

# 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

## Disadvantages

- Slow speed (interpreted and dynamically-typed language)
- Not memory efficient
- Runtime errors

## Advantages

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

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

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Trusted

Python 3



In [ ]:

# Jupyter Notebook

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- Code
- Code
- Markdown
- Raw NBConvert
- Heading



In [ ]:



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## # 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

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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)



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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

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## 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). Below the toolbar, the main area displays a section titled 'Day 02' and 'Python'. It contains a mathematical equation  $\frac{\partial \phi}{\partial t} = x\phi$ . Below the equation are two code cells. The first cell, In [1], contains the assignment `var=2`. The second cell, In [2], contains the command `print(var)`, which outputs the value `3`. A third cell, In [ ], contains the command `print(var)` again, with `var=4` written below it. A fourth cell, In [ ], is currently empty. At the bottom of the notebook, there are navigation icons for back, forward, and search.

# 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

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, Kernel, Next Cell, Previous Cell, Code.
- 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)
- Page Footer:** Navigation icons for back, forward, search, etc.

# Jupyter Notebook - Binder (12 min)

jupyter day02\_python (unsaved changes)

File Edit View Insert Cell Kernel Widgets Help

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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 title "jupyter day02\_python (unsaved changes)". The toolbar includes standard file operations (File, Edit, View, Insert, Cell, Kernel, Widgets, Help), a "Code" dropdown, and various icons for running cells, selecting cell types, and navigating. Two arrows point to specific buttons: a blue arrow points to the "Download" button, and a red arrow points to the "GitHub" button. The main area displays a section titled "Day 02" with a heading "Python". Below the heading is a mathematical equation  $\frac{\partial \phi}{\partial t} = x\phi$ . The notebook contains four cells: In [1] shows the assignment of a variable "var" to 2; In [2] shows the printing of "var", resulting in 3; and In [\*] shows the printing of "var" again, resulting in 4. A fifth cell, In [ ], is shown at the bottom. The status bar at the bottom indicates "Memory: 67 / 2048 MB".

# Jupyter Notebook - Binder

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master 1 branch 0 tags

Go to file Add file Code

**Ernesto-Lima exercises solutions** btdbsza 5 hours ago 27 commits

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

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

Readme

Releases No releases published Create a new release

Packages No packages published Publish your first package

- 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.
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- 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).



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Starting repository: Ernesto-Lima/VeraoLNCC2021.git/HEAD  
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			solutions_day02.ipynb	seconds ago	216 kB
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jupyter day02\_python

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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.

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- 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.