Developing and Deploying Transparent and Reproducible Algorithms for Public Health

R: tidymodels & plumber

Doug Manuel Juan Li Wenshan Li Kitty Chen











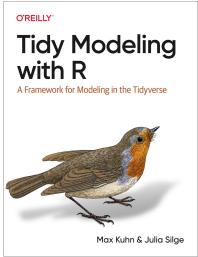
TIDYMODELS

The tidymodels framework is a collection of packages for modeling and machine learning using <u>tidyverse</u> principles.

https://www.tidymodels.org/

https://www.tmwr.org/





PLUMBER

Plumber allows you to create a web API by merely decorating your existing R source code with roxygen2-like comments.

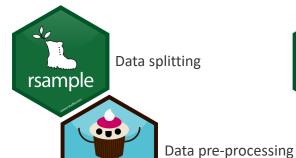
https://www.rplumber.io/



TIDYMODELS Main packages



The meta-package



recipes



Model interface



Model performance

Hyperparameter tuning of your model and pre-processing steps







TIDYMODELS Main packages

rsample

Data splitting Train/test split, (nested) cross validation (CV) etc.



Data pre-processing

The meta-package tidym parsnip

Model ensemble To integrate predictions from many models

Model interface

Model performance

Extra functions for tuning finetŲne

> Hyperparameter tuning of your model and pre-processing steps

> > Creates and manages tuning parameters and parameter grids



workflowsets

The goal of workflowsets is to allow users to create and easily fit a large number of models. workflowsets can create a workflow set that holds multiple workflow objects.



Workflows bundle your pre-processing, modeling, and postprocessing together



Reporting converts the information in common statistical R objects into user-friendly, predictable formats

dials

Demo and assignment overview



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Modules







Grades









Final Assignment

Start Assignment

Due Feb 26 by 11:59pm Points 1 Submitting a file upload

Learners will successfully complete the course by fulfilling the following:

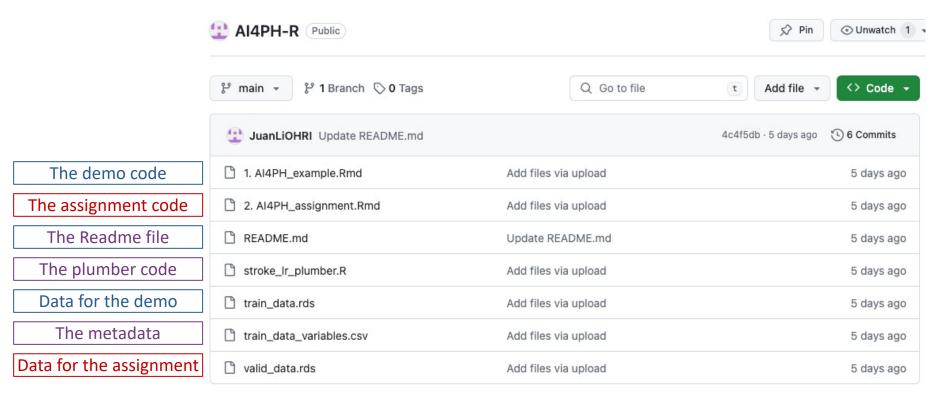
- 1. Develop and deploy an algorithm where a user can input feature values on a web application and the web application will return the score of the algorithm.
- 2. Understand the usage of metadata.
- 3. Validate the already developed model (tidymodels workflow) on another dataset, with some data harmonization steps.

A dataset on stroke will be provided for the assignment.

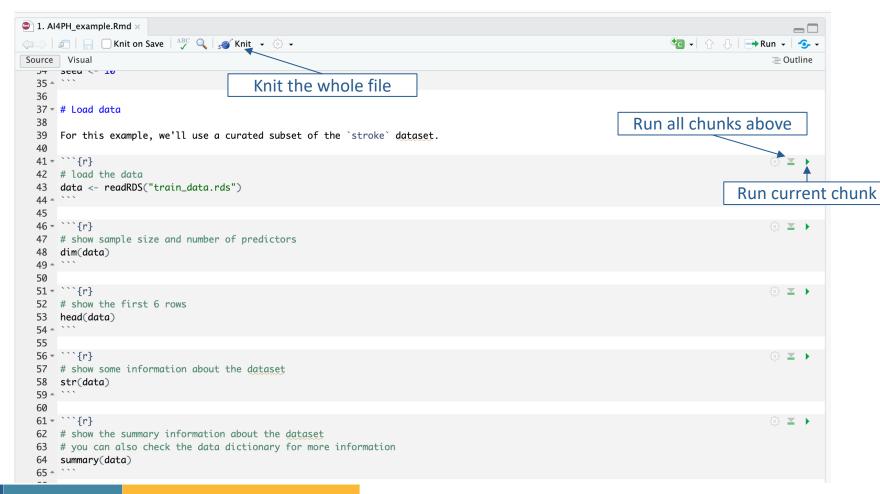
Materials of the demo and assignment can be found on Github: https://github.com/JuanLiOHRI/AI4PH-R/tree/main

To submit your work on the assignment, please send us the assignment file (.Rmd) that includes your code and all the output. Please rename the file as AI4PH_assignment_YourName.Rmd. E.g. my name is Juan Li and I will rename my submission as AI4PH_assignment_JuanLi.Rmd.

Demo and assignment overview— The Github repository (https://github.com/JuanLiOHRI/AI4PH-R/tree/main)



Preparation - R markdown file (.Rmd)



Preparation - Pipe operator: %>%

You can use the pipe operator (%>%) in R to "pipe" together a sequence of operations. This operator is most commonly used in R to perform a sequence of operations on a data frame. The basic syntax for the pipe operator is:

```
df %>%
    operation1 %>%
    operation2 %>%
    operation3
    ...

df_step1 <- operation1(df,...)
    df_step2 <- operation2(df_step1, ...)
    df_step3 <- operation3(df_step2, ...)
    ...</pre>
```

The pipe operator simply feeds the results of one operation into the next operation below it. The advantage of using the pipe operator is that it makes code extremely easy to read.

TIDYMODELS (demo): a subset of the stroke data

```
> data <- readRDS("train_data.rds")
> dim(data)
[1] 4066    11
> head(data)
```

	gender	age	hypertension	heart_disease	ever_married	work_type	Residence_type	<pre>avg_glucose_level</pre>	bmi	smoking_statu	stroke
1	M 4	9.33984	Yes	No	Yes	Private job	Rural	179.89718	27.84435	Never smoke	d 0
2	F 5	0.10903	No	No	Yes	Private job	Urban	136.81856	26.68095	Currently smoke	s 0
3	F 7	6.21449	No	No	No	Self-employed	Urban	201.03038	42.08255	Never smoke	d 0
5	F 6	6.76548	Yes	No	Yes	Private job	Urban	88.45523	25.77091	Never smoke	d 0
6	M 4	3.14164	Yes	No	No	Self-employed	Urban	249.41379	34.42329	Currently smoke	s 0
8	F 6	9.54896	No	No	Yes	${\tt Government\ job}$	Urban	94.31868	28.52712	Formerly smoke	d 0

variable	role	type	min	max	label
gender	predictor	Categorical			F; M
age	predictor	Continuous	40	100	
hypertension	predictor	Categorical			No; Yes
heart_disease	predictor	Categorical			No; Yes
ever_married	predictor	Categorical			No; Yes
work_type	predictor	Categorical			Self-employed; Private job; Government job
Residence_type	predictor	Categorical			Rural; Urban
avg_glucose_level	predictor	Continuous	0	310	
bmi	predictor	Continuous	9	73	
smoking_status	predictor	Categorical			Never smoked; Formerly smoked; Currently smokes
stroke	outcome	Categorical			0; 1

TIDYMODELS (demo): data splitting



```
set.seed(seed) # set seed for reproducibility

# split the data into train and test datasets
stroke_split <- initial_split(data, prop = 0.8, strata = stroke)
stroke_train <- stroke_split %>% training() # retrieve train data
stroke_test <- stroke_split %>% testing() # retrieve test data
```

TIDYMODELS (demo): model initializing



```
set.seed(seed) # set seed for reproducibility

# split the data into train and test datasets
stroke_split <- initial_split(data, prop = 0.8, strata = stroke)
stroke_train <- stroke_split %% training() # retrieve train data
stroke_test <- stroke_split %% testing() # retrieve test data</pre>
```



```
# Initialize a logistic regression object
lr_spec <- logistic_reg() %>%
  # Set the model engine
  set_engine('glm') %>%
  # Set the model mode
  set_mode('classification')
```

TIDYMODELS (demo): data preprocessing





Initialize a logistic regression object
lr_spec <- logistic_reg() %>%
Set the model engine
set_engine('glm') %>%
Set the model mode
set_mode('classification')



```
# Define the data preprocessing recipes
lr_recipe <-
    # define the formula
    recipe(stroke ~ ., data = stroke_train) %>%
    # create dummy variables for all the categorical predictors
    step_dummy(all_nominal_predictors()) %>%
    # center and scale all numeric variables
    step_normalize(all_predictors())
```

TIDYMODELS (demo): define and train the workflow (model with pre-processing steps)



```
set.seed(seed) # set seed for reproducibility

# split the data into train and test datasets
stroke_split <- initial_split(data, prop = 0.8, strata = stroke)
stroke_train <- stroke_split %% training() # retrieve train data
stroke_test <- stroke_split %% testing() # retrieve test data</pre>
```



```
# Initialize a logistic regression object
lr_spec <- logistic_reg() %-%
# Set the model engine
set_engine('glm') %-%
# Set the model mode
set_mode('classification')</pre>
```



```
# Define the data preprocessing recipes
lr_recipe <-
    # define the formula
recipe(stroke ~ ., data = stroke_train) %%
# create dummy variables for all the categorical predictors
step_dummy(all_nominal_predictors()) %%
# center and scale all numeric variables
step_normalize(all_predictors())</pre>
```



```
# Define the workflow
lr_workflow <-
  workflow() %>%
  add_model(lr_spec) **
  add_recipe(lr_recipe) **
```

```
# Train the model with preprocessing steps
lr_workflow_fit <- lr_workflow %>%
fit(data = stroke_train) ## Save the workflow
```

```
```{r}
saveRDS([lr_workflow_fit, "stroke_lr_workflow.rds")
```
```

TIDYMODELS (demo): obtaining the estimated coefficients



```
set.seed(seed) # set seed for reproducibility
# split the data into train and test datasets
stroke_split <- initial_split(data, prop = 0.8, strata = stroke)
stroke_train <- stroke_split %>% training() # retrieve train data
stroke_test <- stroke_split %>% testing() # retrieve test data
```



```
# Define the data preprocessing recipes
lr_recipe <-
    # define the formula
    recipe(stroke ~ ., data = stroke_train) %%
    # create dummy variables for all the categorical predictors
    step_dummy(all_nominal_predictors()) %%
    # center and scale all numeric variables
    step_normalize(all_predictors())</pre>
```



Initialize a logistic regression object
lr_spec <- logistic_reg() %>%
Set the model engine
set_engine('glm') %>%
Set the model mode
set_mode('classification')



Define the workflow
lr_workflow <workflow() %>%
add_model(lr_spec) %>%
add_recipe(lr_recipe)

Train the model with preprocessing steps
lr_workflow_fit <- lr_workflow %>%
 fit(data = stroke_train)

Obtaining the estimated coefficients tidy(lr_workflow_fit)



| # A tibble: 13 × 5 | | | |
|---|-----------------|----------------|-------------------------|
| term | estimate | std.error | statistic p.value |
| <chr></chr> | <dbl></dbl> | <dbl></dbl> | <dbl> <dbl></dbl></dbl> |
| 1 (Intercept) | 0.511 | 0.040 <u>1</u> | 12.7 4.45e-37 |
| 2 age | 0.676 | 0.044 <u>9</u> | 15.1 3.25e-51 |
| <pre>3 avg_glucose_level</pre> | 0.320 | 0.043 <u>3</u> | 7.39 1.50e-13 |
| 4 bmi | -0.148 | 0.042 <u>0</u> | -3.52 4.25e- 4 |
| 5 gender_M | 0.067 <u>1</u> | 0.040 <u>3</u> | 1.67 9.58e- 2 |
| 6 hypertension_Yes | 0.264 | 0.041 <u>8</u> | 6.31 2.70e-10 |
| <pre>7 heart_disease_Yes</pre> | 0.224 | 0.046 <u>4</u> | 4.83 1.34e- 6 |
| <pre>8 ever_married_Yes</pre> | -0.030 <u>7</u> | 0.040 <u>8</u> | -0.754 4.51e- 1 |
| <pre>9 work_type_Private.job</pre> | -0.062 <u>0</u> | 0.046 <u>7</u> | -1.33 1.85e- 1 |
| <pre>10 work_type_Government.job</pre> | -0.040 <u>3</u> | 0.046 <u>2</u> | -0.872 3.83e- 1 |
| 11 Residence_type_Urban | 0.032 <u>4</u> | 0.039 <u>9</u> | 0.812 4.17e- 1 |
| <pre>12 smoking_status_Formerly.smoked</pre> | 0.022 <u>6</u> | 0.043 <u>1</u> | 0.524 6.00e- 1 |
| <pre>13 smoking_status_Currently.smokes</pre> | 0.008 <u>73</u> | 0.042 <u>0</u> | 0.208 8.35e- 1 |

Obtaining the odds ratios tidy(lr_workflow_fit, exponentiate = TRUE)

A tibble: 13×5 term estimate std.error statistic p.value <chr>> <db1> <db1> <dbl> <db1> 12.7 4.45e-37 1 (Intercept) 1.67 0.0401 15.1 3.25e-51 2 age 1.97 0.0449 3 avg_glucose_level 1.38 0.0433 7.39 1.50e-13 -3.52 4.25e- 4 4 bmi 0.862 0.0420 5 gender_M 1.07 0.0403 1.67 9.58e- 2 1.30 0.0418 6.31 2.70e-10 6 hypertension_Yes 7 heart_disease_Yes 1.25 0.0464 4.83 1.34e- 6 0.970 8 ever_married_Yes 0.0408 -0.754 4.51e- 1 -1.33 1.85e- 1 9 work_type_Private.job 0.940 0.0467 10 work_type_Government.job 0.961 0.0462 -0.872 3.83e- 1 11 Residence_type_Urban 1.03 0.0399 0.812 4.17e- 1 0.524 6.00e- 1 12 smoking_status_Formerly.smoked 1.02 0.0431 13 smoking_status_Currently.smokes 0.0420 0.208 8.35e- 1 1.01

TIDYMODELS (demo): predicting on the test data



```
set.seed(seed) # set seed for reproducibility

# split the data into train and test datasets
stroke_split <- initial_split(data, prop = 0.8, strata = stroke)
stroke_train <- stroke_split %% testing() # retrieve train data
stroke_test <- stroke_split %% testing() # retrieve test data</pre>
```



```
# Define the data preprocessing recipes
lr_recipe <-
    # define the formula
    recipe(stroke ~ ., data = stroke_train) %>%
    # create dummy variables for all the categorical predictors
    step_dummy(all_nominal_predictors()) %>%
    # center and scale all numeric variables
    step_normalize(all_predictors())
```



```
# Obtaining the estimated coefficients
tidy(!r_workflow_fit)
# Obtaining the odds ratios
tidy(!r_workflow_fit, exponentiate = TRUE)
```



Initialize a logistic regression object
lr_spec <- logistic_reg() %>%
 # Set the model engine
 set_engine('glm') %>%
 # Set the model mode
 set_mode('classification')



Define the workflow
lr_workflow <workflow() %>%
add_model(lr_spec) %>%
add_recipe(lr_recipe)

Train the model with preprocessing steps
lr_workflow_fit <- lr_workflow %>%
 fit(data = stroke_train)

```
# Combine test data with predictions
test_results <- stroke_test %>%
bind_cols(prediction_class, prediction_prob)
```

TIDYMODELS (demo): model evaluation on the test data



```
set.seed(seed) # set seed for reproducibility
# split the data into train and test datasets
stroke_split <- initial_split(data, prop = 0.8, strata = stroke)</pre>
stroke_train <- stroke_split %>% training() # retrieve train data
stroke_test <- stroke_split %>% testing() # retrieve test data
```



Initialize a logistic regression object lr_spec <- logistic_reg() %>% # Set the model engine set_engine('glm') %>% # Set the model mode set_mode('classification')



Define the data preprocessing recipes lr_recipe <-# define the formula recipe(stroke ~ ., data = stroke_train) %>% # create dummy variables for all the categorical predictors step_dummy(all_nominal_predictors()) %>% # center and scale all numeric variables step_normalize(all_predictors())



Define the workflow lr workflow <workflow() %>% add_model(lr_spec) %>% add_recipe(lr_recipe)

Train the model with preprocessing steps

lr_workflow_fit <- lr_workflow %>%

fit(data = stroke_train)



Obtaining the estimated coefficients tidy(lr_workflow_fit) # Obtaining the odds ratios

custom_metrics <- metric_set(sens, spec, roc_auc)</pre>



tidy(lr_workflow_fit, exponentiate = TRUE) ```{r, message=FALSE}

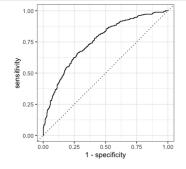


custom_metrics(test_results, truth = stroke, estimate = .pred_class, .pred_0)

A tibble: 3 x 3

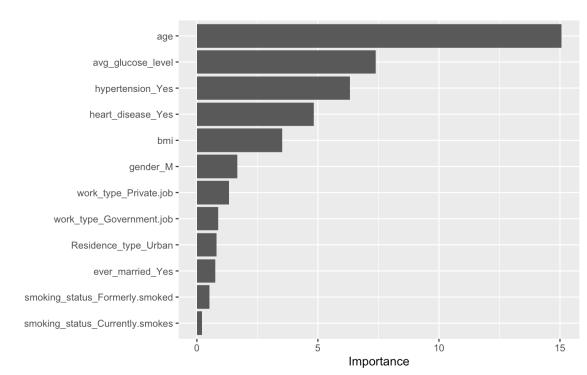
| .metric
<chr></chr> | .estimator
<chr></chr> | .estimate
<dbl></dbl> | |
|------------------------|---------------------------|--------------------------|--|
| sens | binary | 0.5417957 | |
| spec | binary | 0.8126273 | |
| roc_auc | binary | 0.7533750 | |

```{r, message=FALSE} test\_results %>% roc\_curve(stroke, .pred\_0) %>% autoplot()



### **TIDYMODELS (demo): feature importance**

```
'``{r, message=FALSE}
lr_workflow_fit %>%
 extract_fit_parsnip() %>%
 vip::vip(num_features = 20)
```





stroke\_lr\_workflo w.rds

The saved workflow (model with data preprocessing steps) that has been trained on the train data (and hopefully evaluated on the test data).



stroke\_lr\_plumber .R

The plumber script.

```
#* @param gender Your gender, allowed value: F; M
#* @param age Your age, allowed range: 40-100
#* @param hypertension Do you have hypertension? Allowed value: No; Yes
#* @param heart_disease Do you have heart disease? Allowed range: No; Yes
#* @param ever_married Have you ever married? Allowed range: No;Yes
#* @param work_type What kind of work you are doing or have done? Allowed value: Self-employed; Private job; Government job
#* @param Residence_type The type of your residence, allowed range: Rural; Urban
#* @param avg_glucose_level Average glucose level, allowed range: 0-310
#* @param bmi Body mass index, allowed range: 9-73
#* @param smoking_status Smoking, allowed value: Never smoked; Formerly smoked; Currently smokes
#* @get /predict/values
function(gender, age, hypertension, heart_disease, ever_married, work_type,
```

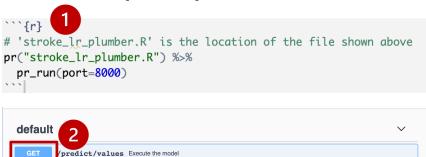
function(gender, age, hypertension, heart\_disease, ever\_married, work\_type, Residence\_type, avg\_glucose\_level, bmi, smoking\_status) {

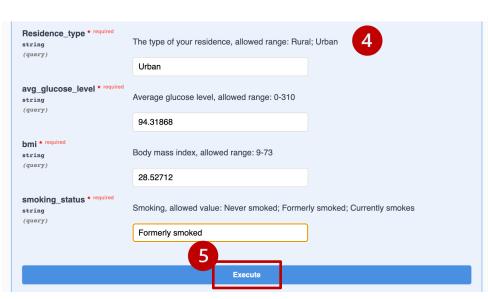
| Parameters                             |                                           |  |  |  |  |
|----------------------------------------|-------------------------------------------|--|--|--|--|
| Name                                   | Description                               |  |  |  |  |
| gender * required<br>string<br>(query) | Your gender, allowed value: F; M          |  |  |  |  |
|                                        | gender - Your gender, allowed value: F; M |  |  |  |  |
| age * required string (query)          | Your age, allowed range: 40-100           |  |  |  |  |
|                                        | age - Your age, allowed range: 40-100     |  |  |  |  |

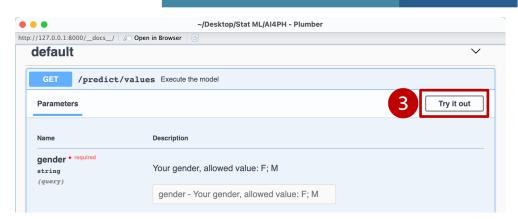
```
read in the saved workflow object
workflow <- readRDS("stroke_lr_workflow.rds")</pre>
 w.rds
assemble the inputs into a data frame
newdata <- data.frame(gender = factor(gender),</pre>
 age = as.numeric(age),
 hypertension = factor(hypertension),
 heart_disease = factor(heart_disease),
 ever_married = factor(ever_married),
 work_type = factor(work_type),
 Residence_type = factor(Residence_type),
 avg_glucose_level = as.numeric(avg_glucose_level),
 bmi = as.numeric(bmi),
 smoking_status = factor(smoking_status)
```

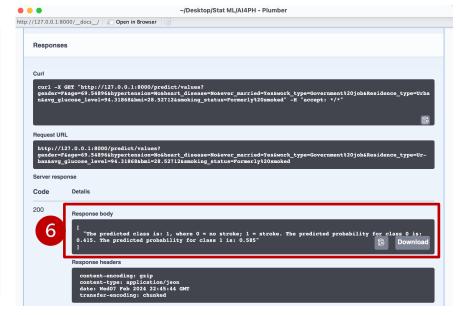
```
predict on the new data - class
prediction_class <- workflow %>%
 predict(new_data = newdata,
 type = 'class')
predict on the new data - probability
prediction_prob <- workflow %>%
 predict(new_data = newdata,
 type = 'prob')
report result
print(paste("The predicted class is: ", prediction_class$.pred_class, ", where 0 = no stroke; 1 = stroke",
 ". The predicted probability for class 0 is: ", round(prediction_prob[1],3),
 ". The predicted probability for class 1 is: ", round(prediction_prob[2],3), sep = ""))
```

| Server respon | nse                                                                                                                                                                      |
|---------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Code          | Details                                                                                                                                                                  |
| 200           | Response body                                                                                                                                                            |
|               | "The predicted class is: 1, where 0 = no stroke; 1 = stroke. The predicted probability for class 0 is: 0.415. The predicted probability for class 1 is: 0.585"  Download |









### Demo

Please copy and paste the below examples and see if the returned results are as expected:

| Example 1             |                         |  |  |  |
|-----------------------|-------------------------|--|--|--|
| gender                | F                       |  |  |  |
| age                   | 69.54896                |  |  |  |
| hypertension          | No                      |  |  |  |
| heart_disease         | No                      |  |  |  |
| ever_married          | Yes                     |  |  |  |
| work_type             | Government job          |  |  |  |
| Residence_type        | Urban                   |  |  |  |
| avg_glucose_level     | 94.31868                |  |  |  |
| bmi                   | 28.52712                |  |  |  |
| smoking_status        | Formerly smoked         |  |  |  |
|                       |                         |  |  |  |
| The observed class: 1 |                         |  |  |  |
| =========             |                         |  |  |  |
| The expected predicte | ed class: 1             |  |  |  |
| The expected probabi  | lity for class 0: 0.415 |  |  |  |

The expected probability for class 1: 0.585

| E                                           | cample 2     |  |  |
|---------------------------------------------|--------------|--|--|
| gender                                      | F            |  |  |
| age                                         | 48.50831     |  |  |
| hypertension                                | No           |  |  |
| heart_disease                               | No           |  |  |
| ever_married                                | Yes          |  |  |
| work_type                                   | Private job  |  |  |
| Residence_type                              | Rural        |  |  |
| avg_glucose_level                           | 61.57483     |  |  |
| bmi                                         | 27.60176     |  |  |
| smoking_status                              | Never smoked |  |  |
|                                             | :            |  |  |
| The observed class: 0                       |              |  |  |
| ==========                                  |              |  |  |
| The expected predicted class: 0             |              |  |  |
| The expected probability for class 0: 0.742 |              |  |  |
| The expected probability for class 1: 0.258 |              |  |  |

| Example 3                                   |                 |  |  |  |
|---------------------------------------------|-----------------|--|--|--|
| gender                                      | M               |  |  |  |
| age                                         | 68.96269        |  |  |  |
| hypertension                                | No              |  |  |  |
| heart_disease                               | No              |  |  |  |
| ever_married                                | Yes             |  |  |  |
| work_type                                   | Self-employed   |  |  |  |
| Residence_type                              | Urban           |  |  |  |
| avg_glucose_level                           | 77.88883        |  |  |  |
| bmi                                         | 25.83863        |  |  |  |
| smoking_status                              | Formerly smoked |  |  |  |
| =======================================     |                 |  |  |  |
| The observed class: 1                       |                 |  |  |  |
| =======================================     |                 |  |  |  |
| The expected predicted class: 1             |                 |  |  |  |
| The expected probability for class 0: 0.371 |                 |  |  |  |
| The expected probability for class 1: 0.629 |                 |  |  |  |

### The final assessment

In this assignment, you will validate the model we developed in class using a different dataset: `valid\_data.rds`. You will run into issues using this dataset as it is because this is a raw dataset without data harmonization, which means that some variables in this dataset are different from the harmonized dataset we used to train and evaluate the model. Your job here is to harmonize the validation data so that it's in the same format as the example data we used in class. You can refer to `train\_data\_variables.csv` to see the format in the harmonized train data.

All materials including this slide deck and the demo code can be found on Github: <a href="https://github.com/JuanLiOHRI/AI4PH-R/tree/main">https://github.com/JuanLiOHRI/AI4PH-R/tree/main</a>

### The final assessment – How to submit



Resources

Pages

People

Assignments



Final Assignment

Start Assignment

Due Feb 26 by 11:59pm

Points 1 Submit

Submitting a file upload

Learners will successfully complete the course by fulfilling the following:

- 1. Develop and deploy an algorithm where a user can input feature values on a web application and the web application will return the score of the algorithm.
- 2. Understand the usage of metadata.
- 3. Validate the already developed model (tidymodels workflow) on another dataset, with some data harmonization steps.

A dataset on stroke will be provided for the assignment.

Materials of the demo and assignment can be found on Github: https://github.com/JuanLiOHRI/AI4PH-R/tree/main

To submit your work on the assignment, please send us the assignment file (.Rmd) that includes your code and all th rename the file as AI4PH\_assignment\_YourName.Rmd). E.g. my name is Juan Li and I will rename my submission as AI4PH\_assignment\_Juanti.Rmd).

## **THANK YOU**

### TIDYMODELS – other packages that might be useful



Some R objects become inconveniently large when saved to disk. The butcher package can reduce the size of those objects by removing the sub-components.

e.g. logistic regression model object that contains the training data. Especially in public health, where the sample size can be huge.



The tidyposterior package enables users to make formal statistical comparisons between models using resampling and Bayesian methods.



infer is a high-level API for tidyverse-friendly statistical inference.

The corrr package has tidy interfaces for working with correlation matrices.