these are again all observations because the test set is the same as the training set). Available statistics are:

"elpd": expected log (pointwise) predictive density (for a new dataset)
(ELPD). Estimated by the sum of the observation-specific log predictive
density values (with each of these predictive density values being a—possibly
weighted—average across the parameter draws). For the corresponding uncertainty interval, a normal approximation is used.

66 summary.vsel

 "mlpd": mean log predictive density (MLPD), that is, the ELPD divided by the number of observations. For the corresponding uncertainty interval, a normal approximation is used.

- "gmpd": geometric mean predictive density (GMPD), that is, exp() of the MLPD. The GMPD is especially helpful for discrete response families (because there, the GMPD is bounded by zero and one). For the corresponding standard error, the delta method is used. The corresponding uncertainty interval type is "exponentiated normal approximation" because the uncertainty interval bounds are the exponentiated uncertainty interval bounds of the MLPD.
- "mse": mean squared error (only available in the situations mentioned in section "Details" below). For the corresponding uncertainty interval, a lognormal approximation is used if deltas is FALSE and a normal approximation is used if deltas is TRUE (or "mixed", in case of plot.vsel()).
- "rmse": root mean squared error (only available in the situations mentioned in section "Details" below). For the corresponding standard error, the delta method is used. For the corresponding uncertainty interval, a log-normal approximation is used if deltas is FALSE and a normal approximation is used if deltas is TRUE (or "mixed", in case of plot.vsel()).
- "R2": R-squared, i.e., coefficient of determination (only available in the situations mentioned in section "Details" below). For the corresponding standard error, the delta method is used. For the corresponding uncertainty interval, a normal approximation is used.
- "acc" (or its alias, "pctcorr"): classification accuracy (only available in the situations mentioned in section "Details" below). By "classification accuracy", we mean the proportion of correctly classified observations. For this, the response category ("class") with highest probability (the probabilities are model-based) is taken as the prediction ("classification") for an observation. For the corresponding uncertainty interval, a normal approximation is used.
- "auc": area under the ROC curve (only available in the situations mentioned in section "Details" below). For the corresponding standard error and lower and upper uncertainty interval bounds, bootstrapping is used. Not supported in case of subsampled LOO-CV (see argument nloo of cv\_varsel()).

type

One or more items from "mean", "se", "lower", "upper", "diff", "diff.lower", "diff.upper", and "diff.se" indicating which of these to compute for each item from stats (mean, standard error, lower and upper uncertainty interval bounds, mean difference to the corresponding statistic of the reference model, lower and upper uncertainty interval bound for this difference, and standard error of this difference, respectively; note that for the GMPD, "diff", "diff.lower", "diff.upper", and "diff.se" actually refer to the ratio vs. the reference model, not the difference). The uncertainty interval bounds belong to uncertainty intervals with (nominal) coverage 1 - alpha. Items "diff", "diff.lower", "diff.upper", and "diff.se" are only supported if deltas is FALSE.

deltas

May be set to FALSE or TRUE. If FALSE, the submodel performance statistics are estimated on their actual scale. If TRUE, the submodel statistics are estimated relatively to the baseline model (see argument baseline). For the GMPD, the term

67 summary.vsel

> "relatively" refers to the *ratio* vs. the baseline model (i.e., the submodel statistic divided by the baseline model statistic). For all other stats, "relatively" refers to the difference from the baseline model (i.e., the submodel statistic minus the

baseline model statistic).

alpha A number determining the (nominal) coverage 1 - alpha of the uncertainty in-

> tervals. For example, in case of a normal-approximation uncertainty interval, alpha = 2 \* pnorm(-1) corresponds to a uncertainty interval stretching by one

standard error on either side of the point estimate.

baseline For summary.vsel(): Only relevant if deltas is TRUE. For plot.vsel(): Al-

> ways relevant. Either "ref" or "best", indicating whether the baseline is the reference model or the best submodel found (in terms of stats[1]), respectively. In case of subsampled LOO-CV, baseline = "best" is not supported.

resp\_oscale Only relevant for the latent projection. A single logical value indicating whether

to calculate the performance statistics on the original response scale (TRUE) or

on latent scale (FALSE).

cumulate Passed to argument cumulate of cv\_proportions(). Affects column cv\_proportions\_diag

of the summary table.

Arguments passed to the internal function which is used for bootstrapping (if

applicable; see argument stats). Currently, relevant arguments are B (the number of bootstrap samples, defaulting to 2000) and seed (see set.seed(), but defaulting to NA so that set.seed() is not called within that function at all).

#### **Details**

The stats options "mse", "rmse", and "R2" are only available for:

- the traditional projection,
- the latent projection with resp\_oscale = FALSE,
- the latent projection with resp\_oscale = TRUE in combination with <refmodel>\$family\$cats being NULL.

The stats option "acc" (= "pctcorr") is only available for:

- the binomial() family in case of the traditional projection,
- all families in case of the augmented-data projection,
- the binomial() family (on the original response scale) in case of the latent projection with resp\_oscale = TRUE in combination with <refmodel>\$family\$cats being NULL,
- all families (on the original response scale) in case of the latent projection with resp\_oscale = TRUE in combination with <refmodel>\$family\$cats being not NULL.

The stats option "auc" is only available for:

- the binomial() family in case of the traditional projection,
- the binomial() family (on the original response scale) in case of the latent projection with resp\_oscale = TRUE in combination with <refmodel>\$family\$cats being NULL.

Note that the stats option "auc" is not supported in case of subsampled LOO-CV (see argument nloo of cv\_varsel()).

#### Value

An object of class vselsummary. The elements of this object are not meant to be accessed directly but instead via helper functions (print.vselsummary()) and performances.vselsummary()).

#### See Also

```
print.vselsummary(), performances.vselsummary()
```

# **Examples**

varsel

Run search and performance evaluation without cross-validation

## **Description**

Run the *search* part and the *evaluation* part for a projection predictive variable selection. The search part determines the predictor ranking (also known as solution path), i.e., the best submodel for each submodel size (number of predictor terms). The evaluation part determines the predictive performance of the submodels along the predictor ranking. A special method is varsel.vsel() which re-uses the search results from an earlier varsel() (or cv\_varsel()) run, as illustrated in the main vignette.

## Usage

```
varsel(object, ...)
## Default S3 method:
varsel(object, ...)
```

```
## S3 method for class 'vsel'
varsel(object, ...)
## S3 method for class 'refmodel'
varsel(
 object,
 d_test = NULL,
 method = "forward",
  ndraws = NULL,
 nclusters = 20,
  ndraws_pred = 400,
  nclusters_pred = NULL,
  refit_prj = !inherits(object, "datafit"),
  nterms_max = NULL,
  verbose = getOption("projpred.verbose", as.integer(interactive())),
  search_control = NULL,
  lambda_min_ratio = 1e-05,
  nlambda = 150,
  thresh = 1e-06,
  penalty = NULL,
  search_terms = NULL,
  search_out = NULL,
  seed = NA,
)
```

# **Arguments**

object	An object of class refmodel (returned by get_refmodel() or init_refmodel()) or an object that can be passed to argument object of get_refmodel().
	For varsel.default(): Arguments passed to get_refmodel() as well as to varsel.refmodel(). For varsel.vsel(): Arguments passed to varsel.refmodel(). For varsel.refmodel(): Arguments passed to the divergence minimizer (see argument div_minimizer of init_refmodel() as well as section "Draw-wise divergence minimizers" of projpred-package) when refitting the submodels for the performance evaluation (if refit_prj is TRUE).
d_test	A list of the structure outlined in section "Argument d_test" below, providing test data for evaluating the predictive performance of the submodels as well as of the reference model. If NULL, the training data is used.
method	The method for the search part. Possible options are "forward" for forward search and "L1" for L1 search. See also section "Details" below.
ndraws	Number of posterior draws used in the search part. Ignored if nclusters is not NULL or in case of L1 search (because L1 search always uses a single cluster). If both (nclusters and ndraws) are NULL, the number of posterior draws from the reference model is used for ndraws. See also section "Details" below.
nclusters	Number of clusters of posterior draws used in the search part. Ignored in case

of NULL, see argument ndraws. See also section "Details" below.

of L1 search (because L1 search always uses a single cluster). For the meaning

ndraws\_pred

Only relevant if refit\_prj is TRUE. Number of posterior draws used in the evaluation part. Ignored if nclusters\_pred is not NULL. If both (nclusters\_pred and ndraws\_pred) are NULL, the number of posterior draws from the reference model is used for ndraws\_pred. See also section "Details" below.

nclusters\_pred

Only relevant if refit\_prj is TRUE. Number of clusters of posterior draws used in the evaluation part. For the meaning of NULL, see argument ndraws\_pred. See also section "Details" below.

refit\_prj

For the evaluation part, should the projections onto the submodels along the predictor ranking be performed again using ndraws\_pred draws or nclusters\_pred clusters (TRUE) or should their projections from the search part, which used ndraws draws or nclusters clusters, be re-used (FALSE)?

nterms\_max

Maximum submodel size (number of predictor terms) up to which the search is continued. If NULL, then min(19, D) is used where D is the number of terms in the reference model (or in search\_terms, if supplied). Note that nterms\_max does not count the intercept, so use nterms\_max = 0 for the intercept-only model. (Correspondingly, D above does not count the intercept.)

verbose

A single integer value from the set  $\{0, 1, 2, 3, 4\}$  (for varse1(), 3 and 4 have the same effect), indicating how much information (if any) to print out during the computations. Higher values indicate that more information should be printed, 0 deactivates the verbose mode. Internally, argument verbose is coerced to integer via as.integer(), so technically, a single logical value or a single numeric value work as well.

search\_control A list of "control" arguments (i.e., tuning parameters) for the search. In case of forward search, these arguments are passed to the divergence minimizer (see argument div\_minimizer of init\_refmodel() as well as section "Draw-wise divergence minimizers" of projpred-package). In case of forward search, NULL causes . . . to be used not only for the performance evaluation, but also for the search. In case of L1 search, possible arguments are:

- lambda\_min\_ratio: Ratio between the smallest and largest lambda in the L1-penalized search (default: 1e-5). This parameter essentially determines how long the search is carried out, i.e., how large submodels are explored. No need to change this unless the program gives a warning about this.
- nlambda: Number of values in the lambda grid for L1-penalized search (default: 150). No need to change this unless the program gives a warning about this.
- thresh: Convergence threshold when computing the L1 path (default: 1e-6). Usually, there is no need to change this.

lambda\_min\_ratio

Deprecated (please use search\_control instead). Only relevant for L1 search. Ratio between the smallest and largest lambda in the L1-penalized search. This parameter essentially determines how long the search is carried out, i.e., how large submodels are explored. No need to change this unless the program gives a warning about this.

nlambda

Deprecated (please use search\_control instead). Only relevant for L1 search. Number of values in the lambda grid for L1-penalized search. No need to change this unless the program gives a warning about this.

thresh Deprecated (please use search\_control instead). Only relevant for L1 search.

Convergence threshold when computing the L1 path. Usually, there is no need

to change this.

penalty Only relevant for L1 search. A numeric vector determining the relative penalties

or costs for the predictors. A value of  $\emptyset$  means that those predictors have no cost and will therefore be selected first, whereas Inf means those predictors will

never be selected. If NULL, then 1 is used for each predictor.

search\_terms Only relevant for forward search. A custom character vector of predictor term

blocks to consider for the search. Section "Details" below describes more precisely what "predictor term block" means. The intercept ("1") is always included internally via union(), so there's no difference between including it explicitly or omitting it. The default search\_terms considers all the terms in the

reference model's formula.

search\_out Intended for internal use.

seed Pseudorandom number generation (PRNG) seed by which the same results can

be obtained again if needed. Passed to argument seed of set.seed(), but can also be NA to not call set.seed() at all. If not NA, then the PRNG state is reset (to the state before calling varsel()) upon exiting varsel(). Here, seed is used for clustering the reference model's posterior draws (if !is.null(nclusters) or !is.null(nclusters\_pred)) and for drawing new group-level effects when predicting from a multilevel submodel (however, not yet in case of a GAMM).

#### **Details**

Arguments ndraws, nclusters, nclusters\_pred, and ndraws\_pred are automatically truncated at the number of posterior draws in the reference model (which is 1 for datafits). Using less draws or clusters in ndraws, nclusters, nclusters\_pred, or ndraws\_pred than posterior draws in the reference model may result in slightly inaccurate projection performance. Increasing these arguments affects the computation time linearly.

For argument method, there are some restrictions: For a reference model with multilevel or additive formula terms or a reference model set up for the augmented-data projection, only the forward search is available. Furthermore, argument search\_terms requires a forward search to take effect.

L1 search is faster than forward search, but forward search may be more accurate. Furthermore, forward search may find a sparser model with comparable performance to that found by L1 search, but it may also overfit when more predictors are added. This overfit can be detected by running search validation (see cv\_varsel()).

An L1 search may select an interaction term before all involved lower-order interaction terms (including main-effect terms) have been selected. In **projpred** versions > 2.6.0, the resulting predictor ranking is automatically modified so that the lower-order interaction terms come before this interaction term, but if this is conceptually undesired, choose the forward search instead.

The elements of the search\_terms character vector don't need to be individual predictor terms. Instead, they can be building blocks consisting of several predictor terms connected by the + symbol. To understand how these building blocks work, it is important to know how **projpred**'s forward search works: It starts with an empty vector chosen which will later contain already selected predictor terms. Then, the search iterates over model sizes  $j \in \{0, ..., J\}$  (with J denoting the maximum submodel size, not counting the intercept). The candidate models at model size j are constructed

from those elements from search\_terms which yield model size j when combined with the chosen predictor terms. Note that sometimes, there may be no candidate models for model size j. Also note that internally, search\_terms is expanded to include the intercept ("1"), so the first step of the search (model size 0) always consists of the intercept-only model as the only candidate.

As a search\_terms example, consider a reference model with formula  $y \sim x1 + x2 + x3$ . Then, to ensure that x1 is always included in the candidate models, specify search\_terms = c("x1", "x1 + x2", "x1 + x3"), for which helper function force\_search\_terms() exists). This search would start with  $y \sim 1$  as the only candidate at model size 0. At model size 1,  $y \sim x1$  would be the only candidate. At model size 2,  $y \sim x1 + x2$  and  $y \sim x1 + x3$  would be the two candidates. At the last model size of 3,  $y \sim x1 + x2 + x3$  would be the only candidate. As another example, to exclude x1 from the search, specify search\_terms = c("x2", "x3", "x2 + x3") (or, in a simpler way that leads to the same results, search\_terms = c("x2", "x3")).

#### Value

An object of class vsel. The elements of this object are not meant to be accessed directly but instead via helper functions (see the main vignette and projpred-package).

#### Argument d\_test

If not NULL, then d\_test needs to be a list with the following elements:

- data: a data. frame containing the predictor variables for the test set.
- offset: a numeric vector containing the offset values for the test set (if there is no offset, use a vector of zeros).
- weights: a numeric vector containing the observation weights for the test set (if there are no observation weights, use a vector of ones).
- y: a vector or a factor containing the response values for the test set. In case of the latent projection, this has to be a vector containing the *latent* response values, but it can also be a vector full of NAs if latent-scale post-processing is not needed.
- y\_oscale: Only needs to be provided in case of the latent projection where this needs to be a vector or a factor containing the *original* (i.e., non-latent) response values for the test set.

#### See Also

```
cv_varsel()
```

## **Examples**

```
# Data:
dat_gauss <- data.frame(y = df_gaussian$y, df_gaussian$x)

# The `stanreg` fit which will be used as the reference model (with small
# values for `chains` and `iter`, but only for technical reasons in this
# example; this is not recommended in general):
fit <- rstanarm::stan_glm(
   y ~ X1 + X2 + X3 + X4 + X5, family = gaussian(), data = dat_gauss,
   QR = TRUE, chains = 2, iter = 500, refresh = 0, seed = 9876</pre>
```

y\_wobs\_offs 73

y\_wobs\_offs

Extract response values, observation weights, and offsets

# **Description**

A helper function for extracting response values, observation weights, and offsets from a dataset. It is designed for use in the extract\_model\_data function of custom reference model objects (see init\_refmodel()).

#### Usage

```
y_wobs_offs(newdata, wrhs = NULL, orhs = NULL, resp_form)
```

## **Arguments**

newdata The data. frame from which at least the response values should be extracted.

wrhs Either a right-hand side formula consisting only of the variable in newdata con-

taining the weights, NULL (for using a vector of ones), or directly the numeric

vector of observation weights.

orhs Either a right-hand side formula consisting only of the variable in newdata con-

taining the offsets, NULL (for using a vector of zeros), or directly the numeric

vector of offsets.

resp\_form If this is a formula, then the second element of this formula (if the formula

is a standard formula with both left-hand and right-hand side, then its second element is the left-hand side; if the formula is a right-hand side formula, then its second element is the right-hand side) will be extracted from newdata (so resp\_form may be either a standard formula or a right-hand side formula, but in the latter case, the right-hand side should consist only of the response variable).

In all other cases, NULL will be returned for element y of the output list.

# Value

A list with elements y, weights, and offset, each being a numeric vector containing the data for the response, the observation weights, and the offsets, respectively. An exception is that y may also be NULL (depending on argument resp\_form), a non-numeric vector, or a factor.

74 y\_wobs\_offs

# See Also

init\_refmodel()

# **Index**

* datasets	<pre>cv_proportions.vsel(), 15</pre>
df_binom, 23	cv_varsel, 16
df_gaussian, 23	cv_varsel(), 4-6, 15, 16, 19, 20, 28, 29, 31,
mesquite, 30	<i>33–35</i> , <i>38</i> , <i>47</i> , <i>48</i> , <i>50–52</i> , <i>55</i> , <i>61</i> , <i>63</i> , <i>65–68</i> , <i>71</i> , <i>72</i>
abbreviate(), <i>36</i> , <i>38</i>	<pre>cv_varsel.default(), 17</pre>
as.factor(), 26, 28, 43, 58	cv_varsel.refmodel(), 14, 17, 55, 59, 60
as.matrix(), $7$	cv_varsel.vsel(), 16, 17
as.matrix.projection,7	cvfolds (cv-indices), 13
as.matrix.projection(), $5$ , $6$ , $9$	cvfolds(), <i>14</i>
as_draws.projection	
$(as\_draws\_matrix.projection), 9$	df_binom, 23
as_draws_matrix.projection,9	df_gaussian, 23
as_draws_matrix.projection(), 5-7, 50	
<pre>augdat_ilink_binom, 11</pre>	example(), $6$
<pre>augdat_link_binom, 11</pre>	$\exp(), 35, 66$
	extend_family, 24
binomial(), 4, 11, 24, 25, 37, 38, 57, 67	extend_family(), 8, 10–12, 25, 26, 28, 42,
<pre>break_up_matrix_term, 12</pre>	43, 53, 58
<pre>brms::bernoulli(), 4</pre>	extra-families, 28
brms::brmsfamily(), 26	
brms::categorical(), 4, 8, 10, 26, 58	family, 28
brms::cumulative(), 4, 41, 44	family(), $24, 53$
<pre>brms::get_refmodel.brmsfit(), 18, 52</pre>	force_search_terms, 29
brms::loo_moment_match(), 21	force_search_terms(), 20, 72
brms::reloo(), <i>21</i>	formula, <i>3</i> , <i>12</i> , <i>54</i> , <i>56</i>
<pre>brms::resp_thres(), 26</pre>	
	gamm4::gamm4(), 4, 54
cbind(), 56	gaussian(), 4, 54
cl_agg, 12	gc(), 6
$cl_{agg}(), 28$	<pre>get_refmodel (refmodel-init-get), 52</pre>
cv-indices, 13	get_refmodel(), 6, 17, 43, 46, 48, 49, 52, 53,
cv_folds (cv-indices), 13	55, 60, 69
cv_folds(), <i>14</i> , <i>59</i> , <i>60</i>	<pre>get_refmodel.default(), 53, 54</pre>
cv_ids (cv-indices), 13	get_refmodel.stanreg(), 18, 52, 53
cv_ids(), <i>14</i>	ggplot2::element_text(), 32, 37
cv_proportions, 15	$ggplot2::geom_linerange(), 36$
cv_proportions(), 6, 16, 32, 33, 37, 48, 52,	<pre>ggplot2::geom_point(), 36</pre>
62, 65, 67	<pre>ggrepel::geom_label_repel(), 36</pre>
cv_proportions.ranking(), 15, 32	<pre>ggrepel::geom_text_repel(), 36</pre>

76 INDEX

glm(), 4	<pre>predictor_terms(), 62</pre>
	print(), 46, 47
<pre>init_refmodel (refmodel-init-get), 52</pre>	<pre>print.data.frame(), 47</pre>
init_refmodel(), 3, 6, 14, 17–19, 24, 26, 28,	<pre>print.default(), 47</pre>
40–44, 46, 50, 52, 53, 55, 59, 60, 69,	print.projection, 46
70, 73, 74	print.refmodel, 46
	print.vsel, 47
lm(), 4	print.vsel(), 6
lme4::glmer(), 4, 54	print.vselsummary, 47
lme4::lmer(), 4, 54	print.vselsummary(), 6, 47, 68
$\log(), 63$	<pre>proj_linpred (pred-projection), 39</pre>
loo::loo-glossary, 21	proj_linpred(), 6, 39–41, 50, 55
<pre>loo::loo_moment_match(), 21</pre>	proj_predict (pred-projection), 39
loo::psis(), 21	proj_predict(), 6, 25, 27, 39–42, 50, 55
loo::sis(), 21	project, 48
	project(), 4, 6–9, 39–41, 45, 46, 49, 50, 52,
MASS::polr(),4	55, 56, 61
<pre>mclogit::mblogit(), 4</pre>	
mesquite, 30	projpred (projpred-package), 3
mgcv::gam(), 4, 54	projpred-package, 3, 17, 19–22, 50, 56, 69,
mgcv::s(), 56	70, 72
mgcv::t2(), 56	ranking, 51
	ranking(), 6, 15, 32, 48, 61
<pre>nnet::multinom(), 4</pre>	ranking.vsel(), <i>15</i>
	refmodel-init-get, 25, 41, 44, 52
ordinal::clmm(), 4	_
0. 0.1	rstanarm::stan_gamm4(), 56
performances, 31	rstanarm::stan_polr(),4
performances(), 6, 31, 33, 65	run_cvfun, 59
performances.vsel(), 31	run_cvfun(), 18, 60
performances.vselsummary(), 31,68	run_cvfun.default(),60
plot(), <i>33</i>	run_cvfun.refmodel(),60
plot.cv_proportions, 32	set.seed(), 14, 19, 37, 40, 49, 60, 67, 71
plot.cv_proportions(), 6, 16, 32, 48, 62	solution_terms, 61
plot.ranking(plot.cv_proportions), 32	solution_terms(), 61
plot.ranking(), 32	
plot.vsel, 33	solution_terms.projection(), 61, 62
plot.vsel(), 6, 18, 31, 34-36, 62-67	solution_terms.vsel(), 61
poisson(), 24, 25	Student_t (extra-families), 28
<pre>posterior::as_draws(), 9</pre>	Student_t(), 29
<pre>posterior::as_draws_matrix(), 9</pre>	suggest_size, 62
posterior::draws_matrix(), 10, 40, 42	suggest_size(), 36, 48, 63, 64
<pre>posterior::resample_draws(), 9</pre>	<pre>suggest_size.vsel(), 6</pre>
posterior::weight_draws(), 10, 40	summary(), 65
pred-projection, 39	summary.vsel, 65
predict(), 43	summary.vsel(), $6$ , $18$ , $31$ , $33$ , $36$ , $47$ , $48$ ,
predict.glm(), 44	62–64, 67
predict.refmodel, 43	iv
predict.refmodel(), 44, 55	unix::rlimit_as(), <i>5</i> , <i>21</i>
predictor_terms, 45	varsel, 68
r · · · · · · · · · · · · · · · · · · ·	· · · <del> ,</del>

INDEX 77