Package: predRupdate (via r-universe)

August 28, 2024

Title Prediction Model Validation and Updating

Version 0.2.0.9000

Description Evaluate the predictive performance of an existing (i.e. previously developed) prediction/ prognostic model given relevant information about the existing prediction model (e.g. coefficients) and a new dataset. Provides a range of model updating methods that help tailor the existing model to the new dataset; see Su et al. (2018) <doi:10.1177/0962280215626466>. Techniques to aggregate multiple existing prediction models on the new data are also provided; see Debray et al. (2014) <doi:10.1002/sim.6080> and Martin et al. (2018) <doi:10.1002/sim.7586>).

License MIT + file LICENSE

Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.2

URL https://github.com/GlenMartin31/predRupdate,

https://glenmartin31.github.io/predRupdate/

BugReports https://github.com/GlenMartin31/predRupdate/issues

Suggests covr, knitr, rmarkdown, testthat (>= 3.0.0)

Config/testthat/edition 3

Imports utils, stats, survival, pROC, ggplot2, rlang, ggpubr

Depends R (>= 2.10)

VignetteBuilder knitr

Language en-US

Repository https://glenmartin31.r-universe.dev

RemoteUrl https://github.com/glenmartin31/predrupdate

RemoteRef HEAD

RemoteSha b05218cb4444d2a65a8d0538aee23fd3e3e6c8c1

Contents

2
3
4
4
6
8
10
13
15
17
19
21

Index

```
dummy_vars
```

Create dummy variables for all categorical/factor variables in a data.frame

Description

Create dummy/indicator variables for all categorical variables in a data.frame. Can be used as a pre-processing step before calling other functions within the package.

Usage

```
dummy_vars(df)
```

Arguments

df

a data.frame on which to make dummy variables for each categorical/factor variable, based on contrasts.

Value

a data.frame matching df but where each categorical variable in df is replaced with indicator variables. All combinations of the indicator/dummy variable are returned. Naming convention of the new dummy variables is variable_level. For example, a factor variable in df named "colour" with levels "red", "green" and "purple" will be replaced with three columns (the new dummy variables), named colour_red, colour_green and colour_purple.

See Also

pred_input_info

inv_logit

Examples

inv_logit

Apply the inverse logit function to an input

Description

inv_logit applies the inverse-logit transformation (expit/ logistic function) to convert a vector of values between -Inf and Inf, to values between 0 and 1. Used to convert the linear predictor of a logistic regression model into a probability.

Usage

inv_logit(x)

Arguments

х

Numeric vector with values between -Inf and Inf.

Value

Numeric vector of probabilities (i.e. values between 0 and 1)

See Also

logit

Examples

```
inv_logit(-2)
inv_logit(c(-2,-1,0,1,2))
```

logit

Description

logit applies the logit transformation to convert a vector of values between 0 and 1, to values between -Inf and Inf. Used to convert a probability from a logistic regression model onto the linear predictor scale.

Usage

logit(p)

Arguments

р

Numeric vector of probabilities (i.e. values between 0 and 1) that will be transformed.

Value

A numeric vector, with values between -Inf and Inf

See Also

inv_logit

Examples

logit(0.5)
logit(c(0.1, 0.2, 0.3))

map_newdata

Map new data to a predinfo object

Description

This function takes a predinfo object and applies (maps) a new data to this object to check there is consistency between the two. This function is not usually called directly, but rather within other functions within the package, such as pred_predict.

map_newdata

Usage

```
map_newdata(
    x,
    new_data,
    binary_outcome = NULL,
    survival_time = NULL,
    event_indicator = NULL
)
```

Arguments

х	an object of class "predinfo".
new_data	data.frame upon which the prediction model should be applied (for subsequent validation/model updating/model aggregation).
binary_outcome	Character variable giving the name of the column in new_data that represents the observed binary outcomes (should be coded 0 and 1 for non-event and event, respectively). Only relevant for model_type="logistic"; leave as NULL otherwise. Leave as NULL if new_data does not contain any outcomes.
survival_time	Character variable giving the name of the column in new_data that represents the observed survival times. Only relevant for model_type="survival"; leave as NULL otherwise. Leave as NULL if new_data does not contain any survival outcomes.
event_indicator	
	Character variable giving the name of the column in new_data that represents the observed survival indicator (1 for event, 0 for censoring). Only relevant for model_type="survival"; leave as NULL otherwise. Leave as NULL if new_data

Details

This function maps a new dataset onto a pred_info object. The new dataset might be a validation dataset (to test the performance of the existing prediction model) and/or it might be the dataset on which one wishes to apply model updating methods to revise the model. In any case, this should be specified in new_data as a data.frame. Each row should be an observation (e.g. patient) and each variable/column should be a predictor variable. The predictor variables need to include (as a minimum) all of the predictor variables that are included in the existing prediction model (i.e., each of the variable names supplied to pred_input_info, through the model_info parameter, must match the name of a variables in new_data).

does not contain any survival outcomes.

Any factor variables within new_data must be converted to dummy (0/1) variables before calling this function. dummy_vars can help with this.

binary_outcome, survival_time and event_indicator are used to specify the outcome variable(s) within new_data, if relevant (use binary_outcome if model_type = "logistic", or use survival_time and event_indicator if model_type = "survival"). For example, if validating an existing model, then these inputs specify the columns of new_data that will be used for assessing predictive performance of the predictions in the validation dataset. If new_data does not contain outcomes, then leave these inputs to the default of NULL.

Returns a list of the predinfo object, the new_data, and outcomes.

Examples

pred_input_info Input information about an existing prediction model

Description

Input coefficient information about one or multiple existing prediction model(s), for use in other functions in the package.

Usage

```
pred_input_info(
  model_type = c("logistic", "survival"),
  model_info,
  cum_hazard = NULL
)
```

Arguments

<pre>model_type</pre>	specifies the type of model that the existing prediction model is based on; pos- sible options are:
	• "logistic" indicates that the existing model was based on a logistic re- gression model (default)

• "survival" indicates that the existing model was based on a survival regression model

If multiple models are being entered, then all models need to be of the same type - otherwise call function multiple times for each type of model.

model_info a data.frame that contains the coefficients of the existing prediction model(s). Each column should be a predictor variable (with the name of the column being the name of the predictor variable), with the values being the coefficients, taken exactly as published from the existing prediction model(s). Multiple existing prediction models should be specified by entering multiple rows. If a predictor variable is not present in a given model then enter that cell of the data.frame as NA. See examples. cum_hazard A data.frame with two columns: (1) time, and (2) estimated cumulative baseline hazard at that time. The first column (time) should be named 'time' and the second (cumulative baseline hazard) should be named 'hazard'. Only relevant if model_type is "survival"; leave as NULL otherwise. If multiple existing models entered, and model_type = survival, then cum_hazard should be supplied as list of length equal to number of models.

Details

This function will structure the relevant information about one or more existing prediction model(s) into a standardised format, such that it can be used within other functions in the package.

First, the existing prediction model(s) will have a functional form (i.e. the linear predictor of the model); this will be taken as being a linear combination of the variables specified by the columns of model_info.

Second, each of the predictor variables of the existing prediction model(s) will have a published coefficient (e.g. log-odds-ratio or log-hazard-ratio), which should each be given as the values of model_info. If entering information about multiple existing prediction models, then model_info will contain multiple rows (one per existing model). Here, if a given model does not contain a predictor variable that is included in another model, then set as NA; see examples of this below.

In the case of model_type = "logistic", then model_info must contain a column named as "Intercept", which gives the intercept coefficient of each of the existing logistic regression models (taken exactly as previously published); this should be the first column of model_info.

If model_type = "survival", then the baseline cumulative hazard of the model(s) can be specified in cum_hazard. If the baseline cumulative hazard of the existing survival model is not available, then leave as NULL; this will limit any validation metrics that can be calculated.

Note, the column names of model_info should match columns in any new data that the existing model(s) will be applied to (i.e. any new data that will be provided to other functions within the package should have corresponding predictor variables entered through model_info). See pred_predict, pred_validate, pred_update and pred_stacked_regression for more information.

Value

pred_input_info returns an object of class "predinfo", with child classes per model_type. This is a standardised format, such that it can be used with other functions in the package. An object of class "predinfo" is a list containing the following components:

- M = the number of existing models that information has been entered about
- model_type = this is the type of model that the existing prediction model is based upon ("logistic" or "survival")
- coefs = this is the set of (previously estimated) coefficients for each predictor variable
- coef_names = gives the names of each predictor variable
- formula = this is the functional form of the model's linear predictor
- cum_hazard = if supplied, this is the cumulative baseline hazard of the existing model(s)

Examples

```
#Example 1 - logistic regression existing model
# create a data.frame of the model coefficients, with columns being variables
coefs_table <- data.frame("Intercept" = -3.4,</pre>
                           "SexM" = 0.306,
                           "Smoking_Status" = 0.628,
                           "Diabetes" = 0.499,
                           "CKD" = 0.538)
#pass this into pred_input_info()
Existing_Logistic_Model <- pred_input_info(model_type = "logistic",</pre>
                                            model_info = coefs_table)
summary(Existing_Logistic_Model)
#Example 2 - survival model example; uses an example dataset within the
              package.
#
pred_input_info(model_type = "survival",
                model_info = SYNPM$Existing_TTE_models[2,],
                cum_hazard = SYNPM$TTE_mod2_baseline)
#Example 3 - Input information about multiple models
summary(pred_input_info(model_type = "logistic",
                        model_info = SYNPM$Existing_logistic_models))
```

pred_predict Make predictions from an existing prediction model

Description

Use an existing prediction model to estimate predicted risks of the outcome for each observation in a new dataset.

Usage

```
pred_predict(
    x,
    new_data,
    binary_outcome = NULL,
    survival_time = NULL,
    event_indicator = NULL,
    time_horizon = NULL
)
```

Arguments

Х	an object of class "predinfo" produced by calling pred_input_info.
new_data	data.frame upon which predictions are obtained using the prediction model.

8

binary_outcome	Character variable giving the name of the column in new_data that represents the observed binary outcomes (should be coded 0 and 1 for non-event and event, respectively). Only relevant for model_type="logistic"; leave as NULL otherwise. Leave as NULL if new_data does not contain any outcomes.
survival_time	Character variable giving the name of the column in new_data that represents the observed survival times. Only relevant for model_type="survival"; leave as NULL otherwise. Leave as NULL if new_data does not contain any survival outcomes.
event_indicator	
	Character variable giving the name of the column in new_data that represents the observed survival indicator (1 for event, 0 for censoring). Only relevant for model_type="survival"; leave as NULL otherwise. Leave as NULL if new_data does not contain any survival outcomes.
time_horizon	for survival models, an integer giving the time horizon (post baseline) at which a prediction is required (i.e. the t at which P(T <t) be="" currently,<="" estimated).="" should="" td=""></t)>

ime_horizon for survival models, an integer giving the time horizon (post baseline) at which a prediction is required (i.e. the t at which P(T<t) should be estimated). Currently, this must match a time in x\$cum_hazard. If left as NULL, no predicted risks will be returned, just the linear predictor.

Details

This function takes the relevant information about the existing prediction model (as supplied by calling pred_input_info), and returns the linear predictor and predicted risks for each individ-ual/observation in new_data.

If the existing prediction model is based on logistic regression (i.e., if x="logistic"), the predicted risks will be the predicted probability of the binary outcome conditional on the predictor variables in the new data (i.e., P(Y=1 | X)). If the existing prediction model is based on a time-to-event/survival model (i.e., if x\$model_type == "survival"), the predicted risks can only be calculated if a baseline cumulative hazard is provided; in this case, the predicted risks will be one minus the survival probability (i.e., 1 - S(T>time horizon | X)).

new_data should be a data.frame, where each row should be an observation (e.g. patient) and each variable/column should be a predictor variable. The predictor variables need to include (as a minimum) all of the predictor variables that are included in the existing prediction model (i.e., each of the variable names supplied to pred_input_info, through the model_info parameter, must match the name of a variables in new_data). Any factor variables within new_data must be converted to dummy (0/1) variables before calling this function. dummy_vars can help with this. See examples.

binary_outcome, survival_time and event_indicator are used to specify the outcome variable(s) within new_data (use binary_outcome if x\$model_type = "logistic", or use survival_time and event_indicator if x\$model_type = "survival").

Value

pred_predict returns a list containing the following components:

- LinearPredictor = the linear predictor for each observation in the new data (i.e., the linear combination of the models predictor variables and their corresponding coefficients)
- PredictedRisk = the predicted risk for each observation in the new data

- TimeHorizon = for survival models, an integer giving the time horizon at which a prediction is made
- Outcomes = vector of outcomes/endpoints (if available).

See Also

pred_input_info

Examples

```
#Example 1 – logistic regression existing model – shows handling of factor variables
coefs_table <- data.frame("Intercept" = -3.4,</pre>
                           "Sex_M" = 0.306,
                           "Smoking_Status" = 0.628)
existing_Logistic_Model <- pred_input_info(model_type = "logistic",</pre>
                                            model_info = coefs_table)
new_df <- data.frame("Sex" = as.factor(c("M", "F", "M", "M", "F", "F", "M")),</pre>
                      "Smoking_Status" = c(1, 0, 0, 1, 1, 0, 1))
#new_df has a factor variable, so needs indicator variables creating before pred_predict:
new_df_indicators <- dummy_vars(new_df)</pre>
pred_predict(x = existing_Logistic_Model,
             new_data = new_df_indicators)
#Example 2 - survival model example; uses an example dataset within the
              package. Multiple existing models
model2 <- pred_input_info(model_type = "survival",</pre>
                          model_info = SYNPM$Existing_TTE_models,
                           cum_hazard = list(SYNPM$TTE_mod1_baseline,
                                                  SYNPM$TTE_mod2_baseline,
                                                  SYNPM$TTE_mod3_baseline))
pred_predict(x = model2,
             new_data = SYNPM$ValidationData[1:10,],
             survival_time = "ETime",
             event_indicator = "Status",
             time_horizon = 5)
```

pred_stacked_regression

Perform Stacked Regression on Existing Prediction Models

Description

This function takes a set of existing prediction models, and uses the new dataset to combine/aggregate them into a single 'meta-model', as described in Debray et al. 2014.

pred_stacked_regression

Usage

```
pred_stacked_regression(
    x,
    positivity_constraint = FALSE,
    new_data,
    binary_outcome = NULL,
    survival_time = NULL,
    event_indicator = NULL
)
```

Arguments

х	an object of class "predinfo" produced by calling pred_input_info contain- ing information on at least two existing prediction models.	
positivity_cons	straint	
	TRUE/FALSE denoting if the weights within the stacked regression model should be constrained to be non-negative (TRUE) or should be allowed to take any value (FALSE). See details.	
new_data	data.frame upon which the prediction models should be aggregated.	
binary_outcome	Character variable giving the name of the column in new_data that represents the observed binary outcomes (should be coded 0 and 1 for non-event and event, respectively). Only relevant for model_type="logistic"; leave as NULL otherwise. Leave as NULL if new_data does not contain any outcomes.	
survival_time	Character variable giving the name of the column in new_data that represents the observed survival times. Only relevant for x\$model_type="survival"; leave as NULL otherwise.	
event_indicator		
	Character variable giving the name of the column in new_data that represents the observed survival indicator (1 for event, 0 for censoring). Only relevant for x\$model_type="survival"; leave as NULL otherwise.	

Details

This function takes a set of (previously estimated) prediction models that were each originally developed for the same prediction task, and pool/aggregate these into a single prediction model (meta-model) using stacked regression based on new data (data not used to develop any of the existing models). The methodological details can be found in Debray et al. 2014.

Given that the existing models are likely to be highly co-linear (since they were each developed for the same prediction task), it has been suggested to impose a positivity constraint on the weights of the stacked regression model (Debray et al. 2014.). If positivity_constraint is set to TRUE, then the stacked regression model will be estimated by optimising the (log-)likelihood using bound constrained optimization ("L-BFGS-B"). This is currently only implemented for logistic regression models (i.e., if x\$model_type="logistic"). For survival models, positivity_constraint = FALSE.

new_data should be a data.frame, where each row should be an observation (e.g. patient) and each variable/column should be a predictor variable. The predictor variables need to include (as a minimum) all of the predictor variables that are included in the existing prediction models (i.e.,

each of the variable names supplied to pred_input_info, through the model_info parameter, must match the name of a variables in new_data).

Any factor variables within new_data must be converted to dummy (0/1) variables before calling this function. dummy_vars can help with this. See pred_predict for examples.

binary_outcome, survival_time and event_indicator are used to specify the outcome variable(s) within new_data (use binary_outcome if x\$model_type = "logistic", or use survival_time and event_indicator if x\$model_type = "survival").

Value

A object of class "predSR". This is the same as that detailed in pred_input_info, with the added element containing the estimates of the meta-model obtained by stacked regression.

References

Debray, T.P., Koffijberg, H., Nieboer, D., Vergouwe, Y., Steyerberg, E.W. and Moons, K.G. (2014), Meta-analysis and aggregation of multiple published prediction models. *Statistics in Medicine*, 33: 2341-2362

See Also

pred_input_info

Examples

```
LogisticModels <- pred_input_info(model_type = "logistic",</pre>
                                    model_info = SYNPM$Existing_logistic_models)
SR <- pred_stacked_regression(x = LogisticModels,</pre>
                               new_data = SYNPM$ValidationData,
                               binary_outcome = "Y")
summary(SR)
#Survival model example:
TTModels <- pred_input_info(model_type = "survival",</pre>
                             model_info = SYNPM$Existing_TTE_models,
                             cum_hazard = list(SYNPM$TTE_mod1_baseline,
                                                    SYNPM$TTE_mod2_baseline,
                                                     SYNPM$TTE_mod3_baseline))
SR <- pred_stacked_regression(x = TTModels,</pre>
                               new_data = SYNPM$ValidationData,
                               survival_time = "ETime",
                               event_indicator = "Status")
summary(SR)
```

pred_update

Description

This function takes an existing (previously developed) prediction model and applies various model updating methods to tailor/adapt it to a new dataset. Various levels of updating are possible, ranging from model re-calibration to model refit.

Usage

```
pred_update(
    x,
    update_type = c("intercept_update", "recalibration", "refit"),
    new_data,
    binary_outcome = NULL,
    survival_time = NULL,
    event_indicator = NULL
)
```

Arguments

x	an object of class "predinfo" produced by calling pred_input_info contain- ing information on exactly one existing prediction model.
update_type	character variable specifying the level of updating that is required.
new_data	data.frame upon which the prediction models should be updated.
binary_outcome	Character variable giving the name of the column in new_data that represents the observed binary outcomes (should be coded 0 and 1 for non-event and event, respectively). Only relevant for model_type="logistic"; leave as NULL otherwise. Leave as NULL if new_data does not contain any outcomes.
survival_time	Character variable giving the name of the column in new_data that represents the observed survival times. Only relevant for x\$model_type="survival"; leave as NULL otherwise.
event_indicator	
	Character variable giving the name of the column in new_data that represents the observed survival indicator (1 for event, 0 for censoring). Only relevant for x\$model_type="survival"; leave as NULL otherwise.

Details

This function takes a single existing (previously estimated) prediction model, and apply various model discrete model updating methods (see Su et al. 2018) to tailor the model to a new dataset.

The type of updating method is selected with the update_type parameter, with options: "intercept_update", "recalibration" and "refit". "intercept_update" corrects the overall calibration-in-thelarge of the model, through altering the model intercept (or baseline hazard) to suit the new dataset. This is achieved by fitting a logistic model (if the existing model is of type logistic) or time-toevent model (if the existing model if of type survival) to the new dataset, with the linear predictor as the only covariate, with the coefficient fixed at unity (i.e. as an offset). "recalibration" corrects the calibration-in-the-large and any under/over-fitting, by fitting a logistic model (if the existing model is of type logistic) or time-to-event model (if the existing model if of type survival) to the new dataset, with the linear predictor as the only covariate. Finally, "refit" takes the original model structure and re-estimates all coefficients; this has the effect as re-developing the original model in the new data.

new_data should be a data.frame, where each row should be an observation (e.g. patient) and each variable/column should be a predictor variable. The predictor variables need to include (as a minimum) all of the predictor variables that are included in the existing prediction model (i.e., each of the variable names supplied to pred_input_info, through the model_info parameter, must match the name of a variables in new_data).

Any factor variables within new_data must be converted to dummy (0/1) variables before calling this function. dummy_vars can help with this. See pred_predict for examples.

binary_outcome, survival_time and event_indicator are used to specify the outcome variable(s) within new_data (use binary_outcome if x\$model_type = "logistic", or use survival_time and event_indicator if x\$model_type = "survival").

Value

A object of class "predUpdate". This is the same as that detailed in pred_input_info, with the added element containing the estimates of the model updating and the update type.

References

Su TL, Jaki T, Hickey GL, Buchan I, Sperrin M. A review of statistical updating methods for clinical prediction models. Stat Methods Med Res. 2018 Jan;27(1):185-197. doi: 10.1177/0962280215626466.

See Also

pred_input_info

Examples

```
#Example 1 – update time-to-event model by updating the baseline hazard in new dataset
model1 <- pred_input_info(model_type = "survival",</pre>
                           model_info = SYNPM$Existing_TTE_models[1,],
                           cum_hazard = SYNPM$TTE_mod1_baseline)
recalibrated_model1 <- pred_update(x = model1,</pre>
                                    update_type = "intercept_update",
                                    new_data = SYNPM$ValidationData,
                                    survival_time = "ETime",
                                    event_indicator = "Status")
```

summary(recalibrated_model1)

Description

Validate an existing prediction model, to calculate the predictive performance against a new (validation) dataset.

Usage

```
pred_validate(
    x,
    new_data,
    binary_outcome = NULL,
    survival_time = NULL,
    event_indicator = NULL,
    time_horizon = NULL,
    level = 0.95,
    cal_plot = TRUE,
    ...
)
```

Arguments

x	an object of class "predinfo" produced by calling pred_input_info.	
new_data	data.frame upon which the prediction model should be evaluated.	
binary_outcome	Character variable giving the name of the column in new_data that represents the observed binary outcomes (should be coded 0 and 1 for non-event and event, respectively). Only relevant for model_type="logistic"; leave as NULL otherwise. Leave as NULL if new_data does not contain any outcomes.	
survival_time	Character variable giving the name of the column in new_data that represents the observed survival times. Only relevant for x\$model_type="survival"; leave as NULL otherwise.	
event_indicator		
	Character variable giving the name of the column in new_data that represents the observed survival indicator (1 for event, 0 for censoring). Only relevant for x\$model_type="survival"; leave as NULL otherwise.	
time_horizon	for survival models, an integer giving the time horizon (post baseline) at which a prediction is required. Currently, this must match a time in x\$cum_hazard.	
level	the confidence level required for all performance metrics. Defaults at 95%. Must be a value between 0 and 1.	
cal_plot	indicate if a flexible calibration plot should be produced (TRUE) or not (FALSE).	

Details

This function takes an existing prediction model formatted according to pred_input_info, and calculates measures of predictive performance on new data (e.g., within an external validation study). The information about the existing prediction model should first be inputted by calling pred_input_info, before passing the resulting object to pred_validate.

new_data should be a data.frame, where each row should be an observation (e.g. patient) and each variable/column should be a predictor variable. The predictor variables need to include (as a minimum) all of the predictor variables that are included in the existing prediction model (i.e., each of the variable names supplied to pred_input_info, through the model_info parameter, must match the name of a variables in new_data).

Any factor variables within new_data must be converted to dummy (0/1) variables before calling this function. dummy_vars can help with this. See pred_predict for examples.

binary_outcome, survival_time and event_indicator are used to specify the outcome variable(s) within new_data (use binary_outcome if x\$model_type = "logistic", or use survival_time and event_indicator if x\$model_type = "survival").

In the case of validating a logistic regression model, this function assesses the predictive performance of the predicted risks against an observed binary outcome. Various metrics of calibration (agreement between the observed risk and the predicted risks, across the full risk range) and discrimination (ability of the model to distinguish between those who develop the outcome and those who do not) are calculated. For calibration, the observed-to-expected ratio, calibration intercept and calibration slopes are estimated. The calibration intercept is estimated by fitting a logistic regression model to the observed binary outcomes, with the linear predictor of the model as an offset. For calibration slope, a logistic regression model is fit to the observed binary outcome with the linear predictor from the model as the only covariate. For discrimination, the function estimates the area under the receiver operating characteristic curve (AUC). Various other metrics are also calculated to assess overall accuracy (Brier score, Cox-Snell R2).

In the case of validating a survival prediction model, this function assesses the predictive performance of the linear predictor and (optionally) the predicted event probabilities at a fixed time horizon against an observed time-to-event outcome. Various metrics of calibration and discrimination are calculated. For calibration, the observed-to-expected ratio at the specified time_horizon (if predicted risks are available through specification of x\$cum_hazard) and calibration slope are produced. For discrimination, Harrell's C-statistic is calculated.

For both model types, a flexible calibration plot is produced (for survival models, the cumulative baseline hazard must be available in the predinfo object, x\$cum_hazard). Specify parameter cal_plot to indicate whether a calibration plot should be produced (TRUE), or not (FALSE). The calibration plot is produced by regressing the observed outcomes against a cubic spline of the logit of predicted risks (for a logistic model) or the complementary log-log of the predicted risks (for a survival model). Users can specify the following additional parameters to pred_validate to modify the calibration plot:

- xlim as a numeric vector of length 2, giving the lower and upper range of the x-axis scale defaults at 0 and 1. Changes here should match changes to the ylim such that the plot remains 'square'.
- ylim as a numeric vector of length 2, giving the lower and upper range of the y-axis scale defaults at 0 and 1. Changes here should match changes to the xlim such that the plot remains 'square'.

- xlab string giving the x-axis label. Defaults as "Predicted Probability".
- ylab string giving the x-axis label. Defaults as "Observed Probability".
- pred_rug TRUE/FALSE of whether a 'rug' should be placed along the x-axis of the calibration plot showing the distribution of predicted risks. Defaults as FALSE in favour of examining the box-plot/violin plot that is produced.
- cal_plot_n_sample numeric value (less than nrow(new_data)) giving a random subset of observations to render the calibration plot over. The calibration plot is always created using all data, but for rendering speed in large datasets, it can sometimes be useful to render the plot over a smaller (random) subset of observations. Final (e.g. publication-ready) plots should always show the full plot, so a warning is created if users enter a value of cal_plot_n_sample.

Value

pred_validate returns an object of class "predvalidate", with child classes per model_type. This is a list of performance metrics, estimated by applying the existing prediction model to the new_data. An object of class "predvalidate" is a list containing relevant calibration and discrimination measures. For logistic regression models, this will include observed:expected ratio, calibration-intercept, calibration slope, area under the ROC curve, R-squared, and Brier Score. For survival models, this will include observed:expected ratio (if cum_hazard is provided to x), calibration slope, and Harrell's C-statistic. Optionally, a flexible calibration plot is also produced, along with a box-plot and violin plot of the predicted risk distribution.

The summary function can be used to extract and print summary performance results (calibration and discrimination metrics). The graphical assessments of performance can be extracted using plot.

See Also

pred_input_info

Examples

```
#Example 1 - multiple existing model, with outcome specified; uses
             an example dataset within the package
model1 <- pred_input_info(model_type = "logistic",</pre>
                           model_info = SYNPM$Existing_logistic_models)
val_results <- pred_validate(x = model1,</pre>
                              new_data = SYNPM$ValidationData,
                              binary_outcome = "Y",
                              cal_plot = FALSE)
```

summary(val_results)

pred_val_probs

Description

This function is included for situations where one has a vector of predicted probabilities from a model and a vector of observed binary outcomes that we wish to validate the predictions against. See pred_validate for the main validation function of this package.

Usage

```
pred_val_probs(binary_outcome, Prob, cal_plot = TRUE, level = 0.95, ...)
```

Arguments

binary_outcome	vector of binary outcomes (coded as 1 if outcome happened, and 0 otherwise). Must be of same length as Prob
Prob	vector of predicted probabilities. Must be of same length of binary_outcome.
cal_plot	indicate if a flexible calibration plot should be produced (TRUE) or not (FALSE).
level	the confidence level required for all performance metrics. Defaults at 95%. Must be a value between 0 and 1.
	further plotting arguments for the calibration plot. See Details below.

Details

This function takes a vector of observed binary outcomes, and a corresponding vector of predicted risks (e.g. from a logistic regression CPM), and calculates measures of predictive performance. The function is intended as a standalone way of validating predicted risks against binary outcomes outside of the usual pred_input_info() -> pred_validate() package workflow. See pred_validate for the main validation function of this package.

Various metrics of calibration (agreement between the observed risk and the predicted risks, across the full risk range) and discrimination (ability of the model to distinguish between those who develop the outcome and those who do not) are calculated. For calibration, the observed-to-expected ratio, calibration intercept and calibration slopes are estimated. The calibration intercept is estimated by fitting a logistic regression model to the observed binary outcomes, with the linear predictor of the model as an offset. For calibration slope, a logistic regression model is fit to the observed binary outcome with the linear predictor from the model as the only covariate. For discrimination, the function estimates the area under the receiver operating characteristic curve (AUC). Various other metrics are also calculated to assess overall accuracy (Brier score, Cox-Snell R2).

A flexible calibration plot is produced. Specify parameter cal_plot to indicate whether a calibration plot should be produced (TRUE), or not (FALSE). See pred_validate for details on this plot, and details of optional plotting arguments.

Value

An object of class "predvalidate", which is a list containing relevant calibration and discrimination measures. See pred_validate for details.

See Also

pred_input_info, pred_validate

SYNPM

Examples

```
# simulate some data for purposes of example illustration
set.seed(1234)
x1 <- rnorm(2000)
LP < -2 + (0.5 \times x1)
PR <- 1/(1+exp(-LP))
y <- rbinom(2000, 1, PR)
#fit hypothetical model to the simulated data
mod <- glm(y[1:1000] ~ x1[1:1000], family = binomial(link="logit"))</pre>
#obtain the predicted risks from the model
pred_risk <- predict(mod, type = "response",</pre>
                       newdata = data.frame("x1" = x1[1001:2000]))
#Use pred_val_probs to validate the predicted risks against the
#observed outcomes
summary(pred_val_probs(binary_outcome = y[1001:2000],
                         Prob = pred_risk,
                         cal_plot = FALSE))
```

SYNPM

SYNthetic Prediction Models (SYNPM) and Validation dataset

Description

A list containing: (1) information on some (synthetic) existing prediction models (representing those available/published, which we want to validate in another independent dataset); and (2) a synthetic dataset that we wish to validate/update the models on.

Usage

SYNPM

Format

A list with six elements.

- 1. The first element is a data frame with the information about three existing binary (logistic regression) models for a binary outcome at one year
- 2. The second element is a data frame with the information about three existing time-to-event (Cox) models for the time-to-event outcome
- 3. The third, fourth and fifth elements are the cumulative baseline hazard information for the three time-to-event model
- 4. The sixth element is the (synthetic) validation dataset on which we want to validate the existing models. The dataset has 20000 rows and 8 variables:

Age The age of the individual at baseline

SexM The sex of the individual (1 = male; 0 = female)
Smoking_Status Indicates whether the individual was or is a smoker (1=previous/ current smoker, 0=non-smoker)
Diabetes Indicates whether the individual has diabetes (1=diabetic, 0=not diabetic)
Creatinine The Creatinine value for the individual (mg/dL)
ETime The time from baseline until either the event or censoring
Status Indicator of whether the patient experienced the event or was censored at ETime
Y Binary indicator of whether the individual experienced the event by 1 time-unit

Source

Simulated Data; see https://github.com/GlenMartin31/predRupdate

Index

* datasets SYNPM, 19

dummy_vars, 2, 5, 9, 12, 14, 16

inv_logit, 3, 4

logit, 3, 4

 $map_newdata, 4$

pred_input_info, 2, 5, 6, 7–18 pred_predict, 7, 8, 9, 12, 14, 16 pred_stacked_regression, 7, 10 pred_update, 7, 13 pred_val_probs, 17 pred_validate, 7, 15, 16–18

SYNPM, 19