Introduction to Python

August, 2024

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# About this Course

## 0.1 Curriculum

The course covers fundamentals of Python, a high-level programming language, and use it to wrangle data for analysis and visualization.

## 0.2 Target Audience

The course is intended for researchers who want to learn coding for the first time with a data science application via the Python language. This course is also appropriate for folks who have explored data science or programming on their own and want to focus on some fundamentals.

## 0.3 Learning Objectives

**Analyze** Tidy datasets in the Python programming language via data subsetting, joining, and transformations.

**Evaluate** summary statistics and data visualization to understand scientific questions.

**Describe** how the Python programming environment interpret complex expressions made out of functions, operations, and data structures, in a step-by-step way.

**Apply** problem solving strategies to debug broken code.

## 0.4 Offerings

This course is taught on a regular basis at [Fred Hutch Cancer Center](https://www.fredhutch.org/) through the [Data Science Lab](https://hutchdatascience.org/). Announcements of course offering can be found [here](https://hutchdatascience.org/training/).

# 1 Intro to Computing

Welcome to Introduction to Python! Each week, we cover a chapter, which consists of a lesson and exercise. In our first week together, we will look at big conceptual themes in programming, see how code is run, and learn some basic grammar structures of programming.

## 1.1 Goals of the course

In the next 6 weeks, we will explore:

* Fundamental concepts in high-level programming languages (Python, R, Julia, etc.) that is transferable: *How do programs run, and how do we solve problems using functions and data structures?*
* Beginning of data science fundamentals: *How do you translate your scientific question to a data wrangling problem and answer it?*
* 
* Data science workflow. Image source: [R for Data Science](https://r4ds.hadley.nz/whole-game).
* Find a nice balance between the two throughout the course: we will try to reproduce a figure from a scientific publication using new data.

## 1.2 What is a computer program?

* A sequence of instructions to manipulate data for the computer to execute.
* A series of translations: English <-> Programming Code for Interpreter <-> Machine Code for Central Processing Unit (CPU)

We will focus on English <-> Programming Code for Python Interpreter in this class.

More importantly: **How we organize ideas <-> Instructing a computer to do something**.

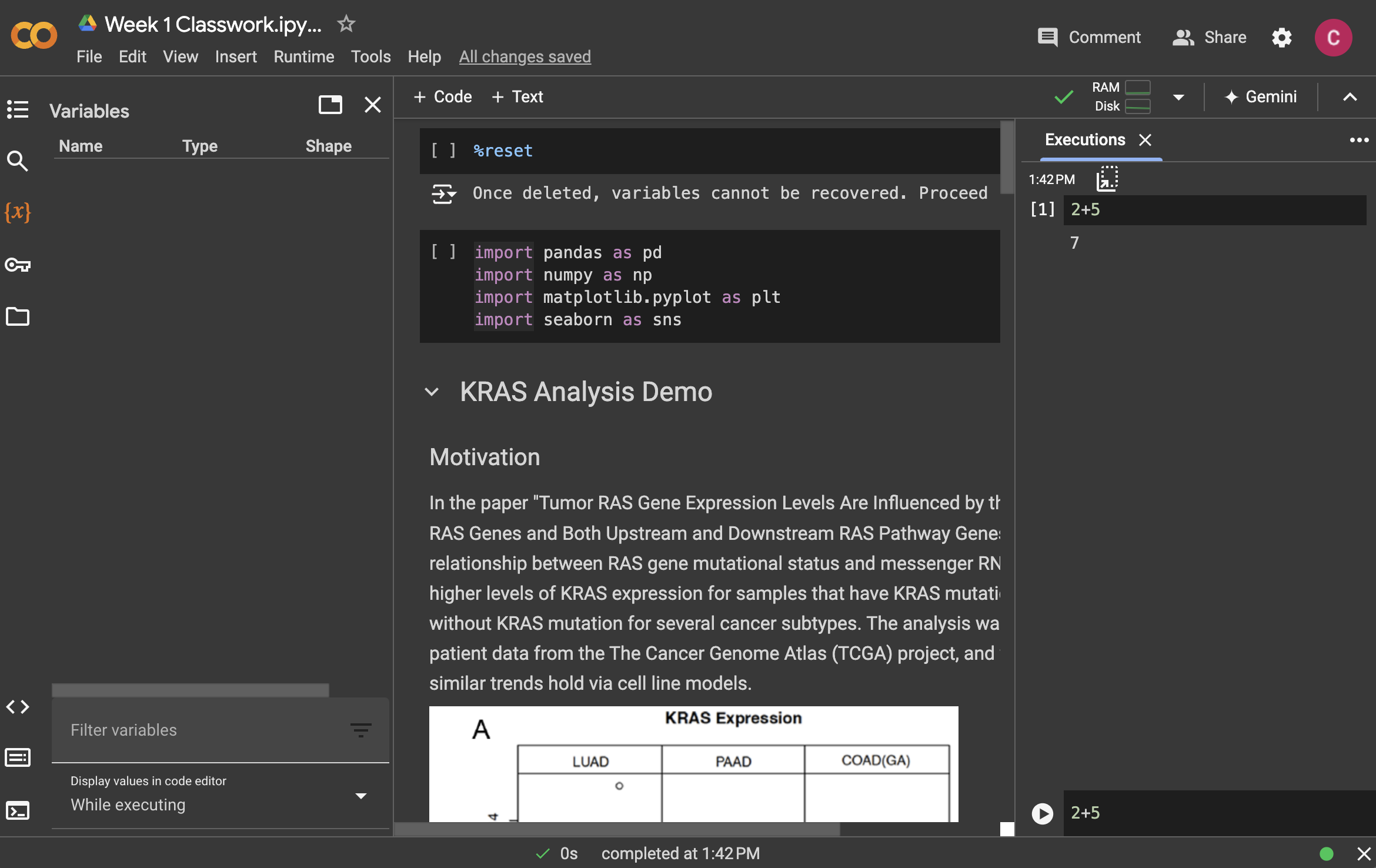
## 1.3 A programming language has following elements:

* Grammar structure to construct expressions; combining expressions to create more complex expressions
* Encapsulate complex expressions via **functions** to create modular and reusable tasks
* Encapsulate complex data via **data structures** to allow efficient manipulation of data

## 1.4 Google Colab Setup

Google Colab is a Integrated Development Environment (IDE) on a web browser. Think about it as Microsoft Word to a plain text editor. It provides extra bells and whistles to using Python that is easier for the user.

Let’s open up the KRAS analysis in Google Colab. If you are taking this course while it is in session, the project name is probably named “KRAS Demo” in your Google Classroom workspace. If you are taking this course on your own time, you can view it [here](https://colab.research.google.com/drive/1_77QQcj0mgZOWLlhtkZ-QKWUP1dnSt-_?usp=sharing).



Today, we will pay close attention to:

* Python Console (“Executions”): Open it via View -> Executed code history. You give it one line of Python code, and the console executes that single line of code; you give it a single piece of instruction, and it executes it for you.
* Notebook: in the central panel of the website, you will see Python code interspersed with word document text. This is called a Python Notebook (other similar services include Jupyter Notebook, iPython Notebook), which has chunks of plain text *and* Python code, and it helps us understand better the code we are writing.
* Variable Environment: Open it by clicking on the “{x}” button on the left-hand panel. Often, your code will store information in the Variable Environment, so that information can be reused. For instance, we often load in data and store it in the Variable Environment, and use it throughout rest of your Python code.

The first thing we will do is see the different ways we can run Python code. You can do the following:

1. Type something into the Python Console (Execution) and click the arrow button, such as 2+2. The Python Console will run it and give you an output.
2. Look through the Python Notebook, and when you see a chunk of Python Code, click the arrow button. It will copy the Python code chunk to the Python Console and run all of it. You will likely see variables created in the Variables panel as you load in and manipulate data.
3. Run every single Python code chunk via Runtime -> Run all.

Remember that the *order* that you run your code matters in programming. Your final product would be the result of Option 3, in which you run every Python code chunk from start to finish. However, sometimes it is nice to try out smaller parts of your code via Options 1 or 2. But you will be at risk of running your code out of order!

To create your own content in the notebook, click on a section you want to insert content, and then click on “+ Code” or “+ Text” to add Python code or text, respectively.

Python Notebook is great for data science work, because:

* It encourages reproducible data analysis, when you run your analysis from start to finish.
* It encourages excellent documentation, as you can have code, output from code, and prose combined together.
* It is flexible to use other programming languages, such as R.

Now, we will get to the basics of programming grammar.

## 1.5 Grammar Structure 1: Evaluation of Expressions

* **Expressions** are be built out of **operations** or **functions**.
* Functions and operations take in **data types**, do something with them, and return another data type.
* We can combine multiple expressions together to form more complex expressions: an expression can have other expressions nested inside it.

For instance, consider the following expressions entered to the Python Console:

18 + 21

## 39

max(18, 21)

## 21

max(18 + 21, 65)

## 65

18 + (21 + 65)

## 104

len("ATCG")

## 4

Here, our input **data types** to the operation are **integer** in lines 1-4 and our input data type to the function is **string** in line 5. We will go over common data types shortly.

Operations are just functions in hiding. We could have written:

from operator import add  
  
add(18, 21)

## 39

add(18, add(21, 65))

## 104

Remember that the Python language is supposed to help us understand what we are writing in code easily, lending to *readable* code. Therefore, it is sometimes useful to come up with operations that is easier to read. (Most functions in Python are stored in a collection of functions called **modules** that needs to be loaded. The import statement gives us permission to access the functions in the module “operator”.)

### 1.5.1 Data types

Here are some common data types we will be using in this course.

| Data type name | **Data type shorthand** | **Examples** |
| --- | --- | --- |
| Integer | int | 2, 4 |
| Float | float | 3.5, -34.1009 |
| String | str | “hello”, “234-234-8594” |
| Boolean | bool | True, False |

A nice way to summarize this first grammar structure is using the function machine schema, way back from algebra class:



Function machine from algebra class.

Here are some aspects of this schema to pay attention to:

* A programmer should not need to know how the function or operation is implemented in order to use it - this emphasizes abstraction and modular thinking, a foundation in any programming language.
* A function can have different kinds of inputs and outputs - it doesn’t need to be numbers. In the len() function, the input is a String, and the output is an Integer. We will see increasingly complex functions with all sorts of different inputs and outputs.

## 1.6 Grammar Structure 2: Storing data types in the Variable Environment

To build up a computer program, we need to store our returned data type from our expression somewhere for downstream use. We can assign a variable to it as follows:

x = 18 + 21

If you enter this in the Console, you will see that in the Variable Environment, the variable x has a value of 39.

### 1.6.1 Execution rule for variable assignment

Evaluate the expression to the right of =.

Bind variable to the left of = to the resulting value.

The variable is stored in the **Variable Environment**.

The Variable Environment is where all the variables are stored, and can be used for an expression anytime once it is defined. Only one unique variable name can be defined.

The variable is stored in the working memory of your computer, Random Access Memory (RAM). This is temporary memory storage on the computer that can be accessed quickly. Typically a personal computer has 8, 16, 32 Gigabytes of RAM.

Look, now x can be reused downstream:

x - 2

## 37

y = x \* 2

It is quite common for programmers to not know what data type a variable is while they are coding. To learn about the data type of a variable, use the type() function on any variable in Python:

type(y)

## <class 'int'>

We should give useful variable names so that we know what to expect! If you are working with sales data, consider num\_sales instead of y.

## 1.7 Grammar Structure 3: Evaluation of Functions

Let’s look at functions a little bit more formally: A function has a **function name**, **arguments**, and **returns** a data type.

### 1.7.1 Execution rule for functions:

Evaluate the function by its arguments if there’s any, and if the arguments are functions or contains operations, evaluate those functions or operations first.

The output of functions is called the **returned value**.

Often, we will use multiple functions in a nested way, and it is important to understand how the Python console understand the order of operation. We can also use paranthesis to change the order of operation. Think about what the Python is going to do step-by–step in the lines of code below:

max(len("hello"), 4)

## 5

(len("pumpkin") - 8) \* 2

## -2

If we don’t know how to use a function, such as pow(), we can ask for help:

?pow  
  
pow(base, exp, mod=None)  
Equivalent to base\*\*exp with 2 arguments or base\*\*exp % mod with 3 arguments  
   
Some types, such as ints, are able to use a more efficient algorithm when  
invoked using the three argument form.

This shows the function takes in three input arguments: base, exp, and mod=None. When an argument has an assigned value of mod=None, that means the input argument already has a value, and you don’t need to specify anything, unless you want to.

The following ways are equivalent ways of using the pow() function:

pow(2, 3)

## 8

pow(base=2, exp=3)

## 8

pow(exp=3, base=2)

## 8

but this will give you something different:

pow(3, 2)

## 9

And there is an operational equivalent:

2 \*\* 3

## 8

We will mostly look at functions with input arguments and return types in this course, but not all functions need to have input arguments and output return. Here are some varieties of functions to stretch your horizons.

| Function call | What it takes in | What it does | Returns |
| --- | --- | --- | --- |
| pow(a, b) | integer a, integer b | Raises a to the bth power. | Integer |
| print(x) | any data type x | Prints out the value of x to the console. | None |
| datetime.now() | Nothing | Gets the current time. | String |

## 1.8 Tips on writing your first code

Computer = powerful + stupid

Computers are excellent at doing something specific over and over again, but is extremely rigid and lack flexibility. Here are some tips that is helpful for beginners:

* Write incrementally, test often
* Check your assumptions, especially using new functions, operations, and new data types.
* Live environments are great for testing, but not great for reproducibility.
* Ask for help!

To get more familiar with the errors Python gives you, take a look at this [summary of Python error messages](https://betterstack.com/community/guides/scaling-python/python-errors/).

## 1.9 Exercises

Exercise for week 1 can be found [here](https://colab.research.google.com/drive/1AqVvktGz3LStUyu6dLJFsU2KoqNxgagT?usp=sharing).

# 2 Working with data structures

In our second lesson, we start to look at two **data structures**, **Lists** and **Dataframes**, that can handle a large amount of data for analysis.

## 2.1 Lists

In the first exercise, you started to explore **data structures**, which store information about data types. You explored **lists**, which is an ordered collection of data types or data structures. Each *element* of a list contains a data type or another data structure.

We can now store a vast amount of information in a list, and assign it to a single variable. Even more, we can use operations and functions on a list, modifying many elements within the list at once! This makes analyzing data much more scalable and less repetitive.

We create a list via the bracket [ ] operation.

staff = ["chris", "ted", "jeff"]  
chrNum = [2, 3, 1, 2, 2]  
mixedList = [False, False, False, "A", "B", 92]

### 2.1.1 Subsetting lists

To access an element of a list, you can use the bracket notation [ ] to access the elements of the list. We simply access an element via the “index” number - the location of the data within the list.

*Here’s the tricky thing about the index number: it starts at 0!*

1st element of chrNum: chrNum[0]

2nd element of chrNum: chrNum[1]

…

5th element of chrNum: chrNum[4]

With subsetting, you can modify elements of a list or use the element of a list as part of an expression.

### 2.1.2 Subsetting multiple elements of lists

Suppose you want to access multiple elements of a list, such as accessing the first three elements of chrNum. You would use the **slice** operator :, which specifies:

* the index number to start
* the index number to stop, *plus one.*

If you want to access the first three elements of chrNum:

chrNum[0:3]

## [2, 3, 1]

The first element’s index number is 0, the third element’s index number is 2, plus 1, which is 3.

If you want to access the second and third elements of chrNum:

chrNum[1:3]

## [3, 1]

If you want to access everything but the first three elements of chrNum:

chrNum[3:len(chrNum)]

## [2, 2]

where len(chrNum) is the length of the list.

When the start or stop index is specified, it implies that you are subsetting starting the from the beginning of the list or subsetting to the end of the list, respectively:

chrNum[:3]

## [2, 3, 1]

chrNum[3:]

## [2, 2]

More discussion of list slicing can be found [here](https://stackoverflow.com/questions/509211/how-slicing-in-python-works).

## 2.2 Objects in Python

The list data structure has an organization and functionality that metaphorically represents a pen-and-paper list in our physical world. Like a physical object, we have examined:

* What does it contain (in terms of data)?
* What can it do (in terms of operations and functions)?

And if it “makes sense” to us, then it is well-designed.

The list data structure we have been working with is an example of an **Object**. The definition of an object allows us to ask the questions above: what does it contain, and what can it do. It is an organizational tool for a collection of data and functions that we can relate to. Formally, an object contains the following:

* **Value** that holds the essential data for the object.
* **Attributes** that store additional data for the object.
* Functions called **Methods** that can be used on the object.

This organizing structure on an object applies to pretty much all Python data types and data structures.

Let’s see how this applies to the list:

* Value: the contents of the list, such as [2, 3, 4].
* **Attributes** that store additional values: Not relevant for lists.
* **Methods** that can be used on the object: chrNum.count(2) counts the number of instances 2 appears as an element of chrNum.

Object methods are functions that does something with the object you are using it on. You should think about chrNum.count(2) as a function that takes in chrNum and 2 as inputs. If you want to use the count function on list mixedList, you would use mixedList.count(x).

| Function method | What it takes in | What it does | Returns |
| --- | --- | --- | --- |
| chrNum.count(x) | list chrNum, data type x | Counts the number of instances x appears as an element of chrNum. | Integer |
| chrNum.append(x) | list chrNum, data type x | Appends x to the end of the chrNum. | None (but chrNum is modified!) |
| chrNum.sort() | list chrNum | Sorts chrNum by ascending order. | None (but chrNum is modified!) |
| chrNum.reverse() | list chrNum | Reverses the order of chrNum. | None (but chrNum is modified!) |

## 2.3 Dataframes

A Dataframe is a two-dimensional data structure that stores data like a spreadsheet does.

The Dataframe data structure is found within a Python module called “Pandas”. A Python module is an organized collection of functions and data structures. The import statement below gives us permission to access the “Pandas” module via the variable pd.

To load in a Dataframe from existing spreadsheet data, we use the function pd.read\_csv():

import pandas as pd  
  
metadata = pd.read\_csv("classroom\_data/metadata.csv")  
type(metadata)

## <class 'pandas.core.frame.DataFrame'>

There is a similar function pd.read\_excel() for loading in Excel spreadsheets.

Let’s investigate the Dataframe as an object:

* What does a Dataframe contain (in terms of data)?
* What can a Dataframe do (in terms of operations and functions)?

### 2.3.1 What does a Dataframe contain (in terms of data)?

We first take a look at the contents:

metadata

## ModelID ... OncotreeLineage  
## 0 ACH-000001 ... Ovary/Fallopian Tube  
## 1 ACH-000002 ... Myeloid  
## 2 ACH-000003 ... Bowel  
## 3 ACH-000004 ... Myeloid  
## 4 ACH-000005 ... Myeloid  
## ... ... ... ...  
## 1859 ACH-002968 ... Esophagus/Stomach  
## 1860 ACH-002972 ... Esophagus/Stomach  
## 1861 ACH-002979 ... Esophagus/Stomach  
## 1862 ACH-002981 ... Esophagus/Stomach  
## 1863 ACH-003071 ... Lung  
##   
## [1864 rows x 30 columns]

It looks like there are 1864 rows and 30 columns in this Dataframe, and when we display it it shows some of the data.

We can look at specific columns by looking at **attributes** via the dot operation. We can also look at the columns via the bracket operation.

metadata.ModelID

## 0 ACH-000001  
## 1 ACH-000002  
## 2 ACH-000003  
## 3 ACH-000004  
## 4 ACH-000005  
## ...   
## 1859 ACH-002968  
## 1860 ACH-002972  
## 1861 ACH-002979  
## 1862 ACH-002981  
## 1863 ACH-003071  
## Name: ModelID, Length: 1864, dtype: object

metadata['ModelID']

## 0 ACH-000001  
## 1 ACH-000002  
## 2 ACH-000003  
## 3 ACH-000004  
## 4 ACH-000005  
## ...   
## 1859 ACH-002968  
## 1860 ACH-002972  
## 1861 ACH-002979  
## 1862 ACH-002981  
## 1863 ACH-003071  
## Name: ModelID, Length: 1864, dtype: object

The names of all columns is stored as an attribute, which can be accessed via the dot operation.

metadata.columns

## Index(['ModelID', 'PatientID', 'CellLineName', 'StrippedCellLineName', 'Age',  
## 'SourceType', 'SangerModelID', 'RRID', 'DepmapModelType', 'AgeCategory',  
## 'GrowthPattern', 'LegacyMolecularSubtype', 'PrimaryOrMetastasis',  
## 'SampleCollectionSite', 'Sex', 'SourceDetail', 'LegacySubSubtype',  
## 'CatalogNumber', 'CCLEName', 'COSMICID', 'PublicComments',  
## 'WTSIMasterCellID', 'EngineeredModel', 'TreatmentStatus',  
## 'OnboardedMedia', 'PlateCoating', 'OncotreeCode', 'OncotreeSubtype',  
## 'OncotreePrimaryDisease', 'OncotreeLineage'],  
## dtype='object')

The number of rows and columns are also stored as an attribute:

metadata.shape

## (1864, 30)

### 2.3.2 What can a Dataframe do (in terms of operations and functions)?

We can use the head() and tail() functions to look at the first few rows and last few rows of metadata, respectively:

metadata.head()

## ModelID PatientID ... OncotreePrimaryDisease OncotreeLineage  
## 0 ACH-000001 PT-gj46wT ... Ovarian Epithelial Tumor Ovary/Fallopian Tube  
## 1 ACH-000002 PT-5qa3uk ... Acute Myeloid Leukemia Myeloid  
## 2 ACH-000003 PT-puKIyc ... Colorectal Adenocarcinoma Bowel  
## 3 ACH-000004 PT-q4K2cp ... Acute Myeloid Leukemia Myeloid  
## 4 ACH-000005 PT-q4K2cp ... Acute Myeloid Leukemia Myeloid  
##   
## [5 rows x 30 columns]

metadata.tail()

## ModelID PatientID ... OncotreePrimaryDisease OncotreeLineage  
## 1859 ACH-002968 PT-pjhrsc ... Esophagogastric Adenocarcinoma Esophagus/Stomach  
## 1860 ACH-002972 PT-dkXZB1 ... Esophagogastric Adenocarcinoma Esophagus/Stomach  
## 1861 ACH-002979 PT-lyHTzo ... Esophagogastric Adenocarcinoma Esophagus/Stomach  
## 1862 ACH-002981 PT-Z9akXf ... Esophagogastric Adenocarcinoma Esophagus/Stomach  
## 1863 ACH-003071 PT-LAGmLq ... Lung Neuroendocrine Tumor Lung  
##   
## [5 rows x 30 columns]

Both of these functions (without input arguments) are considered as **methods**: they are functions that does something with the Dataframe you are using it on. You should think about metadata.head() as a function that takes in metadata as an input. If we had another Dataframe called my\_data and you want to use the same function, you will have to say my\_data.head().

#### 2.3.2.1 Subsetting Dataframes

Perhaps the most important operation you will can do with Dataframes is subsetting them. There are two ways to do it. The first way is to subset by numerical indicies, exactly like how we did for lists. You will use the iloc and bracket operations, and you give two slices: one for the row, and one for the column.

Subset the first 5 rows, and first two columns:

metadata.iloc[:5, :2]

## ModelID PatientID  
## 0 ACH-000001 PT-gj46wT  
## 1 ACH-000002 PT-5qa3uk  
## 2 ACH-000003 PT-puKIyc  
## 3 ACH-000004 PT-q4K2cp  
## 4 ACH-000005 PT-q4K2cp

If we want a custom slice that is not sequential, we can use an integer list. Subset the last 5 rows, and the 1st and 10 and 21th column:

metadata.iloc[5:, [1, 10, 21]]

## PatientID GrowthPattern WTSIMasterCellID  
## 5 PT-ej13Dz Suspension 2167.0  
## 6 PT-NOXwpH Adherent 569.0  
## 7 PT-fp8PeY Adherent 1806.0  
## 8 PT-puKIyc Adherent 2104.0  
## 9 PT-AR7W9o Adherent NaN  
## ... ... ... ...  
## 1859 PT-pjhrsc Organoid NaN  
## 1860 PT-dkXZB1 Organoid NaN  
## 1861 PT-lyHTzo Organoid NaN  
## 1862 PT-Z9akXf Organoid NaN  
## 1863 PT-LAGmLq Suspension NaN  
##   
## [1859 rows x 3 columns]

This is a great way to start thinking about subsetting your dataframes for analysis, but this way of of subsetting can lead to some inconsistencies in the long run. For instance, suppose your collaborator added a new cell line to the metadata and changed the order of the column. Then your code to subset the last 5 rows and the columns will get you a different answer once the spreadsheet is changed.

The second way is to subset by the column name, and this is much more preferred in data analysis practice. You will learn about it next week!

# About the Authors

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| --- | --- |
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| Content Contributor(s) (include section name/link in parentheses) - make new line if more than one section involved | Wrote less than a chapter |
| Content Editor(s)/Reviewer(s) | Checked your content |
| Content Director(s) | Helped guide the content direction |
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| Illustrator(s) | Created graphics for the course |
| Figure Artist(s) | Created figures/plots for course |
| Videographer(s) | Filmed videos |
| Videography Editor(s) | Edited film |
| Audiographer(s) | Recorded audio |
| Audiography Editor(s) | Edited audio recordings |
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| Funder(s) | Institution/individual who funded course including grant number |
| Funding Staff | Staff members who help with funding |

## ─ Session info ───────────────────────────────────────────────────────────────  
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## ui X11  
## language (EN)  
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## httpuv 1.6.14 2024-01-26 [1] RSPM (R 4.3.0)  
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## later 1.3.2 2023-12-06 [1] RSPM (R 4.3.0)  
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## memoise 2.0.1 2021-11-26 [1] RSPM (R 4.3.0)  
## mime 0.12 2021-09-28 [1] RSPM (R 4.3.0)  
## miniUI 0.1.1.1 2018-05-18 [1] RSPM (R 4.3.0)  
## pkgbuild 1.4.3 2023-12-10 [1] RSPM (R 4.3.0)  
## pkgload 1.3.4 2024-01-16 [1] RSPM (R 4.3.0)  
## profvis 0.3.8 2023-05-02 [1] RSPM (R 4.3.0)  
## promises 1.2.1 2023-08-10 [1] RSPM (R 4.3.0)  
## purrr 1.0.2 2023-08-10 [1] RSPM (R 4.3.0)  
## R6 2.5.1 2021-08-19 [1] RSPM (R 4.3.0)  
## Rcpp 1.0.12 2024-01-09 [1] RSPM (R 4.3.0)  
## remotes 2.4.2.1 2023-07-18 [1] RSPM (R 4.3.0)  
## rlang 1.1.4 2024-06-04 [1] CRAN (R 4.3.2)  
## rmarkdown 2.27.1 2024-06-11 [1] Github (rstudio/rmarkdown@e1c93a9)  
## sessioninfo 1.2.2 2021-12-06 [1] RSPM (R 4.3.0)  
## shiny 1.8.0 2023-11-17 [1] RSPM (R 4.3.0)  
## stringi 1.8.3 2023-12-11 [1] RSPM (R 4.3.0)  
## stringr 1.5.1 2023-11-14 [1] RSPM (R 4.3.0)  
## urlchecker 1.0.1 2021-11-30 [1] RSPM (R 4.3.0)  
## usethis 2.2.3 2024-02-19 [1] RSPM (R 4.3.0)  
## vctrs 0.6.5 2023-12-01 [1] RSPM (R 4.3.0)  
## xfun 0.44.4 2024-06-11 [1] Github (yihui/xfun@9da62cc)  
## xtable 1.8-4 2019-04-21 [1] RSPM (R 4.3.0)  
## yaml 2.3.8 2023-12-11 [1] RSPM (R 4.3.0)  
##   
## [1] /usr/local/lib/R/site-library  
## [2] /usr/local/lib/R/library  
##   
## ──────────────────────────────────────────────────────────────────────────────

# 3 References