Virtual Patient Cohorts

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CHAPTER

ONE

MAIN

$main.handle_leftclick(event: Event) \rightarrow None$

Helper function to set the focus to the widget associated with the current event event.

Is used to set the focus to whatever widget is clicked by the user.

Parameters

event (*Event*) – The event, i.e. left mouse click.

main.main()

Main function.

Setting up argparse to catch the --debug flag on startup, running setup_logging() and finally running the program, i.e. its mainloop().

main.setup_logging(debug: bool = False)

Logging setup for the program.

Logs are saved in a ./logs/ directory relative to the current working directory, which will be created if it's not present. Logging config uses a 'logging_config.json' file in this module's directory.

Parameters

 $\begin{tabular}{ll} \textbf{debug } (bool, optional) - flag that gets passed through by argparse to enable logging on debug level, defaults to False \\ \end{tabular}$

2 Chapter 1. main

CTKINTERFACE MODULE

class src.CTkInterface.MainApp

Bases: CTk

Main interface of the program. Providing ways for the user to input information that gets checked for to finally be able to fit a model to data.

Uses a tkinter extension called customtkinter to achieve a modern look.

```
__init__() \rightarrow None
```

Setup of the main interface window seen after starting the program, arranging widgets and setting default values.

```
browse\_files() \rightarrow None
```

Opens a tkinter.filedialog to let the user select a file containing fitting data. Sets internal variables to the file path and name when a file is successfully selected.

$check_inputs_populated() \rightarrow str$

Checks the various fields for missing user input.

Returns

Message with missing or invalid entried, empty if okay.

Return type

str

$\textbf{check_inputs_sensible()} \rightarrow str$

Checks whether the user input 'makes sense', e.g. if there are unfitted constants in the model expression.

Returns

Message with apparent issues in the user's input.

Return type

str

$\textbf{compute_params()} \rightarrow None$

Runs ModelFitter.fit() on the model and data, opens a window with the results.

$confirm_input() \rightarrow None$

Checks inputs and displays any issues. If okay, sets internal variables.

$\textbf{create_interpretation_string}(\textit{model}: \ VPCModel \ | \ \textit{None} = \textit{None}, \ **kwargs: \ \textit{str} \ | \ \textit{None}) \rightarrow \textit{str}$

Creates the interpretation string of the user input.

Parameters

• model (VPCModel, optional) – Model to be iterpreted, defaults to None.

• **kwargs** (*str* / *None*) – Additional keyword arguments, defaults to None.

Returns

A multi-line f-string containing the entered information.

Return type

str

create_tooltip_for(*widget: Widget, msg: str*) → ToolTip

Helper Function to create a ToolTip for and attach it to a tkinter.Widget.

Parameters

- widget (Widget) The tkinter. Widget the ToolTip is binded to.
- **msg** (*str*) What the ToolTip should say.

Returns

A new ToolTip instance.

Return type

ToolTip

$display_interpreted_input(msg: str) \rightarrow None$

Shows the interpretation of the user input.

Parameters

msg(str) – interpretation of the user input

$missing_independent_variables() \rightarrow list[str]$

Returns list of all characters or strings that were entered in the independent parameter field that are not present in the model string. If the field was left empty 't' is defaulted to.

Returns

List of missing symbols.

Return type

list

$remove_compute_tooltip() \rightarrow None$

Removes the tooltip and enables the 'compute parameters' button.

```
reset_state() \rightarrow None
```

Resets the program to an initial state without closing and reopening it.

Raises

AttributeError – if one of the internal attributes that should have been set are not found and therefore couldn't be reset.

$save_results() \rightarrow int$

Saves relevant inputs and outputs of the program in a file.

Returns

0 if FileHandler.write_file() finished normally, 1 otherwise.

Return type

int

CTKRESULTINTERFACE MODULE

```
class src.CTkResultInterface.FailedFitInterface(main window: MainApp)
    Bases: CTkToplevel
```

Intereface for displaying a message for a failed fit.

```
__init__(main_window: MainApp)
```

Initialize the failed fit interface. :param main_window: Parent window. :type main_window: MainApp

 $reset_app() \rightarrow None$

Reset the parent application's state and close this window.

class src.CTkResultInterface.ResultInterface(main_window: MainApp, model: VPCModel, fitted_model: VPCModel, data: list[list[int | float]])

Bases: CTkToplevel

Interface for results created by ModelFitter.

Provides a way to save results locally and view a plot of the residuals of the fit if possible.

Uses a tkinter extension called customtkinter to achieve a modern look.

```
__init__(main_window: MainApp, model: VPCModel, fitted_model: VPCModel, data: list[list[int |
           float]]) \rightarrow None
```

Setup of the result interface window, arranging widgets and setting values.

Parameters

- main_window (MainApp) Parent window.
- model (VPCModel) Model that was fitted to the sample data.
- fitted_model (VPCModel) Fitted model as a means to get easy access to the fitted model's lambda function.
- data (list[list[int | float]]) The data the input was fitted to.

```
create\_difference\_dict(list\_actual: list[tuple[float, ...]], list\_predicted: list[tuple[float, ...]]) <math>\rightarrow dict[int, list[tuple[float, ...]])
                                          list[float]]
```

Used to compute the differences (residuals) of two input lists created by process_lists(). Stores the differences at each index in a dictionary with index:difference pairs.

Parameters

- list_actual (list[tuple[float, ...]]) list of the actual values.
- list_predicted (list[tuple[float, ...]]) list of the predicted values.

Raises

- **ValueError** If the input lists somehow have different lengths.
- **ValueError** If a pair of tuples somehow have different lengths.

Returns

Dictionary with the differences at their corresponding index.

Return type

dict[int,list[float]]

$graph_residuals() \rightarrow None$

Method that uses matplotlib to graph the residuals of the fitted model against the input data after the graph button is pressed.

```
\textbf{process\_lists}(\textit{lst: list[list[float]]}) \rightarrow \textit{list[float]} \mid \textit{list[tuple[float, ...]]}
```

Converts a list of lists of floats into a list of floats, if there is only a single sub-list.

If there are multiple sub-lists inside the input list, will zip them and return a list of tuples of floats.

Parameters

1st (*list*[*list*[*float*]]) – List that is to be converted, typically the data the model was fitted to, or part of it.

Raises

ValueError – If there are types other than list in the outer list.

Returns

List of floats or list of tuples of floats.

Return type

list[float] | list[tuple[float, ...]]

```
reset_app() \rightarrow None
```

Method that calls the parent's reset_state() method to reset the app to an initial state after the reset button is pressed.

```
save_as() \rightarrow None
```

Method that calls the parent's save_results() method and sets the saved_message_label's value accordingly after the save button is pressed.

$set_result_label_text() \rightarrow None$

Method that sets the text inside the results textbox.

FILEHANDLER MODULE

This module provides basic functionality to convert data stored in .xlsx or .csv files into python lists.

class src.FileHandler.**FileExtensions**(*value*, *names=None*, **values*, *module=None*, *qualname=None*, *type=None*, *start=1*, *boundary=None*)

Bases: Enum

Enum class that has all valid file extension names and suffixes.

CSV = 'CSV'

EXCEL = 'XLSX'

 $src.FileHandler.dataframe_tolist(data_frame: DataFrame) \rightarrow list[list[float | int]]$

Convert a pd.DataFrame to a list of lists containing its values.

Parameters

data_frame (pd.DataFrame) – DataFrame to be converted.

Raises

ValueError – If the *data_frame* is None, empty, contains empty cells, or non-numeric values.

Returns

List of lists containing the DataFrame's values.

Return type

list[list[float | int]]

$src.FileHandler.get_valid_filename() \rightarrow str$

Create a valid, hopefully non-duplicate, string to use as a file name.

Returns

Stringified time from datetime.now() in the form of %Y-%m-%d-result-from-%Hh%Mm.

Return type

stı

$\verb|src.FileHandler.is_extension_supported| (\textit{file_path: str}) \rightarrow bool$

Check if the file extension at the given path is supported.

Parameters

file_path (*str*) – Path pointing to the file.

Returns

True if supported, False otherwise.

Return type

bool

$src.FileHandler.read_file(file_path: str) \rightarrow DataFrame$

Read a .csv or .xlsx file from the given path and return it as a pd.DataFrame.

Uses pathlib's *is_file()* method to ensure there is a file at the given path. Then tries to obtain the file's suffix and checks for *.csv* or *.xlsx* formats, for which the corresponding pandas read method is called.

Parameters

file_path (*str*) – Path to the file to be read.

Raises

- **FileNotFoundError** If no file exists at *file_path*.
- **ValueError** If *file_path* has no suffix.
- **TypeError** If the file is not either an Excel table or CSV file.

Returns

A pd.DataFrame containing all information that is read from the excel or csv file.

Return type

pd.DataFrame

```
src.FileHandler.write_file(data_frame: DataFrame, file_format: FileExtensions = FileExtensions.EXCEL, destination: str = '/res'') \rightarrow None
```

Write the provided *pd.DataFrame* as either .xlsx or .csv to the ./res/ directory.

If there is no ./res/ directory relative to where the program was started from, that directory will be created.

Parameters

- data_frame (pd.DataFrame) The data frame to be written.
- file_format (FileExtensions, optional) Format of the written file, defaults to File-Extensions. EXCEL.
- **destination** Destination directory, default to "./res/".

Raises

TypeError – If *file_format* was neither Excel nor CSV.

MODELDATA MODULE

```
class src.ModelData.ModelData(fitted_model: str \mid None = None, fitted_consts: dict[str, float] \mid str \mid None = None, model: str = 'f(t) = ...', user_input_model: str = 'f(t) = ...', parameter: list[str] = \langle factory \rangle, user_input_parameter: str = '...', consts: list[str] = \langle factory \rangle, user_input_path: str = 'path/to/data')
```

Bases: object

Container class that stores information for writing into the results file.

Parameters

- **fitted_model** (*str* / *None*) The fitted model as a string.
- **fitted_consts** (*dict[str, float] | str | None*) Dictionary of constants with keys of type *str* and values of type *float*. Alternatively, a string containing the same information. Defaults to None.
- **model** (str, optional) The model the program worked with. Defaults to " $f(t) = \dots$ ".
- user_input_model (str, optional) The exact model the user entered. Defaults to " $f(t) = \dots$ ".
- **parameter** (list[str], optional) The independent variable the program worked with. Defaults to ["..."].
- user_input_parameter (str, optional) The exact independent variables the user entered. Defaults to "...".
- **consts** (*list[str]*, *optional*) The constants the program worked with. Defaults to ["..."].
- user_input_consts (list[str], optional) The exact constants the user entered. Defaults to ["..."].
- **user_input_path** (*str*, *optional*) The path to the data the user provided. Defaults to "path/to/data".
- **__init__**(fitted_model: $str \mid None = None, fitted_consts: dict[str, float] \mid str \mid None = None, model: <math>str = 'f(t) = ...', user_input_model: str = 'f(t) = ...', parameter: list[str] = <factory>, user_input_parameter: <math>str = '...', consts: list[str] = <factory>, user_input_consts: list[str] = <factory>, user_input_path: <math>str = 'path/to/data') \rightarrow None$

consts: list[str]

```
create\_dataframe\_for(format: FileExtensions = FileExtensions.EXCEL) \rightarrow DataFrame
```

Create a *pd.DataFrame* for the specified format, i.e. either Excel or CSV. The DataFrame contains information about the user inputs into the program and what the program made of those. It also contains the fit of the model if possible. If no fitted model string was given, a warning will be logged and the field in the DataFrame will read 'N/A'.

Parameters

format (FileExtensions, *optional*) — The format for which the DataFrame is constructed. Defaults to FileExtensions.EXCEL.

Returns

A DataFrame containing all input and output information.

Return type

pd.DataFrame

```
fitted_consts: dict[str, float] | str | None = None
fitted_model: str | None = None
model: str = 'f(t) = ...'

parameter: list[str]

user_input_consts: list[str]

user_input_model: str = 'f(t) = ...'

user_input_parameter: str = '...'

user_input_path: str = 'path/to/data'
```

MODELFITTER MODULE

This module provides functions to fit a model to data.

The fitting routines are based on the assumption that the model is of type VPCModel with provided data consisting of a list of lists where each sub-list is a column from a datasheet.

```
src.ModelFitter.\_fit\_ode(model: VPCModel, data: list[list[int | float]]) \rightarrow None
```

Fit a model represented by an ordinary differential equation (ODE) to provided data.

This function sets the internal variables of the model to reflect the fit.

Parameters

- model (VPCModel) The model that is to be fit.
- data (list[list[int | float]]) The provided data to which the model is fitted.

Raises

RuntimeError – If an error occurs during the minimization process or while solving the initial value problem.

```
src.ModelFitter.\_fit\_reg(model: VPCModel, data: list[list[int | float]]) \rightarrow None
```

Fit a model that is not represented by an ordinary differential equation (ODE) to provided data.

This function sets the internal parameters of the model to reflect the fit.

Parameters

- model (VPCModel) The model that is to be fitted.
- data(list[list[int | float]]) The provided data to which the model is fitted.

Returns

Tuple consisting of a callable function, as well as values for the independent variable and their resulting data, taken from the provided input data

Return type

None

$src.ModelFitter.check_model_is_valid_vector(model: VPCModel, columns: int) \rightarrow bool$

Checks if the model is valid when comparing it the the sample data.

A model is an invalid if there are not enough columns in the data to account for all independent variables and the result components.

Parameters

- model (VPCModel) The model to be checked.
- **columns** (*int*) The number of columns in the provided data.

Raises

Exception – If there are too few or too many columns in the data. Too few make it impossible to fit the model, too many make it ambiguous as to what the extra columns are supposed to mean, or which columns are even to be regarded and which ones not.

Returns

Whether the model is a vector.

Return type

bool

 $\verb|src.ModelFitter.evaluate_fit|| pcov: ndarray[Any, dtype[_ScalarType_co]]|) \rightarrow \mathsf{dict}[\mathsf{str}, \mathsf{float}]|$

Evaluate the goodness of fit based on the covariance matrix.

Parameters

pcov (2D-array) – Covariance matrix of the fit.

Returns

Dictionary containing evaluation metrics.

Return type

dict

 $src.ModelFitter.fit(model: VPCModel, data: list[list[int | float]]) \rightarrow None$

Main entry function for the fitting process. Delegates model and data to the correct fitting routine based on whether it's an ordinary differential equation or not.

Parameters

- **model** (VPCModel) The model that is supposed to be fitted.
- data (list[list[int | float]]) The data the model is supposed to be fitted to.

VPCMODEL MODULE

```
class src.VPCModel.VPCModel(_model_string: str, _independent_var: list[str])
      Bases: object
      Dataclass to store a model and extract relevant information from it.
      __init__(\_model\_string: str, \_independent\_var: list[str]) <math>\rightarrow None
      _independent_var: list[str]
      _model_string: str
      \_set\_fitted\_consts(fitted\_consts\_dict: dict[str, float]) \rightarrow None
           Function to set the computed fitted constants to its internal variable.
                Parameters
                    fitted_consts_dict (dict[str, float]) - Dictionary of { 'const_name': value}
      \_set\_resulting\_function(fitted\_function: str) \rightarrow None
           Function to set the computed fitted function to its internal variable.
                Parameters
                    fitted_function (str) – The fitted function string.
      property components: int
           Property to return the number of components the result has, i.e. if it is a vector.
           A property without an accompanying setter is used to prohibit setting this value.
                    Number of components of the model expression.
                Return type
      property constants: list[str]
           Property to return the list of constants in the model expression that are to be fitted.
           A property without an accompanying setter is used to prohibit setting this value.
                Returns
                    List of all constants in the model expression.
                Return type
```

list[str]

```
cut_off_lhs() \rightarrow str
```

Cuts off the left hand side of an equation, indicated by an equals sign. Also strips leading and trailing spaces and replaces some characters if needed.

Returns

Model equation without left hand side, including the equals sign.

Return type

str

$cut_off_rhs() \rightarrow str$

Cuts off the right hand side of an equation, indicated by an equals sign. Also strips leading and trailing spaces and replaces some characters if needed.

Returns

Model equation without right hand side, including the equals sign.

Return type

str

property expression_string: str

Property to return the expression string (right-hand side) of the class instance.

A property without an accompanying setter is used to prohibit setting this value.

Returns

The expression string of the model.

Return type

str

```
extract_symbols(sorting\_prio: list[str] \mid None = None) \rightarrow list[str]
```

Extract all unique symbols out of the model equations right-hand side.

Unique symbols are single or multi-character sequences consisting of letters. If a sorting prio is given, the characters in it are returned at the front of the output, the rest is ordered alphabetically.

Parameters

```
sorting\_prio(list[str] \mid None, optional) - Characters to be placed at the start of the output, defaults to None
```

Returns

All unique symbols in the expression on the right-hand of the equation.

Return type

list[str]

property fitted_consts: dict[str, float]

Property to return the dictionary of fitted constants of the function. If this value is not set at the time of accessing it through this property, an empty dictionary will be returned.

A property without an accompanying setter is used to prohibit setting this value.

Returns

Dictionary with constant:value as its pairs.

Return type

dict[str, float]

format_eq(equation: str) \rightarrow str

Replaces some characters for others in a string. Strips leading and trailing spaces.

Parameters

equation (*str*) – The string in which characters will be replaced.

Returns

Stripped input string with replaced characters.

Return type

st

property independent_var: list[str]

Property to return the list of independent variables of the class instance.

A property without an accompanying setter is used to prohibit setting this value.

Returns

List of all independent variables of the model.

Return type

list[str]

$is_ode() \rightarrow bool$

Determines whether the model is an ODE of at most 2nd order.

Returns

True if at most 2nd order ODE, False otherwise.

Return type

bool

is_vector() → bool

Determine whether the function is a vector based on the number of its components.

Raises

Exception – If components are less than 1.

Returns

True if the model is a vector, False otherwise.

Return type

bool

property model_function: FunctionClass

Property to return the lambdified model function of the class instance.

A property without an accompanying setter is used to prohibit setting this value.

Returns

FunctionClass / lambda expression of the model function.

Return type

sympy.FunctionClass

property model_string: str

Property to return the model string of the class instance.

A property without an accompanying setter is used to prohibit setting this value.

Returns

The model string without leading/trailing spaces and some character replacements.

Return type

str

$model_string_to_function() \rightarrow FunctionClass$

Create a lambda function based on the model equation.

Extracts all symbols from the expression and converts them to SymPy symbols. Finally lambdifies the expression to return a callable model function.

Returns

Lambdified model expression.

Return type

FunctionClass

property resulting_function: str

Property to return the stringified function with the computed constants in it. If this value is not set at the time of accessing it through this property, an empty string will be returned.

A property without an accompanying setter is used to prohibit setting this value.

Returns

The string of the final/resulting function after the fit.

Return type

str

set_fit_information($fitted_consts: dict[str, float] \mid None = None, error: bool = False) <math>\rightarrow$ None Set the fitted model information to the model's internal variables.

Parameters

- **fitted_consts** (*dict[str, float]*) The fitted model constants, defaults to None.
- **error** (*bool*) Indicates if an error occurred during fitting, defaults to False.

property symbols: list[str]

Property to return the list of symbols that are in the expression of the class instance.

A property without an accompanying setter is used to prohibit setting this value.

Returns

List of all symbols in the model expression.

Return type

list[str]

CHAPTER

EIGHT

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