Pharmacokinetics/Pharmacodynamics Modelling

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Table of contents

Preface

This is a Quarto book.

To learn more about Quarto visit https://quarto.org/docs/books/.

1 Course concept

All course content is managed in github. On changes locally the complete content is updated.

Chapter 1. What is the technology behind this course.

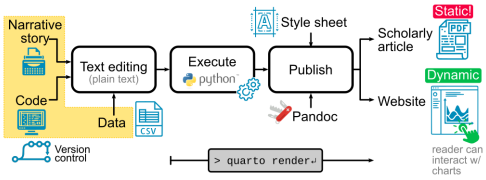

Figure 1: Course writing workflow, starting from plain text (narrative, code and data) all under version control for reproducibility.

1.1 Content

- simple lectures about pharmacokinetics
- short videos
- slides
- simple apps for exploration
- interactive notebook for exploration
- quizzes
- AI tutor

1.2 Form/Technology

- Jupyter notebooks + markdown => cross compilation to
  - HTML (Blog/Webpage) -> hosted on Github.io
  - PDF (handout/book, typst) -> hosted on Github.io for download
  - Presentation (reveal.js) -> hosted on Github.io
  - OpenEdx course: markdown -> OLX (mu), to openedx course format
- figure out how to customize compilation to different targets in Quarto.

1.3 Different classes

- teaching notebooks => rendered to content
- exercise notebooks
- solution notebooks/material

1.4 Version control

- Course content is managed in a GitHub repository (version control)

1.5 Continous integration and deployment

- CI via GitHub actions is used to automatically build and deploy the course content.

1.6 Software and tools

- quatro for conversion;
- openedx (docker container)

1.7 AI support for writing text

- All text creation is supported by ChatGPT.

1.8 Corporate Styling for the course

- use consistent colorschema and logos

1.9 Hosting

- OpenEDX is hosted using the de.NBI cloud (or HU resourses) via OpenStack

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1.10 Notebook and markdown based publishing tools

1.10.1 Quarto

- An open-source scientific and technical publishing system
- https://quarto.org/
- Publish reproducible, production quality articles, presentations, dashboards, websites, blogs, and books in HTML, PDF, MS Word, ePub, and more.
- see: https://gael-close.github.io/posts/2209-tech-writing/2209-tech-writing.html

1.10.1.1 Interactivity

- https://quarto.org/docs/interactive/
- Create custom JavaScript visualizations using Observable JS: https://quarto.org/docs/interactive/ojs/
- Incorporate Jupyter Widgets: https://ipywidgets.readthedocs.io/en/latest/
- Shiny for Python integration: https://quarto.org/docs/dashboards/interactivity/shiny-python/index.html; https://quarto.org/docs/dashboards/interactivity/shiny-python/index.html

1.10.2 jupyterbook

- https://jupyterbook.org/en/stable/intro.html
- Build beautiful, publication-quality books and documents from computational content.
- Similar goal as quarto, but more focused on books.

1.11 Presentations

1.11.1 reveal.js

- reveal.js is an open source HTML presentation framework. It's a tool that enables anyone with a web browser to create fully-featured and beautiful presentations for free.
- Presentations made with reveal.js are built on open web technologies. That means anything you can do on the web, you can do in your presentation. Change styles with CSS, include an external web page using an `iframe` or add your own custom behavior using our JavaScript API.
- The framework comes with a broad range of features including nested slides, Markdown support, Auto-Animate, PDF export, speaker notes, LaTeX support and syntax highlighted code.

- https://revealjs.com/course/
- nice integration with Quarto; https://quarto.org/docs/presentations/revealjs/demo/#/title-slide
- https://github.com/quarto-dev/quarto-web/blob/main/docs/presentations/revealjs/demo/index.qmd

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1.12 Interactive plots

1.12.1 plotly

- https://plotly.com/python/ ### altair
- https://altair-viz.github.io/

1.13 Interactive webapps

1.13.1 Shiny for python

- possible integration with Quarto

1.13.2 Voila

- voila notebooks: https://voila.readthedocs.io/en/stable/
- Voilà allows you to convert a Jupyter Notebook into an interactive dashboard that allows you to share your work with others. It is secure and customizable, giving you control over what your readers experience.

1.13.3 Streamlit

- https://streamlit.io/
- Turn your data scripts into shareable web apps in minutes. All in pure Python. No front-end experience required.

1.13.4 Dash

- Developed by Plotly, Dash is ideal for creating complex, interactive web applications using Python.
- Supports multi-page apps and scales well for large datasets and multiple users.
- Requires knowledge of HTML, CSS, and JavaScript for advanced customization

1.13.5 Panel

- https://panel.holoviz.org/
- Panel is an open-source Python library designed to streamline the development of robust tools, dashboards, and complex applications entirely within Python.

1.13.6 Framework

- https://github.com/observablehq/framework
- Observable Framework is a free, open-source, static site generator for data apps, dashboards, reports, and more. Framework combines JavaScript on the front-end for interactive graphics with any language on the back-end for data analysis. Framework features data loaders that precompute static snapshots of data at build time for dashboards that load instantly.

1.14 Deployment of notebooks

1.14.1 binderhub

- very slow
- https://binderhub.readthedocs.io/en/latest/
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1.14.2 jupyterhub

- JupyterHub brings the power of notebooks to groups of users. It gives users access to computational environments and resources without burdening the users with installation and maintenance tasks. Users - including students, researchers, and data scientists - can get their work done in their own workspaces on shared resources which can be managed efficiently by system administrators.
- https://jupyter.org/hub
- https://tljh.jupyter.org/en/latest/howto/index.html

https://education.github.com/globalcampus/teacher?email_referrer=true

nbgrader: https://nbgrader.readthedocs.io/en/stable/ https://www.youtube.com/watch?v=bEcxnR2V-_8 Otter grader & gradescope

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2 OpenEdx

- https://openedx.org/
- Enable online campuses, instructor-led courses, degree programs, and self-paced courses using a single platform.

2.1 OpenEdx Deployment

- deployment with tutor: https://docs.tutor.edly.io/index.html

2.2 H5P

- Play H5P content in Open edX using h5pxblock
- https://github.com/edly-io/h5pxblock

2.3 OpenEdx Notebook Integration

- openedx notebook integration: https://github.com/parmentelat/nbhosting ?!
- https://github.com/overhangio/jupyter-xblock JupyterHub hosts Jupyter instances with authentication (e.g. OAuth; IDK about using edX users as JupyterHub users with individual Docker image instance containers with nbgrader/xblock) The new jupyter-viewer-xblock (https://github.com/ibleducation/jupyter-viewer-xblock) allows to embed notebooks dynamically from a public URL. Demo here! https://www.youtube.com/watch?v=K8jhWgQnxvI
- https://github.com/overhangio/tutor-jupyter; This is a plugin for Tutor that makes it easy to integrate Jupyter notebooks in Open edX. It achieves the following: 1. Install the official jupyter-xblock in the Open edX LMS and Studio. 2. Run a Docker-based JupyterHub instance with a Docker spawner.

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3 GitHub Global Campus

Focus on teaching with GitHub Classroom Managing and organizing your class is easy with GitHub Classroom. Track and manage assignments, automate grading, and help students when they get stuck— all while using GitHub.

4 Education: Course structure and best practise

4.1 Teaching and Learning with Jupyter

This handbook is for any educator teaching a topic that includes data analysis or computation in order to support learning. - https://jupyter4edu.github.io/jupyter-edu-book/

4.2 Open edX Educators

- Material on how to build and design courses: https://docs.openedx.org/en/latest/educators/index.html
- Instructional Design Concepts: https://docs.openedx.org/en/latest/educators/navigation/creating_course design-concepts

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4.3 Text to speech

4.3.1 Whisper AI

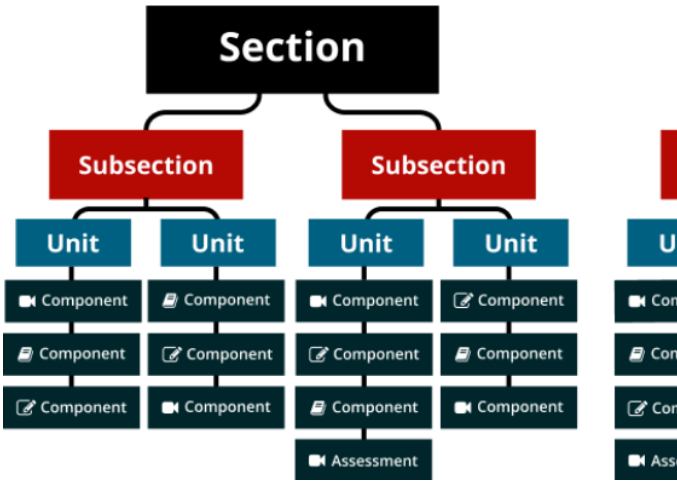
- https://openai.com/index/whisper/

4.3.2 ElevenLabs

- https://elevenlabs.io/

5 Content

Pharmacokinetic modelling is the study of how drugs are absorbed, distributed, metabolised and excreted in the body. The pharmacokinetic modelling course covers topics such as pharmacokinetic principles, drug distribution, clearance and elimination and the factors that influence these processes. Students will learn about different models used to describe pharmacokinetics, such as compartmental models and physiologically based pharmacokinetic models, and how these models can be used to predict drug concentrations and optimise dosing regimens. Other topics that may be covered include pharmacodynamics, drug-drug interactions and the use of pharmacokinetic modelling in drug development and clinical practice. Overall, a course in pharmacokinetic modelling will provide students with a comprehensive understanding of the principles and techniques used to describe the movement of drugs through the body and how this knowledge can be applied to improve drug therapy. For further information please visit: https://livermetabolism.com



The course is structured in sections, subsections and units.

6 Pharmacokinetic Modeling Basics

6.1 Polar Axis

For a demonstration of a line plot on a polar axis, see Figure 6.1.

```
import numpy as np
import matplotlib.pyplot as plt

r = np.arange(0, 2, 0.01)
theta = 2 * np.pi * r
fig, ax = plt.subplots(
  subplot_kw = {'projection': 'polar'}
)
ax.plot(theta, r)
ax.set_rticks([0.5, 1, 1.5, 2])
ax.grid(True)
plt.show()
```

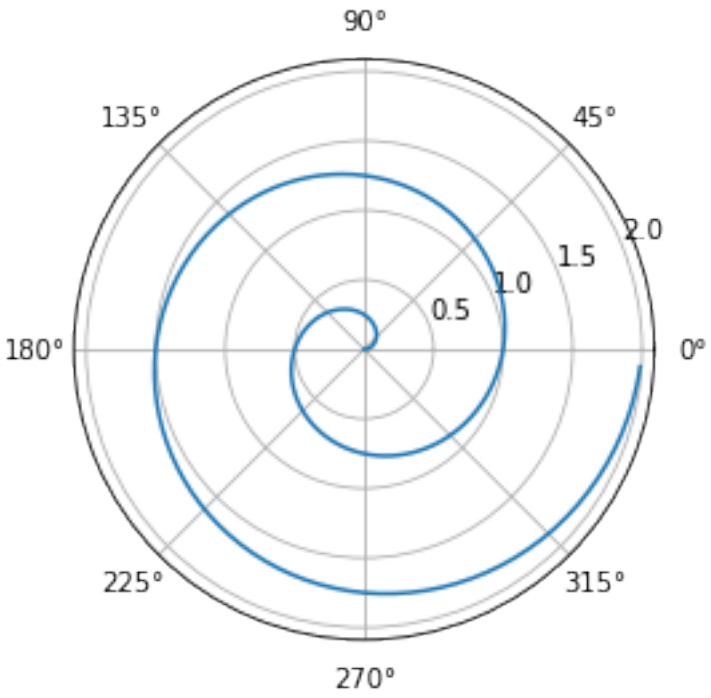


Figure 6.1: A line plot on a polar axis

7 New Section

Testing additional content. Here a citation (Hernandez-Sanchez et al. 2021).

> **Note**
>
> Note that there are five types of callouts, including: `note`, `tip`, `warning`, `caution` and `important`.

7.1 References

Hernandez-Sanchez, Sergio, Victor Moreno-Perez, Jonatan Garcia-Campos, Javier Marco-Lledó, Eva Maria Navarrete-Muñoz, and Carlos Lozano-Quijada. 2021. "Twelve Tips to Make Successful Medical Infographics." *Medical Teacher* 43 (12): 1353–59. https://doi.org/10.1080/0142159X.2020.1855323.