Developing and Deploying Transparent and Reproducible Algorithms for Public Health

R: tidymodels & plumber

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Minicourse team

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- Stacey Fisher Post Doc

Course outline

- 1) Understand open science concepts for algorithms in public health applications.
- 2) Develop an understanding of programming libraries and platforms in R to develop and deploy predictive algorithms. Demo
- 3) Develop and deploy transparent and reproducible machine learning or statistical algorithms.

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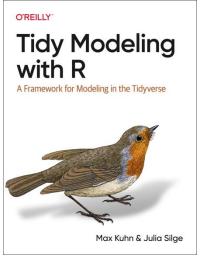
TIDYMODELS

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 (Application Programming Interface) by merely decorating your existing R source code with roxygen2-like comments.

https://www.rplumber.io/



https://phesc.instructure.com/courses/398/assignments/1017





25WI - Developing and Deploying Transpar... > Assignments > Final Assignment



















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Start Assignment

Due Mar 31 by 11:59p.m.

Points 1

Submitting a file upload

Learners will successfully complete the course by fulfilling the following:

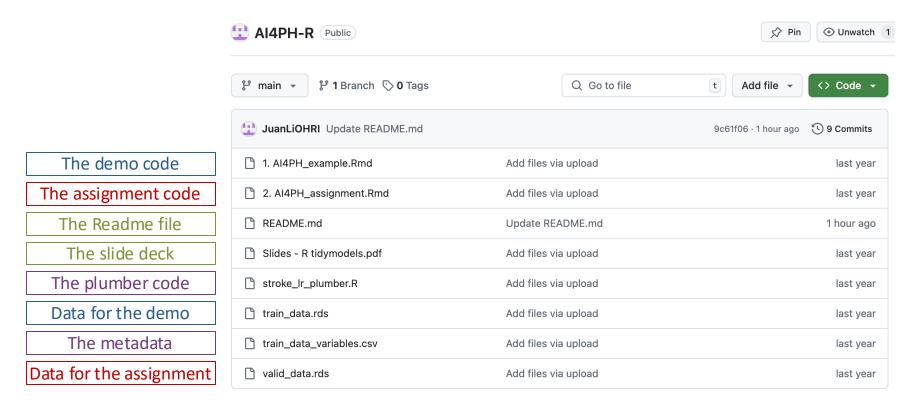
- 1. Develop and deploy an algorithm where a user can input feature values on a web application and the web application will return the score of the algorithm.
- 2. Understand the usage of metadata.
- 3. Validate the already developed model (tidymodels workflow) on another dataset, with some data harmonization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

A dataset on stroke will be provided for the assignment.

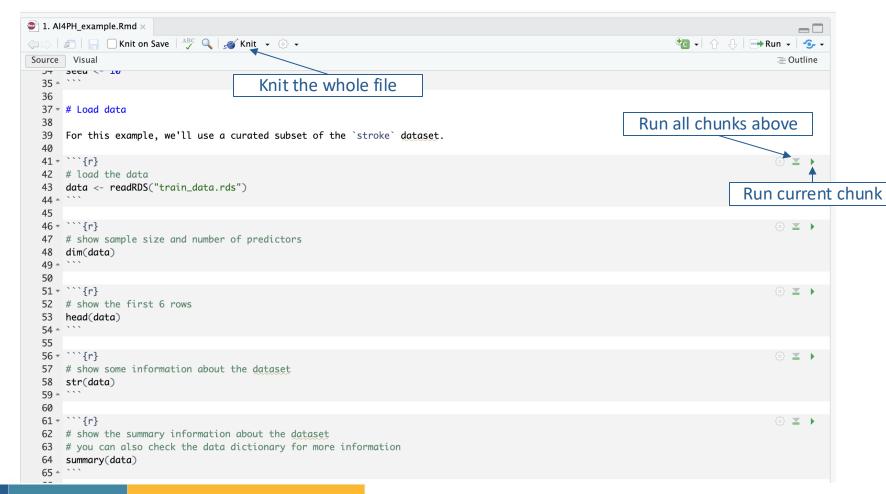
Materials of the demo and assignment can be found on Github: https://github.com/JuanLiOHRI/AI4PH-R/tree/main

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 Main packages

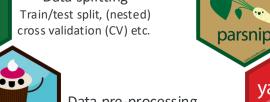


The meta-package



recipes

Data splitting



Data pre-processing



Model interface



Model performance

Hyperparameter tuning of your model and pre-processing steps

> Creates and manages tuning parameters and parameter grids



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



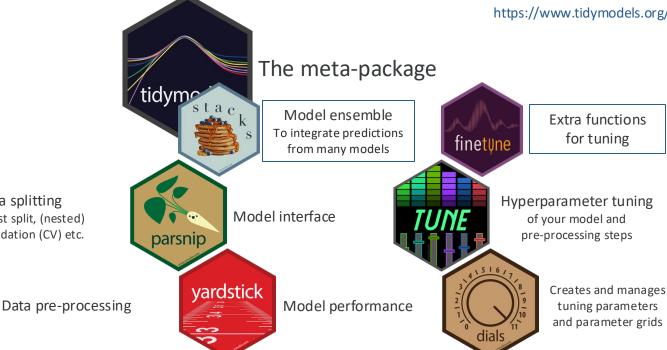
Reporting converts the information in common statistical R objects into user-friendly, predictable formats

dials

TIDYMODELS Main packages

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

recipes



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

TIDYMODELS (demo): a subset of the stroke (CCHS: Canadian Community Health Survey) data

```
> data <- readRDS("train_data.rds")</pre>
```

> 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_status	stroke
1	M 49	33984	Yes	No	Yes	Private job	Rural	179.89718	27.84435	Never smoked	0
2	F 50	0.10903	No	No	Yes	Private job	Urban	136.81856	26.68095	Currently smokes	0
3	F 76	5.21449	No	No	No	Self-employed	Urban	201.03038	42.08255	Never smoked	0
5	F 66	5.76548	Yes	No	Yes	Private job	Urban	88.45523	25.77091	Never smoked	0
6	M 43	3.14164	Yes	No	No	Self-employed	Urban	249.41379	34.42329	Currently smokes	0
8	F 69	54896	No	No	Yes	${\tt Government\ job}$	Urban	94.31868	28.52712	Formerly smoked	0

variable	role	type	min	max	Actual or label	
gender	predictor	Categorical			range. 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; Governn	nent 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; Curre	ntly smokes
stroke	outcome	Categorical			0; 1	

TIDYMODELS (demo): data splitting

For reproducibility, see the random seed. The same seed will be used throughout the demo.



```
```{r, message=FALSE}
seed <- 10</pre>
```

```
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**

```
rsample
```

```
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</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())
```



# 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)

tidy(lr\_workflow\_fit, exponentiate = TRUE)

# Train the model with preprocessing steps
lr\_workflow\_fit <- lr\_workflow %>%
 fit(data = stroke\_train)

# Obtaining the odds ratios

# # Obtaining the estimated coefficients tidy(lr\_workflow\_fit)



| # A tibble: 13 × 5                            |                 |                |                            | # A tibble: 13 × 5                            |             |                |                             |
|-----------------------------------------------|-----------------|----------------|----------------------------|-----------------------------------------------|-------------|----------------|-----------------------------|
| term                                          | estimate        | std.error s    | statistic p.value          | term                                          | estimate    | std.error      | statistic p.value           |
| <chr></chr>                                   | <db1></db1>     | <dbl></dbl>    | <dbl> <dbl></dbl></dbl>    | <chr></chr>                                   | <dbl></dbl> | <dbl></dbl>    | <dbl> <dbl></dbl></dbl>     |
| 1 (Intercept)                                 | 0.511           | 0.040 <u>1</u> | 12.7 4.45e-37              | 1 (Intercept)                                 | 1.67        | 0.040 <u>1</u> | 12.7 4.45e- <mark>37</mark> |
| 2 age                                         | 0.676           | 0.044 <u>9</u> | 15.1 3.25e- <u>51</u>      | 2 age                                         | 1.97        | 0.044 <u>9</u> | 15.1 3.25e-51               |
| 3 avg_glucose_level                           | 0.320           | 0.043 <u>3</u> | 7.39 1.50e-13              | 3 avg_glucose_level                           | 1.38        | 0.043 <u>3</u> | 7.39 1.50e-13               |
| 4 bmi                                         | -0.148          | 0.042 <u>0</u> | -3.52 4.25e- 4             | 4 bmi                                         | 0.862       | 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- <mark>2</mark> | 5 gender_M                                    | 1.07        | 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>6 hypertension_Yes</pre>                 | 1.30        | 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>7 heart_disease_Yes</pre>                | 1.25        | 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>8 ever_married_Yes</pre>                 | 0.970       | 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>9 work_type_Private.job</pre>            | 0.940       | 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            | <pre>10 work_type_Government.job</pre>        | 0.961       | 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             | 11 Residence_type_Urban                       | 1.03        | 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>12 smoking_status_Formerly.smoked</pre>  | 1.02        | 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             | <pre>13 smoking_status_Currently.smokes</pre> | 1.01        | 0.042 <u>0</u> | 0.208 8.35e- 1              |

#### **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 %% training() # 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(lr_workflow_fit)
Obtaining the odds ratios
tidy(lr_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\_fit <- lr\_workflow %>%

fit(data = stroke\_train)

lr workflow <workflow() %>% add\_model(lr\_spec) %>% add\_recipe(lr\_recipe) # Train the model with preprocessing steps



# Obtaining the estimated coefficients tidy(lr\_workflow\_fit) # Obtaining the odds ratios tidy(lr\_workflow\_fit, exponentiate = TRUE)



```
```{r, message=FALSE}
custom_metrics <- metric_set(sens, spec, roc_auc)</pre>
```

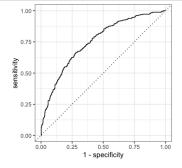
custom_metrics(test_results, truth = stroke, estimate = .pred_class, .pred_0)



A tibble: 3 x 3

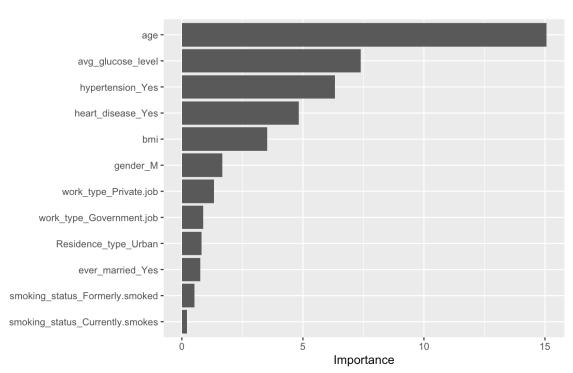
.metric <chr></chr>	.estimator <chr></chr>	.estimate <dbl></dbl>	
sens	binary	0.5417957	
spec	binary	0.8126273	
roc_auc	binary	0.7533750	





TIDYMODELS (demo): feature importance

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

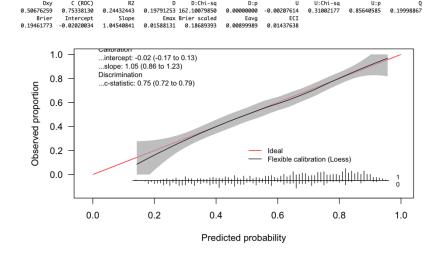


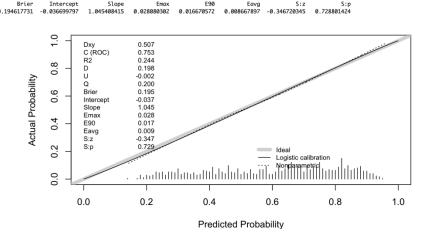
TIDYMODELS (demo): calibration

```
prediction <- test_results$.pred_1 # get the prediction probability
outcome <- as.numeric(as.character(test_results$stroke)) # turn the factor into numerical
CalibrationCurves::val.prob.ci.2(prediction, outcome)

```{r}
rms::val.prob(prediction, outcome)

```</pre>
```





0.856405855 0.199607807

0.197531667 161.790776727



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.

PLUMBER

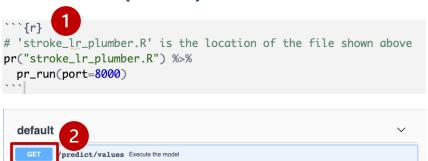
Plumber allows you to create a web API (Application Programming Interface) by merely decorating your existing R source code with roxygen2-like comments. https://www.rplumber.io/

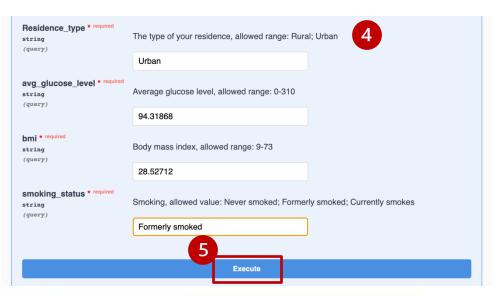


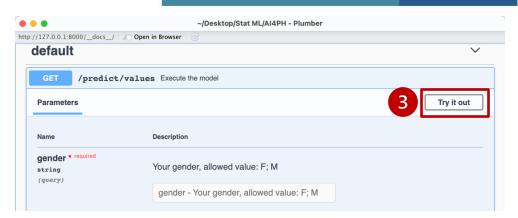
```
# read in the saved workflow object
workflow <- readRDS("stroke_lr_workflow.rds")</pre>
# assemble the inputs into a data frame
newdata <- data.frame(gender = factor(gender),</pre>
                      age = as.numeric(age),
                      hypertension = factor(hypertension),
           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

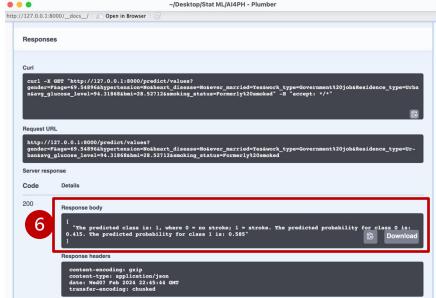
```
# predict on the new data - class
prediction_class <- workflow %>%
  predict(new_data = newdata,
          type = 'class')
# predict on the new data - probability
prediction_prob <- workflow %>%
  predict(new_data = newdata,
          type = 'prob')
# report result
print(paste("The predicted class 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 response	erver response				
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:

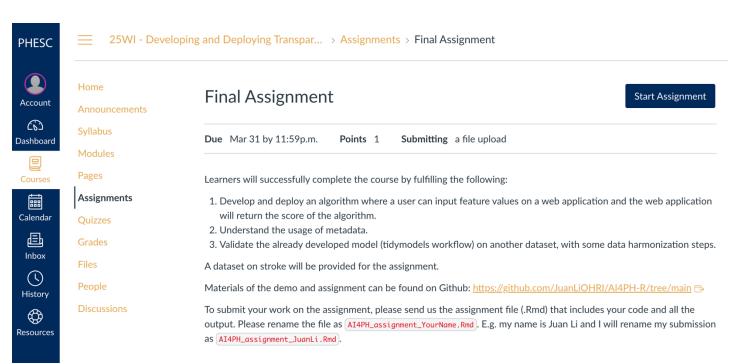
Exa	mple 1
gender	F
age	69.54896
hypertension	No
heart_disease	No
ever_married	Yes
work_type	Government job
Residence_type	Urban
avg_glucose_level	94.31868
bmi	28.52712
smoking_status	Formerly smoked
The observed class:	1
The expected predict	ed class: 1

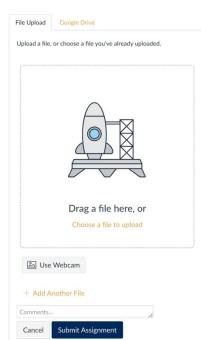
The expected probability for class 0: 0.415 The expected probability for class 1: 0.585

Example 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 predi	cted class: 0			
The expected proba	ability for class 0: 0.742			
The expected proba	ability 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 proba	bility for class 1: 0.629				

The final assessment – How to submit





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: https://github.com/JuanLiOHRI/AI4PH-R/tree/main

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.