33rd CONFERENCE ON
Intelligent Systems for Molecular Biology
AND THE 24th
European Conference on Computational Biology
DATES: July 20 – 24

Computational approaches for deciphering cell-cell communication from single-cell transcriptomics and spatial transcriptomics data

Instructions

July 15th 2025

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Dipartimento di Ingegneria dell'Informazione
Institute for Computational Genomics
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Instructions outline

In the following slides, instructions to download the material and set up the environment are provided.

- **STEP 1: Clone the Git Repository**
- **STEP 2: Set up the Environment**
- **STEP 3: Download the data**
- **STEP 4: Configure resource limits**

⚠️ Please read and complete **all** the steps before the tutorial!

STEP 1: Clone the Git Repository

Step 1: Clone the Git Repository

To get started, you'll need to download tutorial materials available at the **GitLab repository**: https://gitlab.com/sysbiobig/ismb-eccb-2025-tutorial-vt3.

1. Open a terminal or command prompt
2. Navigate to the folder where you want to clone the repo

   For example,
   ```
   cd /home/user
   ```
3. Clone the repository

```
git clone https://gitlab.com/sysbiobig/ismb-eccb-2025-tutorial-vt3.git
```

⚠️ *Make sure you have git installed before running the above commands.*

4. Enter the cloned directory and check the **absolute path** to the repository

UNIX

```
cd ismb-eccb-2025-tutorial-vt3
pwd
```

Windows

```
cd ismb-eccb-2025-tutorial-vt3
cd
```

STEP 2: Set up the Environment

STEP 2: Set up the Environment

For your convenience, we provide a **Docker image** that comes pre-configured with all the tools and dependencies required for the **VT3 tutorial**.

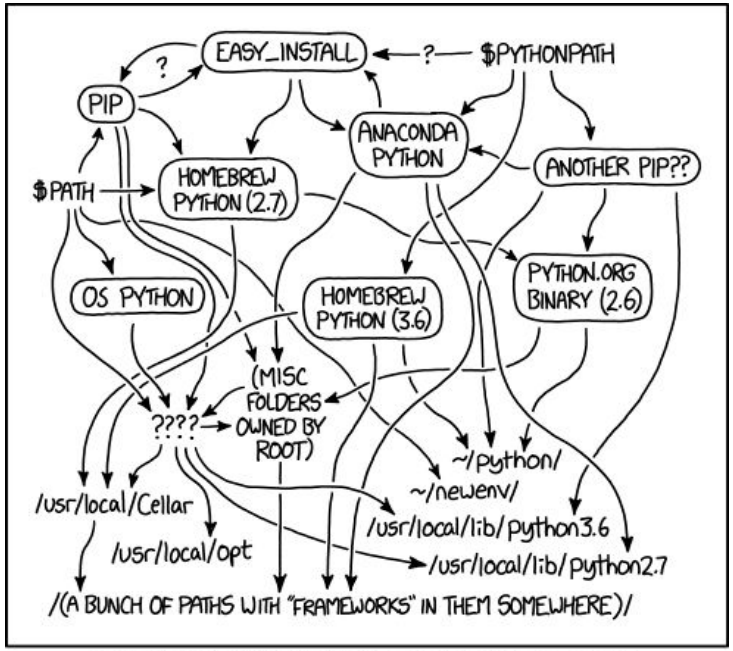
Recommended Option: use the Docker environment

Using the docker environment we ensure reproducibility of results and you don't need to manually install packages.

⚠️ **Using Docker is strongly recommended, but not mandatory.**

Alternative Option: manual setup

If you prefer, you are welcome to set up the environment manually on your own system. See the **"Manual setup" slide** for the list of required packages.



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

https://www.explainxkcd.com/wiki/index.php/1987:_Python_Environment

STEP 2: Set up the Environment

For your convenience, we provide a **Docker image** that comes
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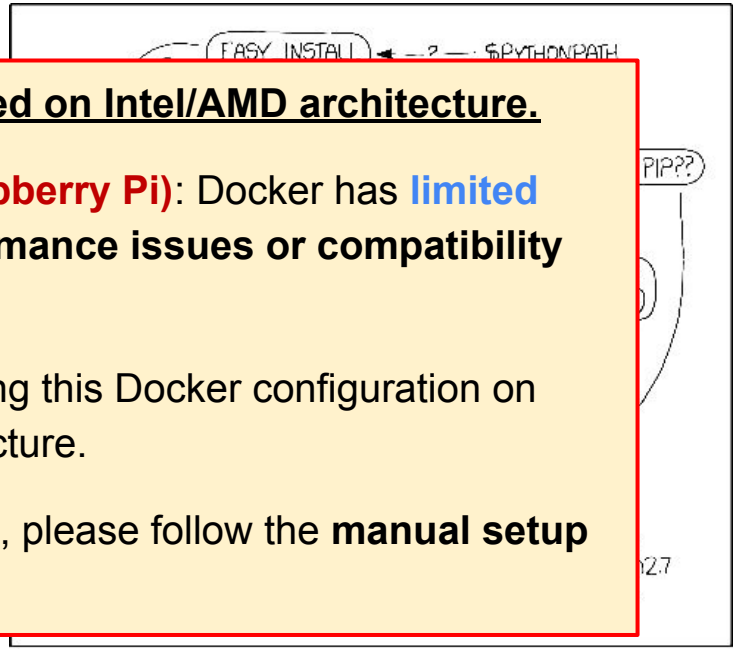
If you
manually on your own system. See the **"Manual setup" slic**
for the list of required packages.

This Docker setup is primarily built and tested on Intel/AMD architecture.

⚠️ **ARM-based Systems (e.g., Apple M1/M2, Raspberry Pi)**: Docker has **limited support** on these systems. It **may work**, but **performance issues or compatibility problems** may occur.

👉 **Recommended Platforms**: We recommend using this Docker configuration on **Linux, Windows or MacOS** with **Intel/AMD** architecture.

If the Docker setup doesn't work on your system, please follow the **manual setup instructions**.



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https://www.explainxkcd.com/wiki/index.php/1987:_Python_Environment

STEP 2: Set up the Environment

⚠️ **Important:** If you're new to Docker or haven’t installed it yet, please follow the setup instructions **well in advance**.
The installation and image download may take time. We expect all environments to be ready **before the tutorial begins**.

For assistance, join our Discord channel: link

Recommended Option: Docker environment

What is Docker?

Docker is one of the most popular and widely used **container engines**. Docker provides the ability to package and run applications in an isolated environment, called a "container". Each container includes: *OS, OS libraries, software dependencies, environmental variables, and tools*.

This is the Docker environment provided for the tutorial:

Ubuntu 22.04 LTS

ismb-eccb-2025-tutorial-vt3

Python 3.10.12

Jupyterlab 4.4.3

R 4.3.1

cellphonedb=5.0.1; liana=1.5.1; nichesphere=0.1.0
scseqcomm=2.0.0; CrossTalkeR=1.4.0; cellchat=2.2.0

Recommended Option: Docker environment

1. **Docker must be installed on your system.** Install Docker on your computer by following the instructions here: https://docs.docker.com/get-started/get-docker/.
   - It contains the step-by-step guides for Mac, Windows and Linux.

Recommended Option: Docker environment

1. **Docker must be installed on your system.** Install Docker on your computer by following the instructions here: https://docs.docker.com/get-started/get-docker/.
   - It contains the step-by-step guides for Mac, Windows and Linux.
2. **Starting the Docker container**
   - Linux users with Docker Engine only: open a **terminal**
   - Docker Desktop users: open the Docker **Desktop terminal** (bottom-right corner)

Recommended Option: Docker environment

1. **Docker must be installed on your system.** Install Docker on your computer by following the instructions here: https://docs.docker.com/get-started/get-docker/.
   It contains the step-by-step guides for Mac, Windows and Linux.

Specify the **absolute path** to the **cloned GitLab repository**
For example: *`/home/user/ismb-eccb-2025-tutorial-vt3`*
This will be used to mount the tutorial files inside the container

   - Docker Desktop users: open the Docker **Desktop terminal** (bottom-right corner)

3. **Run this command** (may take a few minutes)

```
docker run -it -p 8888:8888 --rm --pull=always \
--mount type=bind,src=<path_to_data>,dst=/Tutorial_ISMBECCB2025 \
registry.gitlab.com/sysbiobig/ismb-eccb-2025-tutorial-vt3 \
--ip=0.0.0.0 --port=8888 --allow-root --NotebookApp.token=''
```

This is an **empty string**

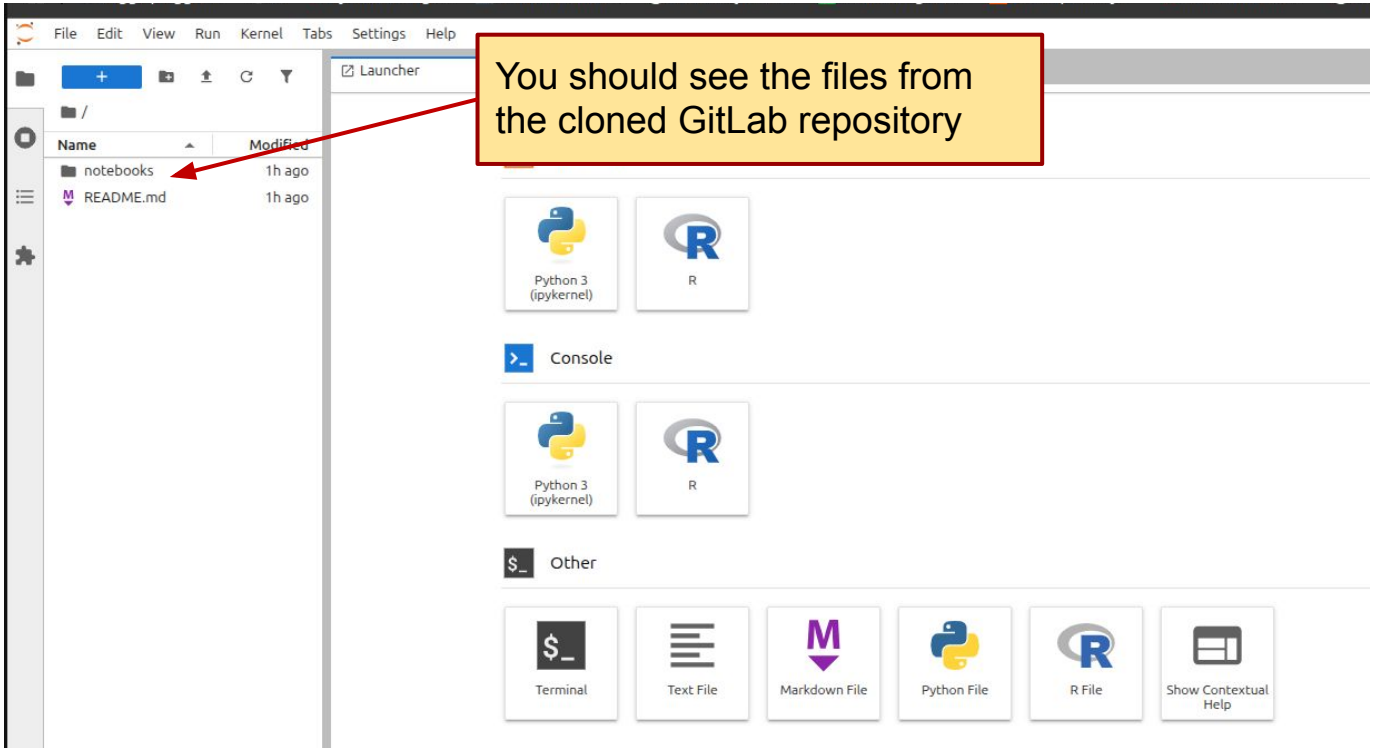
Recommended Option: Docker environment

1. **Docker must be installed on your system.** Install Docker on your computer by following the instructions here: https://docs.docker.com/get-started/get-docker/.
   - It contains the step-by-step guides for Mac, Windows and Linux.
2. **Starting the Docker container**
   - Linux users with Docker Engine only: open a **terminal**
   - Docker Desktop users: open the Docker **Desktop terminal** (bottom-right corner)
3. **Run this command** (may take a few minutes)

4. **Access JupyterLab:** Once the Docker container is running, open your browser and go to: http://127.0.0.1:8888/lab.

Recommended Option: Docker environment

This will open the JupyterLab interface!



Alternative option: Manual setup

You are free to **set up your local environment** independently; however, please note that **we cannot guarantee identical results** across different configurations.

The following tools and packages are required, along with the versions used during the tutorial:

Python(v3.10.12)

- jupyter-lab (v4.4.3)
- cellphonedb (v5.0.1) https://cellphonedb.readthedocs.io/en/latest/
- liana (v1.5.1) https://liana-py.readthedocs.io/en/latest/
- nichesphere (v0.1.0) https://nichesphere.readthedocs.io/en/latest/
    - mudata(v0.3.2) https://mudata.readthedocs.io/en/latest/
    - community_layout(v1.0.6) https://github.com/alexodavies/CommunityLayout/tree/main
    - pygraphviz(v1.14) https://pygraphviz.github.io/

R (v4.3.1)

- scSeqComm (v2.0.0) https://gitlab.com/sysbiobig/scseqcomm
- CrossTalkeR (v1.4.0) https://costalab.github.io/CrossTalkeR/
- CellChat (v2.2.0)
    - https://htmlpreview.github.io/?https://github.com/jinworks/CellChat/blob/master/tutorial/CellChat-vignette.html

STEP 3: Download the data

STEP 3: Download the data

All the tutorial data is hosted on Zenodo: https://zenodo.org/records/15756745

zenodo | Search records... | Communities | My dashboard | Log in | Sign up

Published June 27, 2025 | Version v3

Dataset | Open

ISMB/ECCB25 - VT3 tutorial data

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Show affiliations

Tissues and organs are complex and highly-organized systems composed of diverse cells that work together to maintain homeostasis, drive development and mediate complex disease progression as Myocardial Infarction (Kuppe et al. 2022). A key focus of modern biology is understanding how heterogeneous populations of cells coexist and communicate with each other (intercellular signaling), how they properly respond (intracellular signaling) within a tissue and organ system and how these processes vary across different experimental conditions (comparative analysis). Recently, a rapid expansion of computational tools exploring the expression of ligand and receptor has enabled the systematic inference of cell-cell communication from single-cell transcriptomics and spatial transcriptomics data (Armingol et al. 2021; Armingol, Baghdassarian, and Lewis 2024). These are crucial in unravelling the complex landscape of biological systems.

This tutorial aims to provide a comprehensive introduction to computational approaches for cell-cell communication inference using high throughput transcriptomics data. It covers the fundamental concepts of cellular communication and assumptions underlying analysis focusing on the main computational methods used in the field. This includes computational approaches for inter-cellular communication inference (CellphoneDB (Efremova et al. 2020); LIANA (Dimitrov et al. 2022, 2024)) and for intra-cellular signals communication (scSeqComm (Baruzzo, Cesaro, and Di Camillo 2022); NicheNet (Browaeys, Saelens, and Saeys 2019)). Next, we will describe approaches for comparative analysis of cell-cell networks in distinct biological conditions (CrossTalkeR (Nagai et al. 2021)) and methods for spatially resolved cell-cell communications (Ischia (Regan-KomitoDaniel 2024); DeepCOLOR (Kojima et al. 2024)).

In the first part of the tutorial, participants will be introduced to the theoretical basis of state-of-the-art computational approaches and will learn how to use representative tools for inferring intercellular signaling and intracellular signaling pathways. In the second part, we will focus on the comparative analyses, i.e. changes of cell-cell communication in two conditions, and subsequently highlighting the unique insights spatial transcriptomics data can provide for understanding tissue architecture and cellular communication.

Versions

Version v3 10.5281/zenodo.15756745	Jun 27, 2025
Version v2 10.5281/zenodo.15722171	Jun 23, 2025
Version v1 10.5281/zenodo.15535246	May 28, 2025

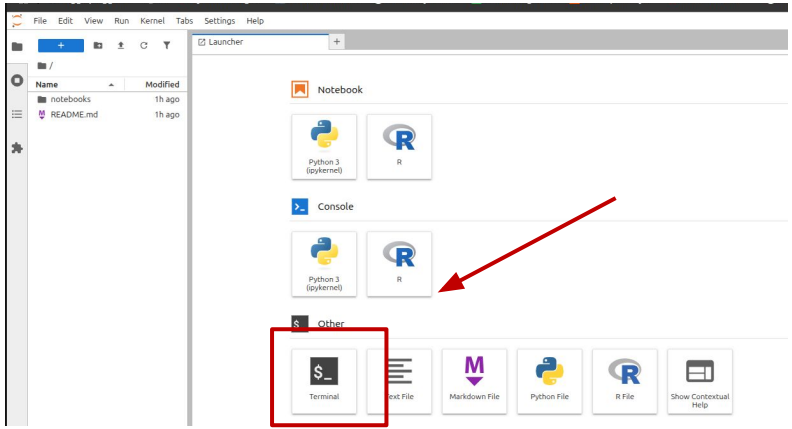
View all 3 versions

Cite all versions? You can cite all versions by using the DOI 10.5281/zenodo.15535245. This DOI represents all versions, and will always resolve to the latest one. Read more.

STEP 3: Download the data

To **download** the data

1. **Open a terminal**
   - Manual setup: open your **local terminal** inside the cloned repository folder
   - Docker setup: open the **JupyterLab terminal** (inside the container)

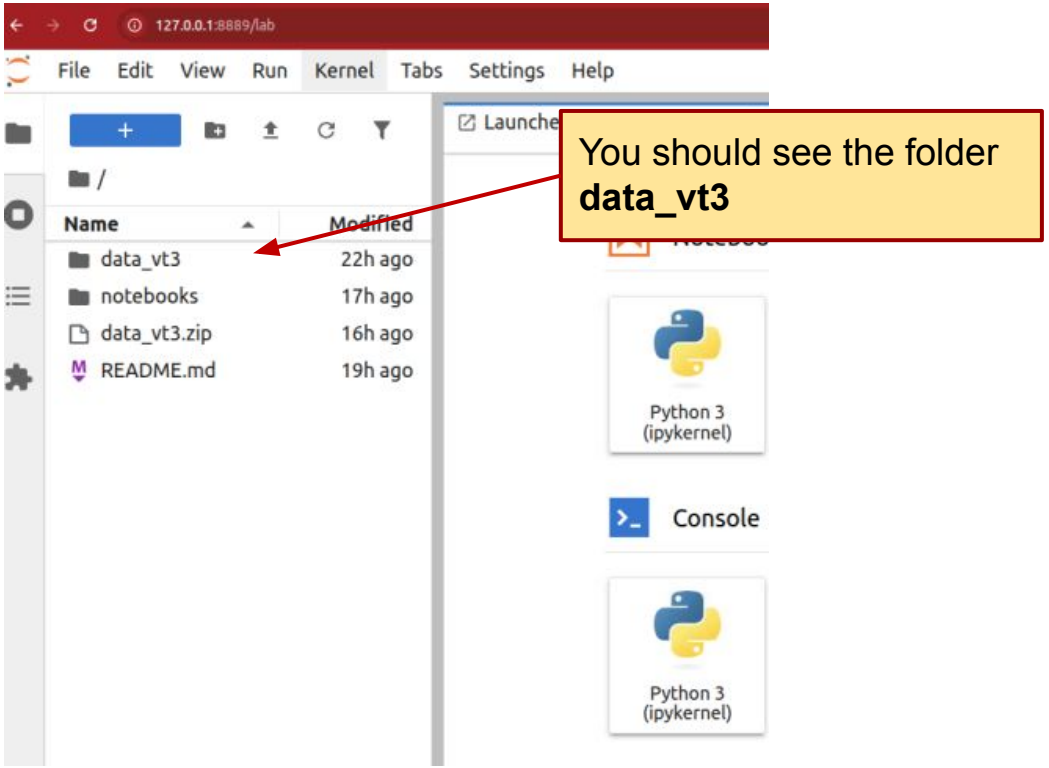


Note that this will download a large file (~2GB) and as such, it will **take some time**.

2. **Run the following command**

```
wget https://zenodo.org/records/15756745/files/data_vt3.zip \
&& unzip data_vt3.zip
```

STEP 3: Download the data



You should see the folder **data_vt3**

STEP 4: Configure resource limits

Configure resource limits (Windows)

Windows users using WSL 2 backend and Docker Desktop app

By default, the WSL 2 VM is assigned 50% of total memory on Windows!
This is maybe not sufficient to run every notebook!
If you have a Windows machine with **<32GB RAM** memory, follow this steps to **configure limits** on the memory.

1) Open any text editor as administrator and create the file **.wslconfig** in your Windows user profile directory, e.g. **C:/Users/<USERNAME>/**
2) Add the following content in the file

```
[wsl2]
memory=13GB
```

Our scripts might take up to **13GB**.

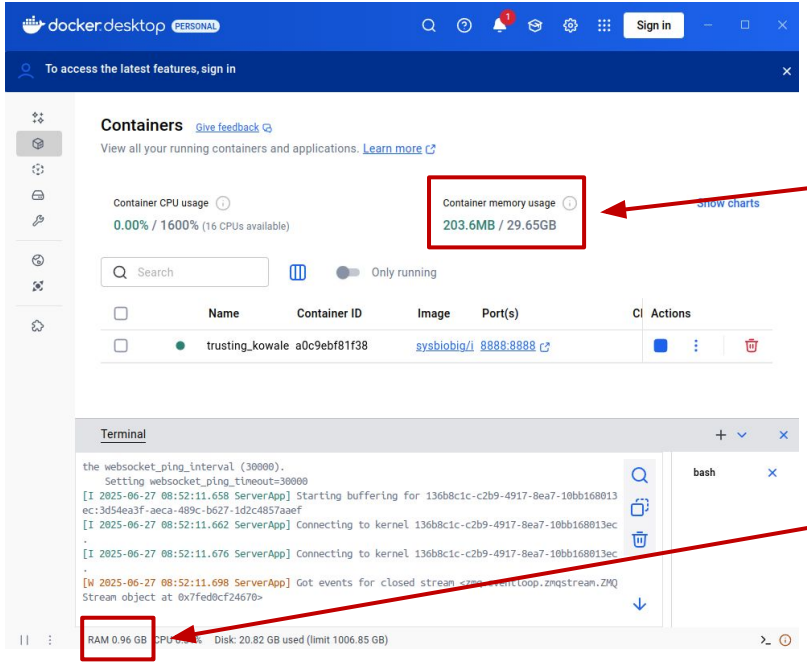
3) Save the file as *.wslconfig* without *.txt* extension.
   ⚠️ *Note that, by default, Windows adds .txt, so make sure to remove it.*
4) Restart WSL2 running the following in the Docker Desktop Terminal, PowerShell, or Command Prompt

```
wsl --shutdown
wsl
```

Configure resource limits (UNIX)

Linux and Mac OS users using Docker Desktop app

You can check how much memory is available for your Docker container in the Docker Desktop dashboard:



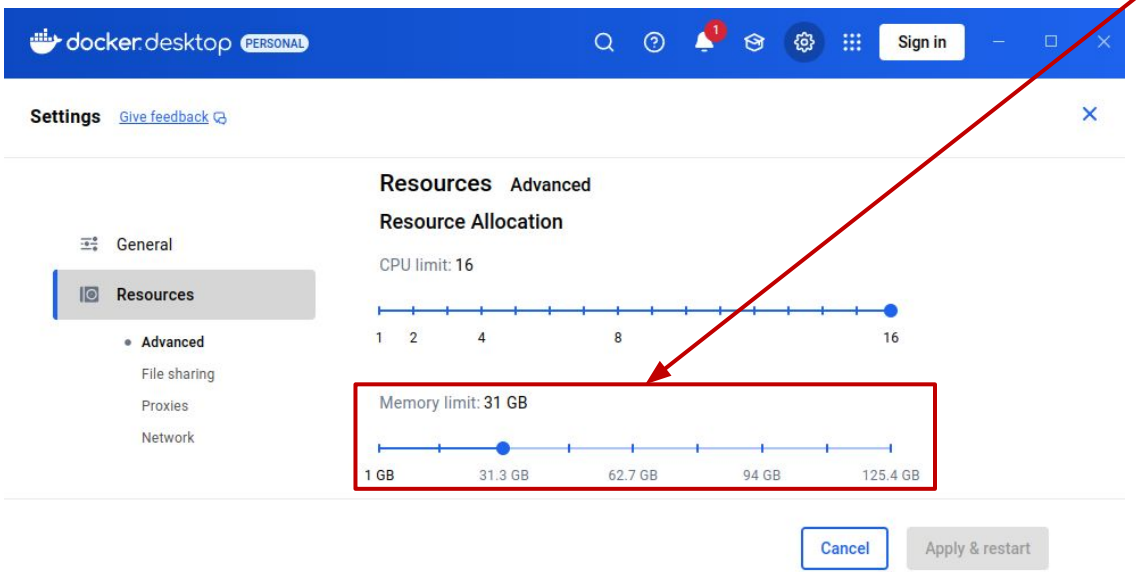
Our scripts might take up to **13GB**. Make sure the available container memory shown here is more than that

If your available memory is less than **13GB**, <u>you can increase it.</u> In **Linux based systems**, clicking here leads you to the dashboard in the next slide…

Configure resource limits (UNIX)

Linux users using Docker Desktop app

You can increase the available container memory using the **slider.** **Don't forget to click "Apply & restart"**



Configure resource limits (UNIX)

Linux users NOT using the Docker Desktop app

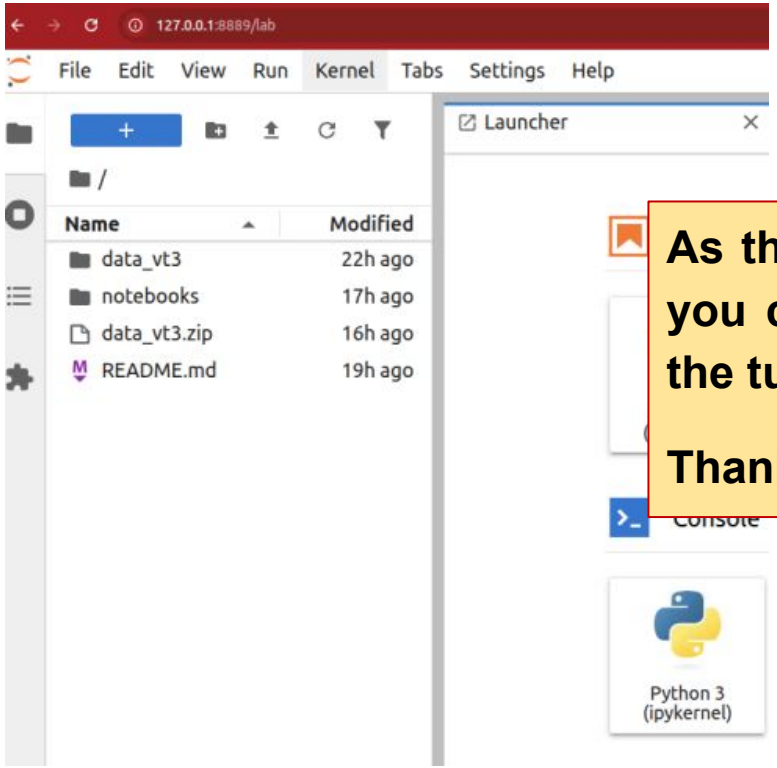
Docker containers on Linux can use **all available system memory** by default. So, if your system has more than **13 GB of RAM**, it should work without issues.

To check your available memory, run the following command in your terminal:

```
sudo docker run [... rest of the docker run command shown previously]
sudo docker ps ### to get the containerID
sudo docker container stats [containerID] ### there you can check what the mem limit is
```

Set up Complete!

If you have followed all the steps, you are now ready for the hands-on part of the tutorial!



As the schedule is very tight, please make sure you complete these steps at least a day before the tutorial begins.

Thank you!