

Development and calibration of tumor models

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MINISTÉRIO DA
CIÊNCIA, TECNOLOGIA
E INOVAÇÕES



Working with Python

- Introduction to Python
- Solving Ordinary Differential Equations

Python advantages and disadvantages

Advantages

- Easy to read, learn, write, and debug
- Dynamically typed
- Free and open-source
- Vast libraries support
- Portability

Disadvantages

- Interpreted language
- Slow speed
- Not memory efficient
- Runtime errors

A web-based, interactive computing tool for capturing the whole computation process: developing, documenting, and executing code, as well as communicating the results.

Jupyter Notebook

jupyter example Last Checkpoint: a few seconds ago (autosaved)



Logout

File Edit View Insert Cell Kernel Help

Trusted

Python 3



In []:

Jupyter Notebook

jupyter example Last Checkpoint: 2 minutes ago (autosaved)



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Python 3

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Code
Code
Markdown
Raw NBConvert
Heading

In []:





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Trusted | Python 3



Day 02 ## Python

```
\begin{equation}
\frac{\partial \phi}{\partial t} = x\phi
\end{equation}
```

In []: var=2

In []: print(var)
var=3

In []: print(var)
var=4

In []:

jupyter example Last Checkpoint: 24 minutes ago (unsaved changes)



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Python 3



Day 02

Python

$$\frac{\partial \phi}{\partial t} = x\phi$$

In [1]: `var=2`

In [2]: `print(var)`
`var=3`

2

In [3]: `print(var)`
`var=4`

3

In []:

Jupyter Notebook

jupyter example Last Checkpoint: 24 minutes ago (unsaved changes)



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Trusted

Python 3



Day 02

Python

$$\frac{\partial \phi}{\partial t} = x\phi$$

In [1]: `var=2`

In []: `print(var)`
`var=3`

In [2]: `print(var)`
`var=4`

2

In []:

jupyter example Last Checkpoint: 24 minutes ago (unsaved changes)



Logout

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Trusted

Python 3



Day 02

Python

$$\frac{\partial \phi}{\partial t} = x\phi$$

In [1]: `var=2`

In [3]: `print(var)`
`var=3`

4

In [2]: `print(var)`
`var=4`

2

In []:

jupyter day02_python (autosaved)

File Edit View Insert Cell Kernel Widgets Help Trusted Python 3 O

Download GitHub Binder Memory: 115 / 2048 MB

Day 02

Python

$$\frac{\partial \phi}{\partial t} = x\phi$$

```
In [1]: var=2
```

```
In [2]: print(var)
var=3
```

```
2
```

```
In [ ]: print(var)
var=4
```

```
In [ ]:
```

The screenshot shows a Jupyter Notebook interface. At the top, there's a toolbar with various icons for file operations like Open, Save, and Run, followed by a dropdown menu labeled 'Code'. To the right of the toolbar is a red box highlighting three buttons: 'Download' (with a cloud icon), 'GitHub' (with a GitHub icon), and 'Binder' (with a circular icon). Above the red box, there are links for 'Visit repo' and 'Copy Binder link'. On the far right, it shows 'Memory: 115 / 2048 MB'. Below the toolbar, the main area contains a section titled 'Day 02' with a heading 'Python'. It displays a mathematical equation $\frac{\partial \phi}{\partial t} = x\phi$. Below the equation are two code cells. The first cell has 'In [1]:' and contains the assignment 'var=2'. The second cell has 'In [2]:' and contains the command 'print(var)'. The output of the second cell is 'var=3'. Below these, there are two more code cells, both starting with 'In []:'. The first one contains 'print(var)' and 'var=4', and its output is 'var=4'. The second one starts with 'In []:' and has an empty input field.

Jupyter Notebook - Binder (10 min)

jupyter day02_python (unsaved changes)

File Edit View Insert Cell Kernel Widgets Help Trusted Python 3 Memory: 67 / 2048 MB

Run Cell Code

Download GitHub Binder

Day 02

Python

$$\frac{\partial \phi}{\partial t} = x\phi$$

```
In [1]: var=2
In [2]: print(var)
var=3
2
In [*]: print(var)
var=4
In [ ]:
```

The screenshot shows a Jupyter Notebook interface with the following details:

- Title Bar:** jupyter day02_python (unsaved changes)
- Toolbar:** File, Edit, View, Insert, Cell, Kernel, Widgets, Help, Trusted, Python 3, Memory: 67 / 2048 MB.
- Toolbar Buttons:** Run (highlighted by a blue arrow), Cell (highlighted by a red arrow), Stop, Clear, Next, Previous, Code, Download, GitHub, Binder.
- Content Area:**
 - Section Headers:** Day 02, Python.
 - Equation:**
$$\frac{\partial \phi}{\partial t} = x\phi$$
 - Code Cells:**
 - In [1]: `var=2`
 - In [2]: `print(var)`
Output: `var=3`
 - In [*]: `print(var)`
Output: `var=4`
 - In []: (empty cell)

Jupyter Notebook - Binder (12 min)

jupyter day02_python (unsaved changes)

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Not Connected Trusted Python 3 Memory: 67 / 2048 MB

Download GitHub Binder

Day 02

Python

$$\frac{\partial \phi}{\partial t} = x\phi$$

```
In [1]: var=2
In [2]: print(var)
var=3
2
In [*]: print(var)
var=4
In [ ]:
```

Jupyter Notebook - Binder

The screenshot shows a GitHub repository page with a dark theme. At the top, there's a search bar and navigation links for 'Pull requests', 'Issues', 'Marketplace', and 'Explore'. Below the header, a large green banner with white text reads 'Learn Git and GitHub without any code!'. A subtext below it says 'Using the Hello World guide, you'll start a branch, write comments, and open a pull request.' A prominent green button labeled 'Read the guide' is centered in the banner. The main content area has a light green background.

The screenshot shows a GitHub repository page for 'Ernesto-Lima / VeraoLNCC2021'. The top navigation bar includes links for 'Code', 'Issues', 'Pull requests', 'Actions', 'Projects', 'Wiki', 'Security', 'Insights', and 'Settings'. On the right, there are buttons for 'Unwatch', 'Star', 'Fork', and a 'Code' dropdown. The main content area displays a list of commits under the heading 'Ernesto-Lima exercises solutions'. Each commit includes a file icon, the file name, a brief description, and the time since the commit. To the right of the commit list, there are sections for 'About', 'Releases', and 'Packages', each with their respective descriptions and links.

About
[MC-CT01] Desenvolvimento e calibração de modelos tumorais

Releases
No releases published
[Create a new release](#)

Packages
No packages published
[Publish your first package](#)

File	Description	Time
README.md	Update README.md	13 days ago
day02_python.ipynb	exercises solutions	5 hours ago
day03_calibration.ipynb	exercises solutions	5 hours ago
requirements.txt	adding tqdm library to use progress indicators with emcee	13 days ago
slides_day03.pdf	updated slides	2 days ago
solutions_day02.ipynb	exercises solutions	5 hours ago
solutions_day03.ipynb	exercises solutions	5 hours ago

- Familiarizar os participantes com a motivação biológica para o uso de diversos modelos de crescimento tumoral;
- Apresentar métodos de resolução de modelos de equações diferenciais ordinárias (EDO's), utilizando Python;
- Calibrar os modelos desenvolvidos via métodos bayesianos.

Ementa:

- Desenvolvimento da parte teória sobre modelagem em câncer (27/11/2021): uma introdução sobre modelagem no contexto do câncer, abordando modelos discretos, contínuos e híbridos. Exemplificação e interpretação de diferentes tipos de funções para a descrição do crescimento tumoral, mortalidade, efeito Allee e terapias, entre outros fenômenos biológicos;
- Introdução à linguagem de programação Python (28/11/2021): resolução de EDO's e diferentes tipos de função, trabalhadas durante o primeiro dia de curso, em Python;
- Desenvolvimento da parte teórica e prática sobre calibração: abordagem de conceitos relacionados à calibração, de forma mais específica à calibração Bayesiana. Os conteúdos teóricos e práticos serão abordados conjuntamente, por meio da calibração de um modelo de EDO, utilizando dados gerados. Nesta atividade, será trabalhada a resolução da EDO e construção de gráficos com os resultados obtidos, usando a biblioteca emcee para calibrar o modelo.

Bibliografia:

- Yin A., Moes D. J., van Hasselt J. G., Swen J. J., Guchelaar H.J. A review of mathematical models for tumor dynamics and treatment resistance evolution of solid tumors. *CPT: pharmacometrics systems pharmacology*. 2019 Oct; 8(10):720-37.
- Oden J. T., Babuska I., Faghihi D. Predictive computational science: Computer predictions in the presence of uncertainty. *Encyclopedia of Computational Mechanics* Second Edition. 2017 Aug 8:1-26.
- Foreman-Mackey D., Hogg D. W., Lang D., Goodman J. emcee: the MCMC hammer. *Publications of the Astronomical Society of the Pacific*. 2013 Feb 25; 125(925):306.
- Silva J. V. de O. Aula1MC03.ipynb. Disponível em: <https://colab.research.google.com/drive/1FgzuhhOwCBXMogBu1mTvjtvEAXV39B3R>. (Material sugerido para iniciantes em Python).
- PythonUFRJ. Departamento de Ciência da Computação - UFRJ. Disponível em: <https://dcc.ufrj.br/~pythonufrj/>. (Material sugerido para iniciantes em programação).



Thanks to Google Cloud, OVH, GESIS Notebooks and the Turing Institute for supporting us! 🎉



Starting repository: Ernesto-Lima/VeraoLNCC2021.git/HEAD
New to Binder? Check out the [Binder Documentation](#) for more information

Build logs

show

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[Upload](#)[New](#)

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<input type="checkbox"/>	/		
<input type="checkbox"/>	day02_python.ipynb	seconds ago	16.2 kB
<input type="checkbox"/>	day03_calibration.ipynb	seconds ago	17.3 kB
<input type="checkbox"/>	solutions_day02.ipynb	seconds ago	216 kB
<input type="checkbox"/>	solutions_day03.ipynb	seconds ago	1.14 MB
<input type="checkbox"/>	README.md	seconds ago	2.67 kB
<input type="checkbox"/>	requirements.txt	seconds ago	101 B
<input type="checkbox"/>	slides_day02.pdf	seconds ago	7.39 MB
<input type="checkbox"/>	slides_day03.pdf	seconds ago	1.58 MB

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Files Running Clusters

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<input type="checkbox"/>	day02_python.ipynb	Running 2 minutes ago	16.2 kB
<input type="checkbox"/>	day03_calibration.ipynb	2 minutes ago	17.3 kB
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<input type="checkbox"/>	slides_day03.pdf	2 minutes ago	1.58 MB

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Day 02

Introduction to Python and ODE Solver

A web-based, interactive computing tool for capturing the whole computation process: developing, documenting, and executing code, as well as communicating the results.

- Ctrl-Enter: run cell in-place
- Shift-Enter: run cell
- Alt-Enter: run cell, insert below

Indentation matters!

Capitalization is important!

In []: M

Jupyter Notebook - Binder and Discord

<https://github.com/ernesto-lima/veraoIncc2021>

The screenshot shows a Discord interface for a channel named '#mini-course-1'. The channel has a message count of 1,000 messages. The channel description reads: 'Este é o começo do canal #mini-course-1, MC01-CT: Development and Calibration of Tumor Models (Desenvolvimento e Calibração de Modelos Tumorais).'. The channel has several messages from users like Anna Claudia Resende, Emanuelle Paixão, and others. The left sidebar shows a tree view of channels under 'EMMCT 2021' and 'MC01-CT'. The right sidebar lists various users categorized by role: HELPDESK—2, ORGANIZER—2, PANELIST—1, and DISPONÍVEL—7.

EMMCT 2021

mini-course-1

MC01-CT: Development and Calibration of Tumor Models (Desenvolvimento e Calibração de Modelos Tumorais).

HELPDESK—2

Anna Claudia Resende

Emanuelle Paixão

ORGANIZER—2

Luciana Barros

Regina Almeida

PANELIST—1

Heber Rocha

AlejandroHerrera

eyeS

FelipeCandidan

LeoSouza

Oscar Antezana

Valerio

VzMedivh

DISPONÍVEL—7

JucasDC_

AlejandroHerrera

Alfredo Scalf

Allan Costa

Bem-vindo(a) a #mini-course-1!

Este é o começo do canal #mini-course-1, MC01-CT: Development and Calibration of Tumor Models (Desenvolvimento e Calibração de Modelos Tumorais).

Anna Claudia Resende 22/01/2021

Professores:

Ernesto Lima (UT at Austin) e Emanuelle Arantes Paixão (LNCC).

Horários:

De quarta (27/01) a sexta (29/01) das 11:00h às 12:30h.

Os principais objetivos deste minicurso são:

- Familiarizar os participantes com a motivação biológica para o uso de diversos modelos de crescimento tumoral;
- Apresentar métodos de resolução de modelos de equações diferenciais ordinárias (EDO's), utilizando Python;
- Calibrar os modelos desenvolvidos via métodos Bayesianos.

Ementa:

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- Introdução à linguagem de programação Python (28/01): resolução de EDO's e diferentes tipos de função, trabalhadas durante o primeiro dia de curso, em Python;
- Desenvolvimento da parte teórica e prática sobre calibração (29/01): abordagem de conceitos relacionados à calibração, de forma mais específica à calibração Bayesiana. Os conteúdos teóricos e práticos serão abordados conjuntamente, por meio da calibração de um modelo de EDO, utilizando dados gerados. Nesta atividade, será trabalhada a resolução da EDO e construção de gráficos com os resultados obtidos, usando a biblioteca emcee para calibrar o modelo.