Working with Google Colab and GitHub

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Introduction to Google Colab

- Colaboratory (Colab) is a free, cloud-based service by Google.
- Replicates Jupyter Notebook functionalities in the cloud.
- Accessible via: https://colab.research.google.com/notebooks/welcome.ipynb
- No installation required.

Using Google Colab

- Functions similarly to desktop Jupyter Notebook.
- Requires a free Google account for full feature access.
- Utilizes a cell-oriented paradigm for tasks.
- Example source code may vary due to version differences and hardware.

Features of Google Colab

- Write and run code.
- Create associated documentation.
- Display graphics.
- Works with .ipynb files, similar to Jupyter Notebook.
- Best used with Chrome or Firefox.
- Suitable for data science and Python projects.

Executing Code in Colab

- Select the cell.
- Click the Run button (right-facing arrow).
- Current cell remains selected after execution.

Managing Cell Outputs

- Clear output of individual cells using the block next to the output.
- Hovering over the block shows execution details (e.g., who executed the content).

Additional Cell Options

- Click the vertical ellipsis on the right side of the cell.
- Access a menu of options specific to that cell.

• Uploading and Saving Code

- Upload code from your local drive.
- · Save to Google Drive or GitHub.
- Access code from any device via these sources.

Syncing Across Devices

- Use Chrome and sync settings across devices.
- · Code is available on desktop, tablet, and smartphone.
- · Same repository and Chrome setup, different devices.

Flexibility vs. Performance

- · Colab offers flexibility but may trade off speed and ergonomics.
- · Local Notebook generally executes code faster.
- · Viewing and editing code on smaller devices can be challenging.

File Download Options

- · Colab supports .ipynb and .py file downloads.
- · Notebook offers additional formats: HTML, LaTeX, PDF.
- Limited presentation creation options in Colab.

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Using Local Runtime Support

- Benefits of Local Runtime
- Improved speed and resource access.
- Access to local files on your machine.
- Control over the Notebook version used for execution.
- Setting Up Local Runtime
- Colab connects to a local copy of Notebook.
- Requires installation of Notebook on your local system.
- Better speed compared to cloud-based execution.
- Requirements for Local Runtime
- Compatible with Windows, Linux, or OS X.
- Requires an appropriate browser (not Internet Explorer).
- Security Considerations
- Risk of infection from Notebook code.
- Trust the source of the code.
- Your machine is not open to others sharing code; they use their own runtimes.

Working with Notebooks

New Notebook

Creating a New Notebook

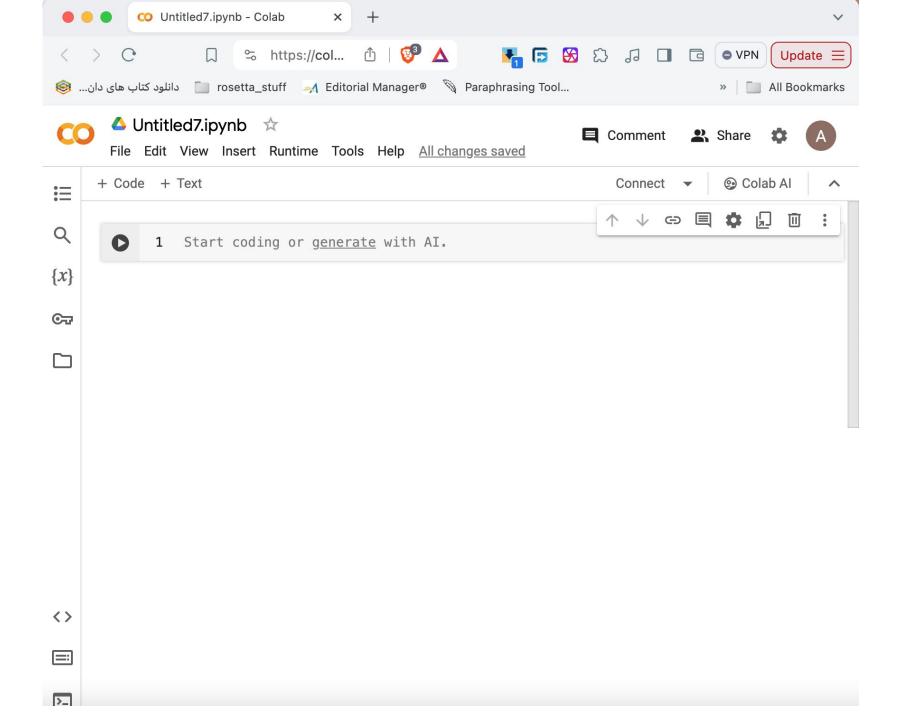
Go to: https://colab.research.google.com/notebooks/welcome.ipynb

- - Choose `File

 New Notebook`.
- - A new Python 3 notebook will open.
- - Click on the filename to change it.

Running Code in Colab

- - Click the right-pointing arrow on the left side of the cell.
- - Cell focus does not change to the next cell automatically.



Opening Existing Notebooks

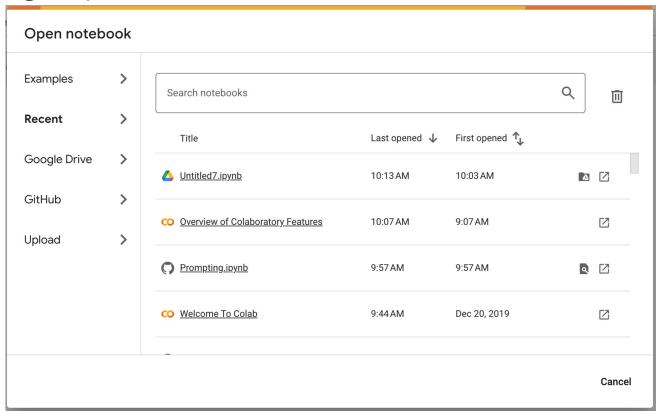
Steps to Open Notebooks

- - Choose `File

 Open Notebook`.
- A dialog box appears (as shown in Figure)

Sources for Existing Notebooks

- - Local storage
- - Google Drive
- - GitHub
- Colab examples



Saving Notebooks

- Cloud-Based Saving Options**
- - Colab offers various cloud-based saving options.
- - Local drive saving requires downloading the file.

- Using Google Drive**
- - Default storage location: Google Drive (https://drive.google.com/).
- - Choose `File □ Save` to save to the root directory.
- - Select a different folder in Google Drive if needed.

Using GitHub to Save Notebooks

Introduction to GitHub

- Alternative to Google Drive for saving content.
- Organized method for sharing code for discussion, review, and distribution.
- GitHub link: https://github.com/

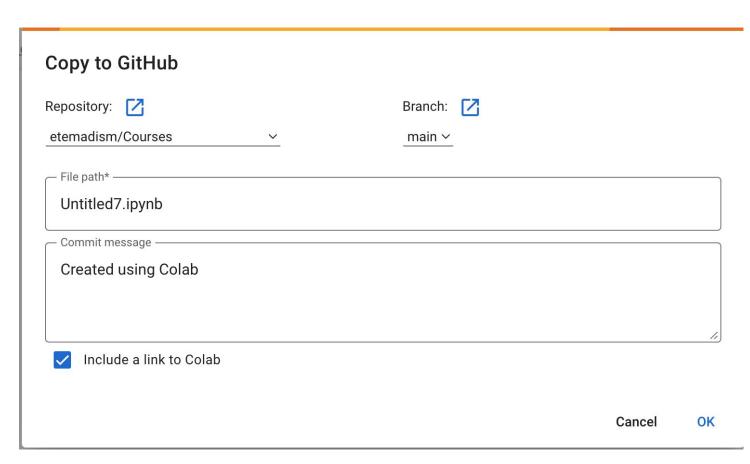
Saving a File to GitHub

- Choose File

 Save a Copy in GitHub.
- Sign in to GitHub if prompted.

GitHub Save Dialog Box

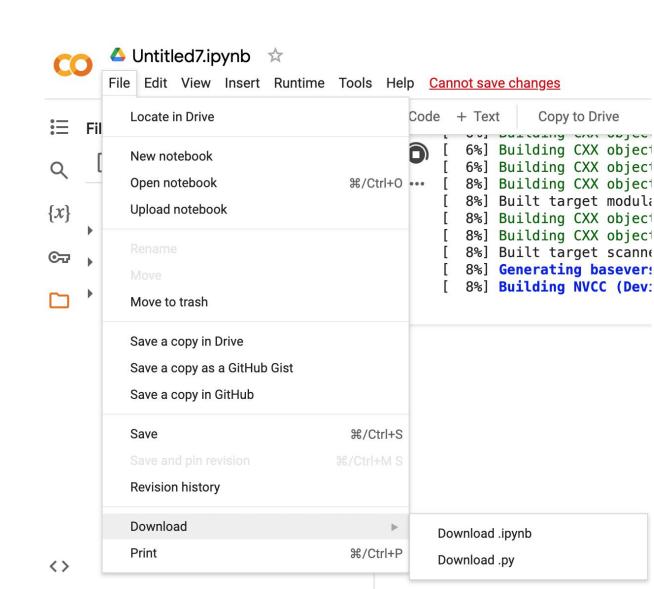
- After signing in, a dialog box appears (as shown in Figure).
- Select repository and specify details for saving the file.



Downloading notebooks

Colab supports two methods for downloading notebooks to your local drive:

- .ipynb files (using File → Download .ipynb)
- and .py files (using File → Download .py).
- In both cases, the file appears in the default download directory for your browser; Colab doesn't offer a method for downloading the file to a specific directory.



Performing Common Tasks

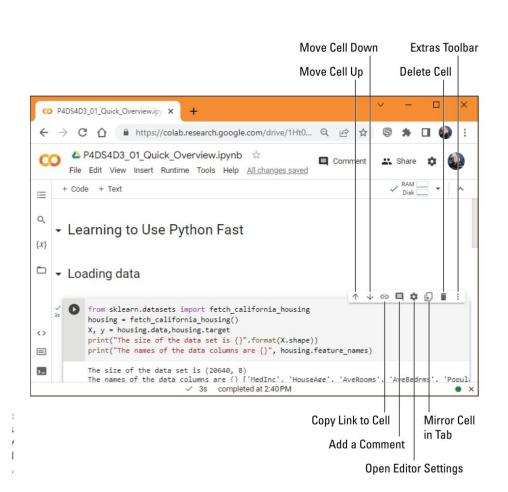
Creating Code Cells

Initial Code Cell**

- First cell in Colab is a code cell.

Accessing Extra Options

- Vertical ellipsis at the rightmost end of the toolbar.
- 1. **Move Cell Up**: Moves the cell up by one position.
- 2. **Move Cell Down**: Moves the cell down by one position.
- 3. **Copy Link to Cell**: Places a link to the cell on the Clipboard.
- 4. **Add a Comment**: Creates a comment balloon to the right of the cell.
- 5. **Open Editor Settings**: Modify Colab's behavior.
- **Slide 69: More Extra Features**
- 6. **Mirror Cell in Tab**: Creates a mirror view of the cell in a side window.
- 7. **Delete Cell**: Removes the cell from the notebook.

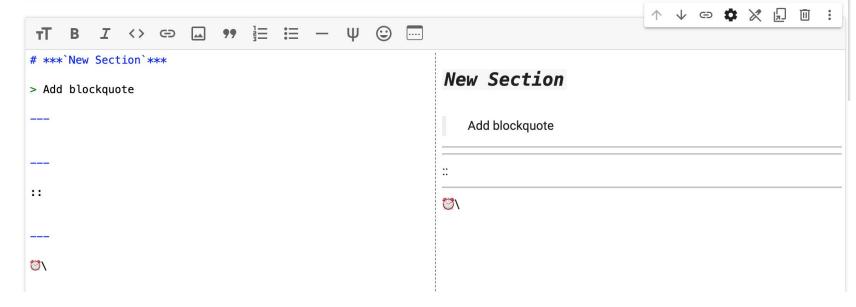


Creating Text Cells

New section
New subsection
New sub-subsection

* * Italic ** ** Bold *** *** Italic an Bold

Reference



Markdown	Preview
bold text	bold text
italicized text or _italicized text_	italicized text
`Monospace`	Monospace
~~strikethrough~~	strikethrough
[A link](https://www.google.com)	<u>A link</u>
![An image](https://www.google.com/images/rss.png)	<u></u>

Enabling Hardware Acceleration

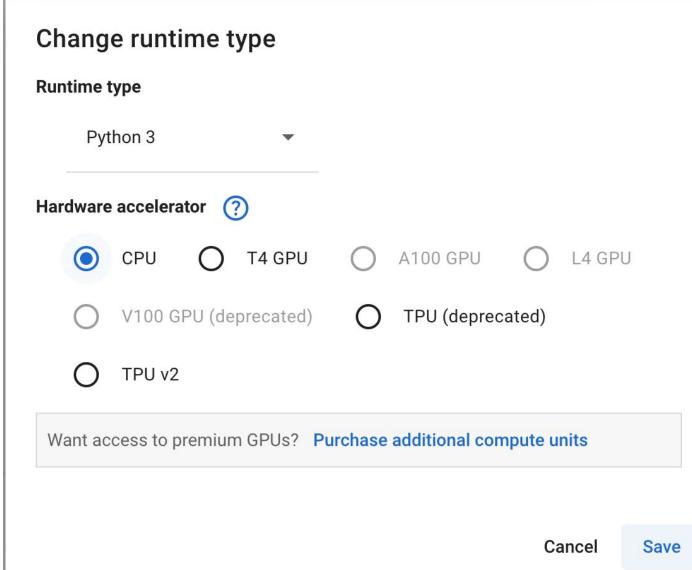
- Go to Edit

 Notebook

 Settings to open the

 Notebook Settings dialog

 box.
- Options to add GPU and TPU for enhanced performance.



Executing the Code

• Run Current Cell:

• Click the right-pointing arrow or choose Runtime

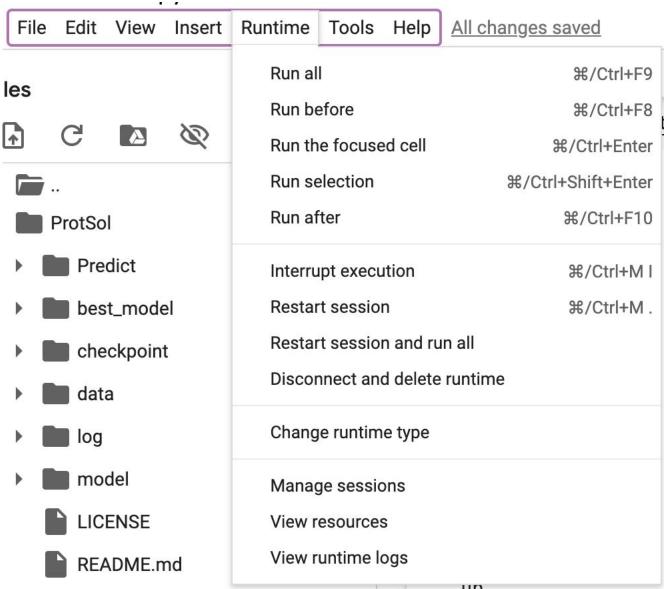
Run the Focused Cell.

Run Other Cells:

 Options to run next, previous, or selected cells from the Runtime menu.

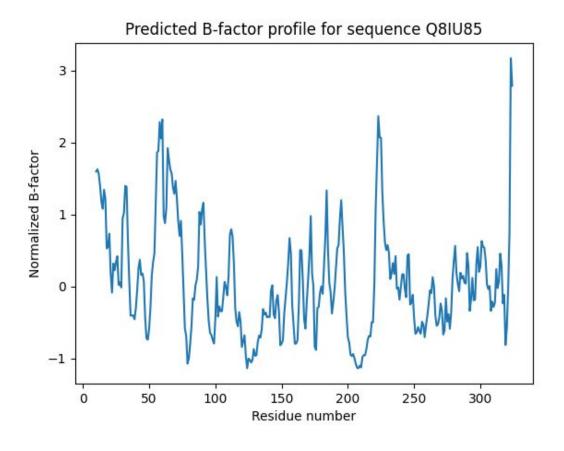
Run All Cells:

- Choose Runtime
 □ Run All to execute
 all code from the top to the bottom of the
 notebook.
- Interrupt execution anytime with Runtime
 □ Interrupt Execution.



Make a colab for running FlexAmino

- Go to
 https://github.com/upcmarina/flexamino
- And install it on Colab
- Make a run test on this protein: <u>https://www.uniprot.org/uniprotkb/</u> <u>Q8IU85/entry</u>
- You must make a result out of it like the figure in write side.



GitHub

Introduction

 GitHub is a web-based platform that uses Git for version control, allowing multiple people to work on projects simultaneously. It is widely used for software development and version control, providing a range of tools for collaboration, code review, and project management.

Cloning a Repository

1. Copy the Repository URL:

• Go to the GitHub repository page you want to clone, like:

https://github.com/upcmarina/flexamino.git

Click the "Code" button and copy the URL.

2. Clone the Repository Locally:

- 1. In your terminal, navigate to the directory where you want to store the cloned repository.
- 2. Use the **git clone** command followed by the URL you copied:

git clone https://github.com/upcmarina/flexamino.git

1. Sign Up for GitHub:

1. Go to GitHub and sign up for an account.

2. Install Git:

1. Download and install Git from Git's official site.

Linux: apt-get install git

Mac: brew install git

1. After installation, configure your Git with your GitHub credentials using the following commands in your terminal:

```
git config --global user.name "Your Name" git config --global user.email "your.email@example.com"
```

Create a New Repository

- 1. Log in to your GitHub account.
- 2. Click the "+" icon in the top right corner and select "New repository".
- 3. Name your repository, add a description (optional), choose public or private, and click "Create repository".

Locally on Your Machine:

- 1. Open your terminal (in VS code) or Git Bash.
- 2. Navigate to the directory where you want to create your project.
- 3. Initialize a new Git repository with: git init

Making Changes and Committing

1. Make Changes:

Open your project in VS code and make changes to your files.

2. Stage Changes:

1. In your terminal, stage the changes using:

git remote add origin

https://github.com/your-username/your-repository.git

Push to GitHub

 Push your code to the remote repository git push -u origin main

In nutshell

```
# Navigate to your project directory
cd path/to/your/project
configure your Git with your GitHub credentials using the following commands in your terminal:
              git config --global user.name "Your Name"
              git config --global user.email "your.email@example.com"
# Initialize Git
git init
# Add GitHub repository as remote
git remote add origin https://github.com/your-username/your-repositor
y.git
```

```
# Add files to staging git add .

# Commit the changes git commit -m "Initial commit"

# Push to GitHub git push -u origin main
```

GitHub Codespaces

• GitHub Codespaces is a cloud-based development environment provided by GitHub, allowing developers to write, run, and debug their code directly from a web browser. It is built on top of Visual Studio Code and integrates seamlessly with GitHub repositories, making it an excellent tool for collaborative development and contributing to open-source projects.

Enable GitHub Codespaces for Your Repository

1. Navigate to Your Repository:

1. Go to <u>GitHub</u> and navigate to the repository where you want to use Codespaces. https://github.com/upcmarina/flexamino

2. Enable Codespaces:

- 1. Click the "Code" button on the repository page.
- 2. In the dropdown menu, select the "Codespaces" tab.
- 3. Click "New codespace" to create a new Codespace.

Step 2: Creating and Launching a Codespace

1. Create a Codespace:

2. After clicking "New codespace," GitHub will start creating your Codespace environment. This may take a few moments.

2. Launch the Codespace:

2. Once the environment is ready, you will be redirected to a web-based Visual Studio Code interface.