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# Home

### **Project Overview**

Materials science is a complex field that focuses on the study of physical materials and their properties. MatMiner is an existing Python library that combines materials data with Machine Learning strategies and models to study material properties without the need for time-consuming physical experimentation. Our project, Hacking Materials ("HA"), aims to build an easy and intuitive user interface to the MatMiner library \* to eliminate the need for its users to have substantial Python or machine learning knowledge or experience.

Materials engineering is a field in which physical materials (e.g. metals, ceramics, polymers, composites, etc.) are studied to understand their composition, characteristics and properties. In many industries, such as mining, manufacturing and others, finding the right material for each job is essential for success. Materials engineers and scientists follow many different methods to compare candidate materials and make recommendations based on how they each satisfy the specific use case requirements. Some of these methods include physical experimentation, which can in some cases take up to 20 years to complete.

To avoid this, computer simulations (based on existing databases of known material properties and machine learning algorithms) can be used to compare materials in a much more efficient way. One such tool for this approach is the Python library MatMiner, which allows easy access to ready-made datasets and integrates well with other machine learning Python libraries. However, to use this library, the user must have a substantial level of specialised knowledge in machine learning and programming, which most materials engineering do not have. To help them overcome this, the solution proposed by the client describes a simple and intuitive user interface that would act as a bridge between the user and the MatMiner library in the backend. The vision of this product is to make machine learning methodologies more accessible within the materials science and engineering industry as a whole, minimising the time and financial costs involved and leading to a more efficient industry.

### **Project Personnel**



Dr Christian Brandl
Client

### Team Members



Alastair Daivis (Alastair Daivis)

Team Representative



Sanjeevani "Sanjee" Avasthi (Sanjeevani Avasthi)

Developer

### **Useful Links**

Trello	GitHub

# **Key Pages**

| Specifications

| Meetings

| Assessments

| Resources



Mamta Lopes (Mamta Ritesh Lopes

Developer



Ghina Yashar (Ghina Yashar)

Frontend Development Lead



Chunbaixue "Caitlyn" Yang (Chunbaixue Yang)

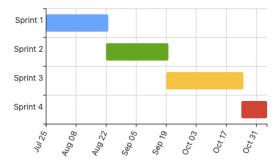
Scrum Master

Supervisor: Mauro Mello Jr

Lecturer: Cristoph Treude

COMP90082 Software Project Subject Coordinator: Eduardo Araújo Oliveira

## **Project Timeline**



## **Project Scope**

At this stage in development, we are focusing on a minimal set of features applicable to all users of the product. We have worked with Dr. Brandl to identify a set of core features, and to cleanly separate these from "pro-user" and other nice-to-have features. These high-priority features are identified in the User Stories list.

For now, only the high-priority features are definitely in scope for development. Other nice-to-have features may be developed once the high priority features have been finished and a minimum viable product has been deployed.

This project is intended to be generally useful to a broad range of potential users, including:

- Educators, who may use it to demonstrate the Matminer library and its capabilities
- Students, who may use it to learn about these tools and experiment with them
- Materials engineers, who will need to be able to access more advanced features including downloading generated code and customising workflow components

## Core technologies used

### Front-end

This project is primarily accessed via a website, which we're building with ReactJS and Styled Components. The development language is Typescript.

We are using Storybooks to automate documentation and previewing for developed UI components.

### Back-end

The front-end is supported by a Flask application, which interacts with Matminer on the user's behalf and surfaces required information in the UI.

The development language is Python. We're also using Pytest and Sphinx for running unit tests and generating documentation.

Key libraries we're using include Matminer and SQLAlchemy.

Our database is Postgres, and all back-end services are built as Docker containers. We have not yet selected a deployment technology, and are discussing options with the Melbourne University IT department.

\*Ward, L., Dunn, A., Faghaninia, A., Zimmermann, N. E. R., Bajaj, S., Wang, Q., Montoya, J. H., Chen, J., Bystrom, K., Dylla, M., Chard, K., Asta, M., Persson, K., Snyder, G. J., Foster, I., Jain, A., Matminer: An open source toolkit for materials data mining. Comput. Mater. Sci. 152, 60-69 (2018).

# | Specifications

- | Project Overview | Personas
- Motivational Model

- | User Stories | Low-fidelity Prototype | Notes on provided material Notes on provided mAcceptance Criteria

# | Project Overview

## The Problem

Materials engineering is a field in which physical materials (e.g. metals, ceramics, polymers, composites, etc.) are studied to understand their composition, characteristics and properties. In many industries, such as mining, manufacturing and others, finding the right material for each job is essential for success. Materials engineers and scientists follow many different methods to compare candidate materials and make recommendations based on how they each satisfy the specific use case requirements. Some of these methods include physical experimentation, which can in some cases take up to 20 years to complete.

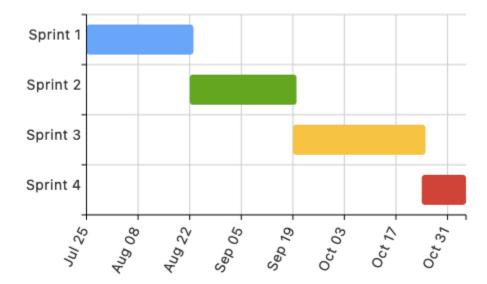
To avoid this, computer simulations (based on existing databases of known material properties and machine learning algorithms) can be used to compare materials in a much more efficient way. One such tool for this approach is the Python library MatMiner, which allows easy access to ready-made datasets and integrates well with other machine learning Python libraries. However, to use this library, the user must have a substantial level of specialised knowledge in machine learning and programming, which most materials engineering do not have. To help them overcome this, the solution proposed by the client describes a simple and intuitive user interface that would act as a bridge between the user and the MatMiner library in the backend. The vision of this product is to make machine learning methodologies more accessible within the materials science and engineering industry as a whole, minimising the time and financial costs involved and leading to a more efficient industry.

## The Client

The client of this project is **Dr Christian Brandl**, who is a senior Mechanical Engineering lecturer at the University of Melbourne and has a Ph.D. in Materials Science & Engineering. Aside from his scholarly work, Dr Brandl also acts as a Materials Consultant to clients who come to him seeking recommendations as to which materials may fit their specific needs, or with questions regarding the properties and characteristics of different materials. Dr Brandl hopes to use the product of this project to demonstrate to his clients the capabilities of machine learning and the possibilities it creates in the materials science field.

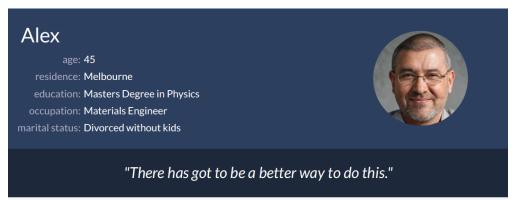
## Schedule

The project will run over four sprints, with the dates of each outlined below.



# | Personas

# Pro User - Prepared by Team RedBack



Motivation: As an experienced Materials Engineer, Alex's job requires him to narrow down candidate materials by performing physical experiments to choose a material which can takes years to do. He needs a tool that can speed up the process by narrowing down candidate materials for experimentation using Machine Learning and simulations.

### **Comfort With Technology**

PROGRAMMING WITH PYTHON

MACHINE LEARNING

**CLOUD BASED STORAGE** 

MATERIAL SCIENCE

### **Criteria For Success:**

Alex can find the right materials efficiently, with accurate results and that matches the client's requirements.

### Needs

- Products to accelerate his workflow
- Access to wide variety of related tools and resources

### Values

- Extensibility
- Accuracy
- Reliability
- Responsiveness
- Scalability
- Transparency

### Wants

- Suitable models and featurizers for different use cases
- Demonstrate reproducible results to his clients
- Share resources with others
- Refining generated workflow to reuse

#### **Fears**

- Tool is too inflexible
- · Losing access to progress on his work
- Not being able to verify his results
- Not having support with the tool

Student - Prepared by team BoxJelly

## **Assol Anahita**

age: 22

residence: Melbourne

education: Material Engineering

occupation: Student marital status: Single



"It's SO time consuming to do material researches and get decent results through just a semester."

Motivation: As a material engineering graduate student, Assol gets frustrated and demotivated when she can't make sense of the data she has because she doesn't have a tool or sufficient programming/machine learning skills to process the material data. She is also frustrated that she can't use machine learning algorithms to help her engineer new materials even though she is told by her supervisor that this idea works in theory.

#### **Comfort With Technology**

PROGRAMMING WITH PYTHON

MACHINE LEARNING

CLOUD BASED STORAGE

MATERIAL SCIENCE

### **Criteria For Success:**

Assol can perform materials data requests/retrievals and accurate materials property predictions supported by Machine Learning technology with easy to follow steps button clicks user interface.

#### Needs

- Easy-to-use interface Material science data processing and retrieval application
- A tool to predict property of a material with assistance of Machine Learning technology without prior knowledge of Python and Machine Learning programming

### Values

- Convenience
- Quickness
- Safety
- Understandable

#### Wants

- A data mining application that helps her researches
- A better understanding on how Machine Learning can help her to learn more about a material
- Ability to use ML algorithms as a black box
- Freedom to select features on her own terms
- A tool to accelerate research progress

#### Fears

- Spends hours without getting anything done because she neither has an adequate tool to do data mining, nor the programming skill to analyse the data herself
- Have to conduct countless experiments to figure out the properties of the materials
- Hard to choose suitable ML algorithms

Industry User - Prepared by team BlueRing

# **Gray Zhou**

age: 28

residence: Ningde, Fujian, China

education: Master of Material Engineering occupation: R & D Engineer of Polymer

marital status: Single



"It is fantastic to apply a multi-function online tool with ML methods if it is efficient and reliable. Nobody will refuse a tool that can save his time"

Motivation: Gray Zhou is a R & D Engineer of polymer in a battery factory. His work is searching for better materials for battery production. Gray spends lots of time testing different materials, but some of tests are waste of time because of the poor performance observed. He needs a system that can predict some useful properties of materials so that he can remove samples with low predicted performance and boost the research. His company provides some solutions, but they are awkward and only have limited functions.

### **Comfort With Technology**

PROGRAMMING WITH PYTHON

MACHINE LEARNING

CLOUD BASED STORAGE

MATERIAL SCIENCE

### **Criteria For Success:**

Provide a website or online-tool with quick, visual interface which can help him in daily development of new materials.

A successful product should help him save noticeable time on data processing and provide reliable prediction of properties.

#### Needs

- Retrieve and extract required data, process the data with ML methods to get some properties
- Provide graphs which can be modified with interface about predicted properties
- Help finding the material with best predicted properties

## Wants

- Ability to interact with the graph to further compare serval materials in detail
- Upload data from his lab for predicting
- Explain what ML method the system applied and how it helps the prediction
- Continue his work on mobile devices without gaps of interaction

### Values

- Easy to get started on both desktop and mobile
- · Efficient back-end process
- Abilities to select functions and filter results
- Well organized visualization of interface and graphs

#### Fears

- Not enough guidance in the web or tool so him may feel confused to find functions he wants.
- Lackingunderstandofwhatthesystemdone, then reducing the confidence level of his report
- Frequently unavailability

# | Motivational Model

- Do/Be/Feel listsGoal Model

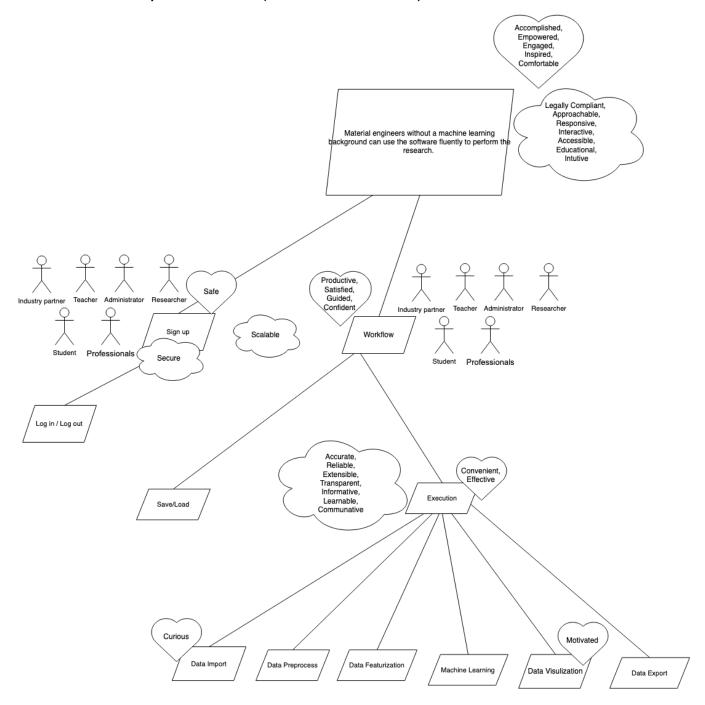
# Do/Be/Feel lists

# Version 1.1 - (cross-team effort)

Who (users)	Do (functional goals)	Be (qualitative goals)	Feel (emotional goals)
Students	Add more database, machine learning method and plot types	Accessible	Accomplished
Administra tors	Compare data using tables & plots	Accurate	Comfortable
Profession als	Data Pre-processing: Calculate descriptive statistics	Approachable	Confident
Industry Partners	Data Pre-processing: Consider anonymized data	Communicative	Convenient
Teachers	Data Pre-processing: Overview of the current import data	Educational	Curious
Researcher	Data Pre-processing: Reduces noise and eliminates ambiguity	Extensible	Effective
Code maintainers	Data Pre-processing: Standardizing data to bring it into the formatting range	Informative	Empowered
	Data Visualization: Data processing: Tabular data & Plotted Graph	Interactive	Engaged
	Edit python code directly in the interface	Intuitive	Guided
	Export input data	Learnable	Inspired
	Export jupyter notebook file	Legally Compliant	Motivated
	Export output data tables and figures	Reliable	Productive
	Featurization data: Add multiple composition-based features	Responsive	Safe
	Featurization data: Add multiple simple density features	Scalable	Satisfied
	Import Data: Creat working spaces when importing	Secure	
	Import Data: Drag and drop import of files	Transparent (progress, error messages, notebook export)	
	Import Data: Import data files (CSV, XES, Parquet) from local system		
	Log in/Log out		
	Machine Learning: Define input data and output data: Splitting data into training, test, and validation sets		
	Machine Learning: Determining model features and training the model: Configure and adjust hyperparameters for optimum performance		
	Machine Learning: Evaluate model performance and establish benchmarks: Continuous measurement and monitoring of model performance		
	Machine Learning: Evaluate model performance and establish benchmarks: Evaluate models using validation methods and validation datasets		
	Machine Learning: Get model results: The most important features of the current ML model		
	Machine Learning: Select the machine learning model to be used		
	Maintain software		
	save/load workflows		
	Sign up		

# **Goal Model**

# Version 1.1 - Sprint 3 Final (cross-team effort)



# | User Stories

- Version 1.3 (cross-team effort)Epics & Owning team allocation

  - User Stories
- Change log

# Version 1.3 - (cross-team effort)

# Epics & Owning team allocation

	Epic	Total Size	Highest Priority within Epic	Assigned Team
1	Input Data	27	1 - Must Have	RedBack
2	Administration	31	1 - Must Have	BoxJelly
3	Machine Learning	16	1 - Must Have	BlueRing
4	Data Visualisation	13	1 - Must Have	BlueRing
5	Jupyter Notebook	20	2 - Should Have	Unassigned - stretch goal
6	External Data	8	2 - Should Have	Unassigned - stretch goal

## **User Stories**

ID		Role		Action		Goal	Epic	Size (days)	Priority
30	As a	general user	l want to	be able to view the citations for used featurizers	so that			1	1 - Must have
32	As a	general user	l want to	browse and select built-in featurizers	so that I can discover ways of manipulating my data				1 - Must have
34	As a	general user	l want to	browse built-in datasets	so that	I can discover data to experiment with		1	1 - Must have
19	As a	student	l want to	quickly browse the Materials available in the database for retrieval and simulations	so that	I can quickly perform queries.		3	2 - Should have
21	As a	general user	I want to	be able to select datasets from exisiting databases	so that	I do not have to worry about how the data is loaded		3	1 - Must have
37	As a	general user	l want to	be able to preview the output of each execution	xecution so that I could explore the data		1	1 - Must have	
41	As a	general user	l want to	view the columns of the saved dataset and select the column I want to featurize	that I can provide the correct input to the featurizer		3	1 - Must hav	
25	As a	general user	l want to	Select specific features from a dataset	so that	I can improve the precision of my model		3	2 - Should have
13	As a	Pro user	l want to	add new features	so that	they can be reused in the future		5	2 - Should have
28	As a	general user	l want to	be able to reference / view citation for original data sources	so that			1	3 - Could have
18	As a	pro user	I want to	be able to apply new featurizers	so that			3	3 - Could have
1	As a	student	I want to	clean and tune data input	so that			5	3 - Could have
29	As a	student	I want to	save project specific data/checkpoints	so that	I can pick up where I left off for specific projects	Administra tion	1	1 - Must have

35	As a	pro user	l want to	export model selections, parameters, and data flows	so that	I can save my work and share it with others		1	1 - Must have
36	As a	pro user	I want to	import exported model selections, parameters, and data flows	so that	I can continue work I had previously saved		1	1 - Must have
20	As a	student	I want to	Create an account using single-sign on, restricted to the *.unimelb.edu.au domain	so that	my research remains private		3	1 - Must have
23	As a	pro user	I want to	Control job execution	so that I can start, view progress of, and cancel jobs related to my project		3	1 - Must have	
10	As a	pro user	I want to	be able to opt in to pro-user features	so that	I can access pro user features		5	1 - Must have
38	As a	pro user	I want to	have my pro user settings persist on each visit	so that	I don't have to reconfigure settings to use the features I need		1	2 - Should have
24	As a	student	I want to	receive provided hints and guidance for new users	so that	I can quickly learn how to use software		3	2 - Should have
14	As a	pro user	I want to	easily find and read documentation on the pro features	so that	I can use them with ease		5	2 - Should have
17	As a	pro user	I want to	Be kept informed about job status	so that	I can avoid polling my workspace to check for results		3	3 - Could
6	As a	pro user	I want to	have access to more processing power	so that	I can run more complex operations or use more data		5	3 - Could
31	As a	general user	I want to	able to select a Machine Learning model	so that	I could use it to train and run the data	Machine Learning	1	1 - Must have
33	As a	general user	I want to	browse built-in ML models  so that  I can discover ways of manipulating my data			1	1 - Must have	
39	As a	user	I want to	be able to select split ratio of data  so that  to train and test the model			1	2 - Should	
26	As a	pro user	I want to	have the option to change the hyperparameters used in the machine learning model				3	2 - Should
15	As a	pro user	I want to	be able use additional ML models	so that	I can improve accuracy		5	2 - Should have
7	As a	pro user	I want to	combine multiple models together	so that	I can model more complex data manipulations		5	3 - Could have
22	As a	general user	I want to	see clear annotation or explanation of data points and features	so that	I can understand the results of the analysis	Data Visualisati on	3	1 - Must have
40	As a	general user	I want to	select features used for x and y axis	so that	I can plot the chart based on features I'm interested in		1	1 - Must have
8	As a	student	I want to	use different type of plotting graphs	so that	I have flexibility to visualize data according to my needs.		5	1 - Must have
9	As a	general user	I want to	able to view and plot the results of the model	so that	I could analysis and visualise the effects of the model		5	1 - Must have
12	As a	student	I want to	export my work to a Jupyter Notebook	so I can extend my work beyond the capability of the hotebook Jupyter Notebook		5	2 - Should	
2	As a	general user	I want to	attach comments to workflow objects	so that	I can document my work		5	3 - Could
4	As a	Pro user	I want to	edit python code on the interface	so that	I can have control how the ML algorithms works			3 - Could
5	As a	Pro user	I want to	upload my own script (in python) if possible	so that	I can extend the tool to support custom models and featurizers		5	3 - Could have
27	As a	pro user	I want	be able to access new databases	so that	I can access addional data	External Data	3	2 - Should

3	As a	Pro user	l want to	be able to add new datasets in the future	so that	if there's a new dataset that can be used on a new project, it can be added instantly		5	3 - Could have
11	As a	student	l want to	analyze the relationship between different features	so that	I can identify which features I need to select for my analysis	?	5	2 - Should have
16	As a	general user	l want to	add specific materials to the workflow for analysis	so that	compare the performance of the specific material my client or I choose with other material	?	3	3 - Could have

# Change log

Version date Version Editor		Editor	Comment
19 Sep 2022	1.3	Chunbaixue Yang	Update US 32 to include featurizer selection as well
23 Sep 2022	1.4	Chunbaixue Yang	Update user stories after cross team meeting

# | Low-fidelity Prototype

The prototype was created in Marvel and can be viewed here.



## **Descriptive Notes**

- · Landing page:
  - Static page with information about the app and project
  - Link to access the app
    - · On click, it opens a login modal
    - Once user is logged in, they're redirected to the app
- Single page app:
  - Top bar:
    - User profile button at the top opens a menu to give the user the option to log out
    - Menu button at the top has options to import or save a workflow, download it in different formats, start over, a link to the
      documentation and a toggle to enable pro view.
  - General user
    - The workflow is divided into major and minor steps. Each major step would have its own page. User can go back and forth between the major steps as needed.
    - Left panel:
      - All the minor steps are numbers and named to guide the user
      - Inputs can be of different types
      - Each step has a tooltip button that would open a modal with guidance information about the step
      - The steps and options in the left panel should always be the same no matter what selections the user made in previous steps. Any step that requires customised inputs would open in a modal.
        - Example 1: Step 3.1 might be "Selecting a plot type". As there is a known, limited list of different plot types, this step may be a drop-down menu that is displayed directly in the left panel.
        - Example 2: Step 3.2 might be customising the selected plot's configuration options. As different plot types
          may need different configuration options, these options will not be displayed in the panel directly. Instead, the
          panel will include only a button that says "Configure plot", which would open a modal with the specific options
          applicable to the selected plot type.
      - Pinned buttons at the bottom of the panel: navigate between the different major steps. Last step page may also have a button to download the full workflow.
    - Viewing window:
      - At the top of the viewing window, the user can see the progression of major steps with the current step highlighted.
      - The output of each minor step is labelled with the step number and contained inside a box. The output inside the box is the same output produced by running the python code, simply copied over for transparency.
      - The outputs from the previous pages are also always displayed, so it's not just the outputs of the current page.
      - Where a resource with citations is used, the citations will be automatically printed after the output of the step where the
        resource was selected.
  - Pro user:
    - Left panel: has all the same options as a general user, plus additional buttons to configure their own settings as needed
    - Viewing window: the window has 2 tabs:
      - Output: same the as the viewing window of the general user
      - Python source code:
        - An editable view of all the code generated by their selections, looks similar to a Jupyter notebook.
        - User can add new cells as desired
        - Brings up the following question: what happens if the user edits the code generated by one of the steps? This
          may lead to inconsistencies between what is shown in the step's input field and what the code now actually
          does. This is an implementation decision so is not a major concern right now, but one option that we decided
          to show in the prototype is that the step's input in the left panel would change to say "Custom" or something
          similar, indicating that the configuration was changed.

# | Notes on provided material



#### Note on below content

The bullet points below were copied directly from the notes provided by the client and are not edited at all for transparency (except for the additions of headings to divide the groups).

## **Organized Wishlist**

As described in the provided notebook and the rough prioritization described in the kickoff meeting.

### **High priority features:**

- Save, load and modify workflow within interface
- · Web interface with user logins
- Server based online application
- Documentation Assumed

### Low priority features:

- Create new features based on existing features (Pro user?)
- Interface to interact with python code directly (Pro interface)
- Extendable to include more databases, machine learning methods and plot types (e.g., by Pro user)
- Hints on sensible/possible next steps and interaction with UI
- List all required citation </aside>

### **Unknown priority features:**

- Define a set of user defined features
- Generates corresponding python code (or jupyter file with markdown)
- Download and upload files to/from server (jupyter file?)
- Interaction with visualisation, e.g., click on data point in plot and open corresponding data entry </aside>

### **General characteristic:**

 Should be usable by engineer or postgrad engineering students without programming experience and just wikipedia knowledge of machine learning

## MatMiner example workflow Requirements

#### Key

Not described by the client, just a suggestion from within the team

Requirement suggested in the relevant step within the Jupyter notebook

Requirement included in the wishlist

#	Workflow step	Requirement
1.0 A	Select dataset from built in datasets with matminer.dataset	UI to select dataset from available options
1.0 B	Select a dataset from an online resource with <i>matminer</i> . data_retrieval	UI to set up the connection to the online databases
1.1	Preview DataFrame to explore or clean it	"Preview data" button prints same result?
1.2	Remove unneeded columns	Allow user to remove columns from list?
1.3	Review descriptive statistics of the data with describe()	"Describe" button prints same result?
2.1, 2.2, 2.3	Featurization: convert inputs into numbers that meaningfully represent the underlying physical quantity using the descriptors library	Select from possible features available
2.1	Printing citation for each featurizer using citations()	List required citation (. citation() result) for all used featurizers
3.1	Define input and output data of the ML model	Select output column from list of columns? All remaining numerical featurized data assumed as input?
3.2.1	Pick, train and run the ML model to generate predictions	Select from list of possible models?
3.2.2	Display the fitting score and cross-validation score	Automatically print results after predictions?
3.2.3	Plot results using plotting library	Select plot type? Select plotting library? Interaction with visualisation (e.g.,click on data point in plot and open corresponding data entry)
3.3.1	Repeat 3.2.1 with different models	Save previous results and allow to run more models?
3.3.2	Plot training error instead of test error (optionally)	Pick which data to plot?
3.3.3	See which features were most important in the model	"Analyse" option?

# | Acceptance Criteria

## Acceptance Criteria

USER STORY ID	USER STORY	GIVEN	WHEN	THEN
32	Browse built-in featurizers	I'm at the featurizer selection step	I click on the dropdown menu	I see a list of all built-in featurizers with readable names
32	Select built-in featurizers	I'm at the featurizer selection step and I can see a list of featurizers	I select one of the featurizers and click on submit	I should receive some feedback on whether the action is successful or not
34	Browse built-in datasets	I'm at the dataset selection step	I click on the dropdown menu	I see a list of all built-in datasets with readable names
21	Select datasets from exisiting databases	I'm at the dataset selection step and I can see a list of datasets	I select one of the datasets and click on submit	I should receive some feedback on whether the action is successful or not
37	Preview the output of each execution			
41	View the columns of the saved dataset			
41	Select the column I want to featurize			
20	Create User Database and Endpoints	I have a registered account for use of this software	I update any relevant personal information	That updated information persists in the database and is linked to my account
			I make changes to my workflow	That workflow data can be saved in the database and is linked to my account
			I delete my account	All linked data is deleted from the database
20	Create an account using single-sign on, restricted to the *.unimelb.edu.au domain	I own a Unimelb account and would like to access the web application features	I click in the login button	I can sign-in using my unimelb.edu.au email as a form authentication
		I am a first time user and don't own a Unimelb account	I click in the login button	If I try to sign-in using a non-unimelb email I receive a notification that only unimelb.edu.au emails are allowed
29	Save project specific data/checkpoints	I am logged into my account	I make changes to my workflow	That data can be saved to the database under my user account
35	Export model selections, parameters, and data flows	I am logged into my account	I click on the export button	I can download a file that has all the data needed to recreate my current workflow state
36	Import exported model selections, parameters, and data flows	I am logged into my account	I click on the import button	I can upload a previously exported workflow state
		I have uploaded a previously exported workflow state	The file passes all data integrity checks	My UI will match the state represented in the imported file
10	opt in to pro-user features	I am a pro user and would like to access my pro-user features	I click in the opt button	I jump in a new window with all pro-user features accessible
23	Control job execution	I have a task in progress	I click in the start, view and cancel buttons	The running tasks can be started, viewed and canceled

# **Change Log**

Date	Version	Author	Comment
14 Oct 2022	1	Chunbaixue Yang	Moved acceptance criteria from User Story to a separate page, also merged BoxJelly's work

# | Development

- | Quality Assurance Guidelines | Development Process
- | Frontend workspace structure proposal

# | Quality Assurance Guidelines

### Work quality guidelines

- Code should be able to run, there's no syntax error
- If test(s) are included in the pull request, they should pass
- All previous tests should still pass with the new changes in the pull request
- A branch should not be put up for a pull request if it has merge conflicts with main, all conflicts should be resolved before that
- Code should be understandable and contain documentation
- Code should not include global state

### Code review guidelines

- Has to be reviewed by 1 member from other 2 teams
- Pull request should have assigned reviewers within 24 h once it's no longer DRAFT and should be reviewed (either approve or require changes) within 48h
- Pull requests should include commit messages describing the work you've done and steps you did to verify your work
- Pull request will be reviewed by using the Review Changes button under the Files changed tab
- Pull request should only be merged/rebased by the creator of pull request
- Branch that has been successfully merged/rebased to main should be deleted by the creator of the pull request
- Reviewers should follow the work quality guideline to review the code

#### Acceptance criteria definition guidelines

- It should be defined from the user's point of view
- It should contain a list of steps to test the desired functionality

### Definition of done (for user story)

- Acceptance criteria should be defined for the user story and pass
- All related code has passed code review and merged to main

# | Development Process

- · All tests are required to pass in CI before landing a pull request
- · Sprint lifecycle:
  - Sprint Kickoff:
    - · Review and re-estimate tasks: user stories get t-shirt size and priority
  - Development:
    - Feature kickoff:
      - · Specify test cases and acceptance criteria
      - Tasks are estimated in number of days to complete using the magic estimation approach
    - · Code reviews:
      - Require tests pass in CI before merging
      - At least one other RedBack member must approve the pull request before it can be merged
      - At least one BoxJelly member working on the same piece of technology must approve the pull request before it can be merged
      - At least one BlueRing member working on the same piece of technology must approve the pull request before it can be merged
      - All test cases and acceptance criteria identified in kickoff must be satisfied
    - · Use auto-formatters to maintain code quality
    - Branching
      - Use the format feature/t-<ticket> as a feature branch template, where <ticket> is the Trello card number
      - <username>/idea for scratch / experimenting branches
      - main is the main branch
      - We will follow the following guidelines: https://www.atlassian.com/git/tutorials/comparing-workflows/gitflow-workflow (we probably only need main, release, scratch, and feature branches)
  - Release management:
    - Deploy as required

# | Frontend workspace structure proposal

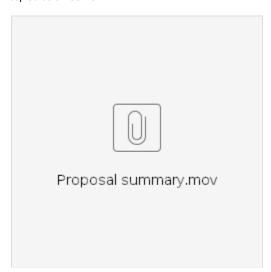
Proposed by	Ghina Yashar
Presented to	All frontend contributors from teams RedBack, BlueRing and BoxJelly
Proposal date	September 1 2022
Status	- September 2 2022
Approvers	<ul> <li>Mamta Lopes(RedBack): 1/9/2022</li> <li>Felipe Lin (BoxJelly): 2/9/2022</li> <li>Rui Zhang (BlueRing): 2/9/2022</li> </ul>

# **Proposed Structure**

Please note: All the names used below can be replaced if needed, the focus of this proposal is more on the structure rather than the naming.

# Summary video

If you don't like reading, please watch the video below for a quick overview of the proposed structure. The sample code snippets shown in the video are copied below as well.



## Summary in writing

The structure I'm proposing would follow this rough directory tree:

## Sample directory structure \_assets \_src \_components |\_exampleComponent \_examples.tsx \_index.tsx \_test.tsx |\_styled.tsx \_ dropdownSelectStepType \_examples.tsx \_index.tsx \_test.tsx \_styled.tsx \_steps \_datasetSelection // (e.g.) \_index.tsx \_test.tsx \_HelpModal \_index.tsx \_styled.tsx \_sections \_appHeader \_index.tsx . . . \_appBody |\_InputPanel \_index.tsx \_ViewingWinow \_index.tsx \_index.tsx \_appFooter // amendment suggested by Felipe |\_App.tsx . . . \_package.json \_README.md

The main ideas of this are as follows:

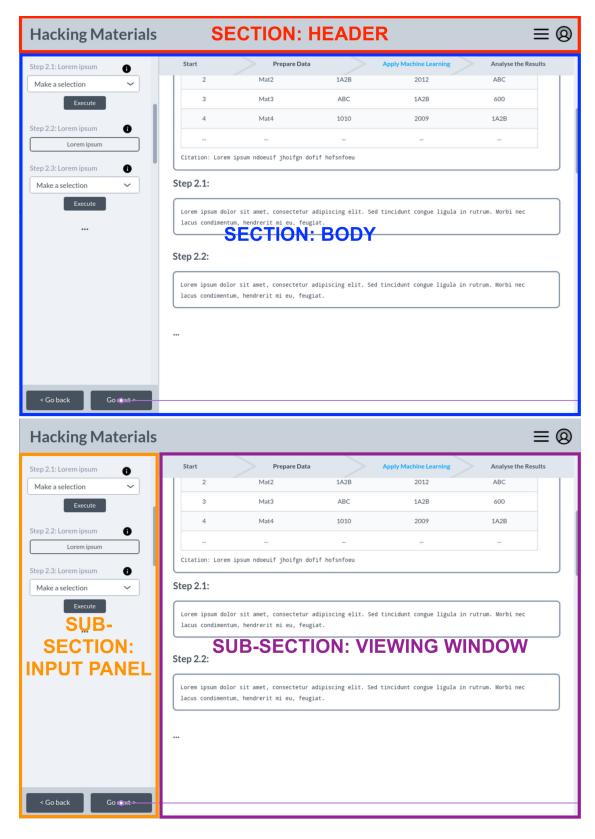
### Sections

By referring to the low-fidelity prototype created earlier in the project, we divide the main application page into 2 main sections:

- Header: the top bar, which does not need to have context of what stage the user is up to and what's happening at any given point.
- Body: Includes 2 subsections that both need to know which stage the user is at (e.g. "Pre-process data" or "Apply machine learning"):
  - Left-side panel: named in the structure as InputPanel. Example code for this panel and how it shows the workflow steps is included in the sample code section below.
  - Main window on the right: named in the structure as `ViewingWindow`

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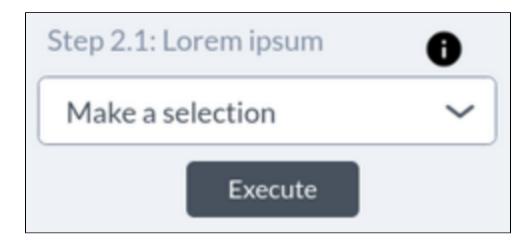
 $\label{prop:poter} \textit{Felipe Lin (HA-BoxJelly) suggests potentially adding an \textit{appFooter} as well. No objections to this so far.}$ 



### Components

This folder will mainly contain all reusable components, e.g. Button, Tooltip, Modal, etc.

Notably, some of these reusable components would be "step types", e.g. <code>DropdownSelectStepType</code>. This example step type refers to the entire object shown below, including a step number, title, tooltip, dropdown list, button and whatever else may be needed. We would create this as a reusable component because many steps have similar requirements, e.g. selecting a dataset and selecting a featurizer should both be dropdown list type steps.



### Steps

The word "steps" in this section refers specifically to the workflow steps that would be shown in the input panel, e.g. Dataset Selection step, Featurizer Selection step, etc.

A separate folder is created for these so that there would be a clear pattern that is easy to follow whenever more steps need to be added. Each step would use a step type component that is imported from the /components folder. E.g. the DatasetSelectionStep would use the DropdownSelectStepType, as shown in the sample code snippet below.

## Sample code snippets

```
Sample src/steps/datasetSelection/index.tsx
import DropdownSelectStepType from '../../components/dropdownSelectStepType';
import HelpModal from './HelpModal';
const DatasetSelectionStep = (props) => {
        const STEP_KEY = "dataset_selection"
        const options = api_call_here() // calls backend API to get the dataset options
        const onSubmit = selected_value => send_to_backend() // send to backend using api
        return (
                <DropdownSelectStepType</pre>
                        stepNumber={props.stepNumber}
                         title="Select Dataset"
                        description="bla bla"
                         tooltipContent={HelpModal}
                        options={options}
                        onSubmit={onSubmit}
                />
        );
};
```

### Sample src/sections/appBody/InputPanel/index.tsx

```
import DatasetSelectionStep from '../../steps/datasetSelectionStep';
import FeatuirzerSelectionStep from '../../steps/featuirzerSelectionStep';
const InputPanel = (props) => {
        const { stage } = props;
        if (stage === 1) {
               return (
                        <div>
                                 <DatasetSelectionStep</pre>
                                         stepNumber="1.1"
                                         data={data}
                                        handleChange={handleChange}
                                 />
                                 <FeatuirzerSelectionStep</pre>
                                         stepNumber="1.1"
                                         data={data}
                                        handleChange={handleChange}
                                 />
                        </div>
                );
        } else if (stage === 2) {
                return (
                        <div>
                        </div>
                );
        }
};
```

# | Project Progress

# **Sprint 2 summary**

### Overview

- User stories 21-selecting a dataset, 32-browsing featurizers, 34-browsing datasets are in progress and close to completion
- Majority of the foundational development has been completed, including:

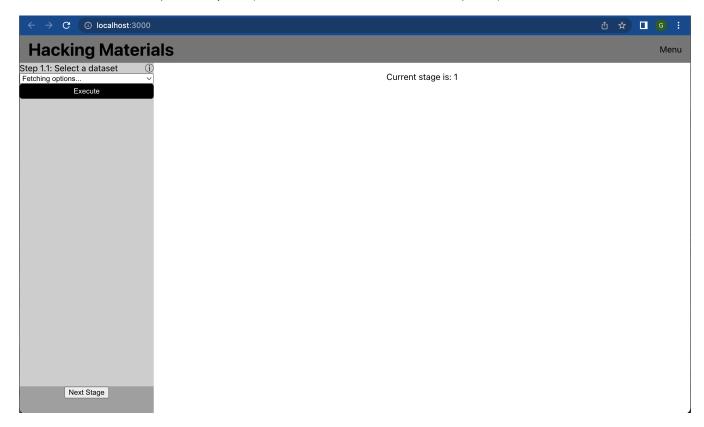
Running development services for both frontend and backend
Running postgress database
Test framework
Docker set up for backend and database services

Documentation generation

Page skeleton

Frontend input collection architecture

Frontend components Storybooks (for automated documentation on reusable components)



# **Analysis**

Most of the tasks derived from our assigned user stories are either done or under review. However, we are slightly behind schedule for multiple reasons.

- One of them is that we found there are varying levels of experience with the technologies we chose. As such, a lot of time was spent on learning
  and gathering tutorials for members across all 3 teams. Moreover, the experienced team members dedicated a lot of their time to make sure
  everyone can get to the level required for making meaningful contribution. Going forward, we expect that this should be less of an issue as team
  members become more comfortable with the technologies.
- As we were getting started with the development, we realized we need to spend some time to standardize processes and practices. Since this
  work has been completed now, it should no longer be a problem for the next sprint.
- During the sprint, code reviews were taking longer than expected as people were initially hesitant about code reviews, because they did not feel
  confident enough to assess the work of others. The situation was getting better as people gaining more knowledge about the technologies. We
  are trying to address this issue by introducing code review guidelines.

# | Resources

- | Links and Tools
  | Contact Information
  | Learning Resources
  Docker
  Git
  GitHub

# | Links and Tools

- GitHub organisation: https://github.com/orgs/COMP90082-2022-SM2/teams
- GitHub team: https://github.com/orgs/COMP90082-2022-SM2/teams/ha-redback
- Confluence: https://confluence.cis.unimelb.edu.au:8443/display/COMP900822022SM2HARedBack/Home
- When2Meet: https://www.when2meet.com
- Our pre-filled one based on our regular schedules: https://www.when2meet.com/?16293461-QLKH3
   Trello board: https://trello.com/b/jZLcqPMi/agile-sprint-board
- Other tools not yet set up.
- https://edstem.org/au/courses/8857/discussion/
- This Person Does Not Exist: https://thispersondoesnotexist.com/
- Persona design tools: Xtensio: https://xtensio.com/, UXpressia: https://uxpressia.com/
- https://www.conventionalcommits.org/en/v1.0.0/ for a guide on writing commit messages
   https://www.atlassian.com/git/tutorials/comparing-workflows/gitflow-workflow for a guide on "Git Flow", a branching strategy

# | Contact Information

Name	Calling name	Email	GitHub	Student ID	Discord
Alastair Daivis (Team rep)	Alastair	adaivis@student.unimelb.edu.au	alaroldai	359 101	alaroldai
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Ghina Yashar	Ghina	gyashar@student.unimelb.edu.au	GhinaY	1274878	Ghinaenae
Chunbaixue Yang	Caitlyn	chunbaixue@student.unimelb.edu.au	ycbx1993	1208333	KitKat

## Client

Name	Calling name	Email	GitHub
Dr Christian Brandl		christian.brandl@unimelb.edu.au	

# Staff

Name	Calling name	Email	GitHub
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# Sibling team contacts: BlueRing

Name	Calling name	Email	GitHub	Student ID	Discord
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Xinle Yu		xinley@student.unimelb.edu.au			
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# Sibling team contacts: BoxJelly

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Radhimas Djan		djanr@student.unimelb.edu.au			
Felipe Leefu Huang Li		fleefuhuangl@student.unimelb.edu.au			

# | Learning Resources

# **Backend**

- Pytest: https://docs.pytest.org/en/7.1.x/getting-started.html
   SQLAlchemy: https://docs.sqlalchemy.org/en/14/dialects/postgresql.html
- Flask:

  - https://flask.palletsprojects.com/en/2.2.x/https://www.tutorialspoint.com/flask/index.htm
  - https://youtu.be/Z1RJmh\_OqeA(Quick guide from setup, creating virtual env similar to the Developer.md, connecting to SQLAlchemy and the frontend)
  - https://github.com/realpython/discover-flask

# Frontend

- React: https://reactjs.org/tutorial/tutorial.html
- Style components: https://www.robinwieruch.de/react-styled-components/
- Testing:
  - **RTL Cheat sheet**
  - RTL + Jest tutorial
  - Jest cheat sheet
- TypeScript:
  - TS Cheat sheetTS tutorial

  - TS + React tutorial
- Storybooks:
  - Tutorial (start from step 2)
  - Official "how to write stories" guide

# **Docker**

### Docker

Docker is a tool for managing isolated runtime environments (called "containers"). You can install Docker by following the Docker guide (linked below).

You can think of it as a combination of:

- · A way to run virtual machines
  - But it's much more efficient
  - · And makes it easier to access host machine resources, for example network ports and filesystems
- A way to build custom virtual machines, just like make can be used to build binaries or applications
  - The build instructions are described by the Dockerfile file

Bear in mind though that containers are not virtual machines - that analogy is useful for describing an overview of what Docker does, but it is not

The two most important things you can do with Docker are:

- Build container images, for example by running: docker image build -t flask-docker .
  - A container *image* is like a compiled program: it does nothing unless it is run
  - · Unlike a program though, it doesn't exist in an obvious way on the filesystem. The Docker runtime is responsible for managing images.
  - -t flask-docker tells Docker to "tag" the image with the string "flask-docker". You can refer to Docker objects (including images) by their hash, but naming them makes it easier.
  - . The . tells Docker to use the Docker file in the current directory. You could provide a path to another directory instead.
- Run a container image, for example by running docker run -d -p 80:5000 flask-docker
   Running an image produces an object called a "container" this is like a process, just as an image is like a compiled program.
  - The -d argument tells Docker to "detach" the container to run it in the background and not show it's output.
  - The -p 80:5000 argument tells Docker to map port 80 on the host machine to port 5000 inside the container. If you're building a Flask application (which by default listens for requests on port 5000), this means that you would access the application by navigating to port 80 on the host machine.
  - flask-docker is the tag of the image we want to run.

Once a container is running, it is given a tag by the Docker runtime. This tag is separate to the tag of the image.

You can view running containers by running docker ps.

When you're finished with a container, you can kill it by running docker kill <container-tag>

For more information, you can go through the Docker getting started guide, or refer to their reference documentation.

### **Docker-Compose**

An alternative to Docker approach detailed above

Docker-compose can automate the process of setting up & managing multiple containers. see Install Docker Compose

Before running the command below create a .env file in this directory and add the following lines

```
POSTGRES_USER="db_user"
POSTGRES_PASS="somehardpassword"
PGA_USER="user@gmail.com'
PGA_PASS="anotherhardpassword"
```

Replace the text inside the inverted commas with appropriate email/password/usernames

Then create a .pgpassfile in the postgres-init folder and add the following line

```
pg_db:5432:ha_db:username:password
```

Replacing username and password with the postgres username and password chosen above

For security, ensure .env & .pgpassfile is added to .gitignore

Running docker-compose up -d in this folder will set up 3 containers with persistant storage

- Flask app as defined in **Dockerfile**, available at 127.0.0.1:5000.
- postgres database available at at 127.0.0.1:5432.
- PGAdmin, a UI to easily manage the database 127.0.0.1:5050. pgAdmin 4 Docs

## Using a Docker Development Container

While it's a little unusual, you can also use Docker to set up a development container. This is a container that you would use to create an isolated environment for software development - for example, if your main machine is a Windows machine, but you want to use a Linux development environment.

Visual Studio Code includes some tools for this: https://code.visualstudio.com/docs/remote/containers

In this kind of setup, you would create a separate container for your development environment, and connect to it from Visual Studio Code.

From the VSCode terminal, you would be able to access the container via a shell just as you could on a normal Linux machine.

Inside the container you could install Docker and develop as normal. However, there could be some issues with accessing web services hosted inside the development container. It may be simpler to use the **Windows Subsystem for Linux** instead: https://code.visualstudio.com/docs/remote/wsl

## **Git**

### Git

### Introduction

I strongly recommend learning how to use Git from the command-line. You can find good resources for doing this on the internet, but one of the best places to start in my opinion is the Atlassian Git tutorial.

The initial part of this tutorial is mainly about setting up a repository, which we have already done and might not be so useful to you. I would recommend starting with Saving Changes, which introduces the "three trees" of Git. Understanding how those trees work together is fundamental to understanding how Git works and how to use it effectively.

A second, also excellent resource is Thoughtbot's Git Tutorial, which comes with written tutorials, recorded videos, and example repositories. In particular, their end-to-end feature example very closely matches how I like to use Git.

### Branching strategy

Branches are key to using Git effectively. While the tutorials above give some good advice on using them, every team has a slightly different branching strategy so I'll mention some good guidelines here:

- Always use a branch. Branches keep you safe by making sure you can get back to a given state of the repository. If you're about to do
  something risky (for example, a git amend or git rebase command), make a branch first so that if it goes wrong you can check out the
  "before" version of your code and undo the mistake.
- Do not modify the history of shared branches. If you are sharing work on a branch with other developers, using a command like git commit commit rebase can cause your version of the branch to become different from the version that the other developers have.
- · Adopt a common strategy for naming branches. I like to use the following formula:
  - Use a slash (/) to separate different parts of the branch name
  - A brief description of the kind of work being done on the branch (feat for new feature development, style for code style changes, doc
    for adding documentation, tests for adding unit tests, and so on)
  - · A short description of the actual work being done on the branch, for example feat/backend-featurizer-list-endpoint

### Resources

- The official git tutorial
- Atlassian's git cheatsheet
- Dangit, Git!?! is a good resource for figuring out how to fix a mistake you've made using Git

### **Tools**

While your IDE may have built-in Git support, I recommend using a stand-alone tool. They tend to be more stable and provide a good overview of the state of the repository.

I use Sublime Merge, but other popular tools include:

- SourceTree, by Atlassian
- Tower
- tig, a command-line UI

Again though, I strongly recommend becoming familiar with Git's command-line interface. Often the GUI interfaces are convenient but hide information that can help you actually understand what they are doing, and knowing the command-line interface will help you use them more effectively.

Related to the above, if you are not yet familiar with a command-line editor I would strongly recommend learning one.

By far the most popular of these are Vim and Emacs, but both of these have quite steep learning curves. If you are looking for a command-line editor to get started with, the easiest is probably nano, which comes installed on most MacOS and Linux machines (I'm not sure about Windows, sorry!).

For those of you who are already confident with Git, some other tools you might find interesting / useful include:

- Interactive Rebase Tool, a more convenient interface for using git rebase -i.
- Trail, a tool I developed for rebasing feature branches on top of an amended commit after responding to code review feedback.

# **GitHub**

# GitHub

### Introduction

GitHub fills two key roles in our project:

- · Code hosting server: it acts as a Git server from which we can push and pull commits, and by doing so share our work
- Code review platform: it acts as a way for us to share feedback on each other's work, facilitating quality control, collaboration, and knowledge distribution.

If you're familiar with Git already, most of GitHub should not be new to you. The exception to this is GitHub's **Pull Request workflow**, which covers the process of merging changes from a feature branch into the main branch.

With this in mind, I recommend reading GitHub's documentation on this topic.

### **Tools**

- GitHub's command-line interface is very good
- GitHub Desktop is a desktop application, which you may find more convenient than using GitHub's website.

# **Sprint 3 Submission Checklist**

1. Verification and Val	
	3 checklist V&V, returned to MMJ with proposed changes and comments on or before Mon 03/10/2022 22:00  .1.1. All BlueRing team members reviewed and know their
	roles
	assigned activities
	buddy or stand-in
	Each assignee adds [due date and time] to check items owned
• 1.	1.2. All BoxJelly team members reviewed and know their
	assigned activities
	buddy or stand-in
	Each assignee adds [due date and time] to check items owned
• 1.	.1.3. All RedBack team members reviewed and know their
	roles
	assigned activities
	buddy or stand-in
	Each assignee adds {due date and time] to check items owned
	(Alastair Daivis added): Check exported artefacts haven't somehow been translated into any other language (?!)
• 1.2. Mon 1	0/10/2022 22:00: Dry run prior to sprint 3 deliverables submission and final date for making any changes to the checklist (sent
to MMJ) • 1.	.2.1. BlueRing
	Completed dry run of all submission activities prior to pressing Upload
	Changes to checklist, if any, attached and returned to MMJ
• 1.	.2.2. BoxJelly
	Completed dry run of all submission activities prior to pressing Upload
	Changes to checklist, if any, attached and returned to MMJ
• 1.	.2.3. Redback
	Completed dry run of all submission activities prior to pressing Upload
	Changes to checklist, if any, attached and returned to MMJ
■ 2. General items	
_	ntation – spelling and grammar, names pelling: full document checked
	Frammar: full document checked
	company and product names, trademarks, professional titles, technical terms, acronyms and abbreviations checked (in full first
tir	me, abbreviated thereafter, capitalization, spelling, trademarks, etc.): full document checked
U	Init names and use: full document checked (e.g., AUD500 or A\$500, 16 MB, 16 Mbit/sec, etc.)
_	contact UoM IT services to find out the correct names for cloud services/servers/platform
_	atting and visual presentation (mostly Confluence) content produced by merging artifacts from different teams is presented in a consistent way across all documents
_ S	maller icons (or links) for Slack, Trello, Github and other products
_ C	content of pages fits onto Confluence export page (resize if required)
A	dd document description including file name/purpose/changelog
M	lake sure titles are detailed and avoid using general-purpose titles.
_ C	confluence pages header and footer reflect current sprint
_ C	confluence exported pages include header and footer
•	ring and packaging documents for submission
	ag and resources (exported Confluence package) for current sprint verified and validated by the QA lead and one other team nember
A	ssessments page should not be included in the exported documentation
F	ilter and rename Assessments Page so that it does not include references to course-related terminology
P	rior versions of artifacts should not be included in the Confluence export for the current sprint

• 2.4. It is	clear which teams were responsible for which deliverables
	There is a deliverables summary list separate from the process action items in the checklist
• 2.5 Deli	very mechanism for each item is known and assigned to team members with due dates  Confluence: team members allocated
	Confluence: due date confirmed
	GitHub: team members allocated
	GitHub: due date confirmed
3. Sprint-specific 3.1. Cor	nfluence (infrastructure)
	Clear, easy to navigate structure with indicative page names (see item 2 above)
	Minimize depth (more on each page, fewer clicks)
	No multiple versions of content (handled by built-in versioning)
	Visible and editable content (e.g., minutes saved directly, diagrams can be updated without referring to an external editor)
	nfluence (project contents and consistency) 3.2.1. Project definition description
	scope
	stakeholders
	team members
	team roles with
	responsibilities
	technology used
	user stories
	test cases
•	<ul><li>3.2.2. General activities</li><li>Weekly team meeting with agenda, meeting minutes, decisions, action items</li></ul>
	Sprint planning, sprint review and sprint retrospective meetings for each sprint
	Stand-up meetings at least twice per week (documented on Confluence only)
	Product and project-related communication from client (documented on Confluence only)
	Recordings and notes from knowledge sharing meetings are documented in Confluence
	Team representatives meeting notes include review of open PRs (to enforce 24/48h code review deadline) (Use filter: -is:pr -label:DRAFT is:open)
• 3.3. Tas	· ·
	Product backlog kept along with a (low-level) sprint backlog
	Tasks in sprint backlog have adequate (low) level of granularity
	Tasks in sprint backlog are linked to their user stories
	Tasks in sprint backlog include effort estimate and due date
	Tasks in sprint backlog include dependencies to other tasks
	Team members assigned to tasks and responsible for moving them along the lanes of the board in a timely manner
	Team members assigned to tasks
	Due dates assigned to tasks
	Documented estimation process (in Confluence)
	Documented workflow (in Confluence)
• 3.4. Ver	sion control  Good quality code: coding standard described (in Confluence) and followed throughout
	Test code and cases clearly identified
	Instructions or infrastructure to build and run the product
	Instructions or infrastructure to run test cases
	Sensible log messages in all commits, including references to tracked issues
	Documented commit and branching policy (in Confluence)
	2 55 5 1. The state of the stat

• 3.5. Well-defin	ed code review policy					
revie	wers					
timefr	timeframes					
check	dist for review (such as this one)					
• 3.6. Sensible p	policy on tagging for system versions					
miles	tone versions					
ability	to repeat tests					
• 3.7. Product						
	Product outcomes for sprint 3 commensurate with project difficulty					
• 3.7.1.	Outcomes of product show					
	Clear and demonstrable use of standards throughout project					
	Structure and content clearly visible (relevant) to client					
	Structure and content clearly visible (relevant) to assessors					
• 3.7.2.	Each requested/proposed functional and non-functional feature can be  Demonstrated to client					
	Demonstrated to assessors					
	Assessed for feedback					
	Product is deployed					
• 3.8. GitHub						
	GitHub folders are structured					
	IF DRY RUN: Artifacts uploaded to GitHub have a "-dry-run" suffix in the name.					
• 3.8.1.	GitHub sprint 3 documents Updated					
	Exported from Confluence					
	Added to repository					
• 3.8.2.	GitHub README file updated to					
	Explain team's repository					
	New release					
• 3.8.3	GitHub baseline tag					
	Generated					
	Resources confirmed					
	Courtesy link sent to MMJ after submission (which is well before the deadline)					