Get Your Laptop Ready for the Workshop on

Big Data Machine Learning Methods for Metabolomics

June 20, 2022

The hands-on session in this workshop will use **RStudio** and **R** (as well as some **R** packages), which are publicly available. Please follow the instructions stated in the below to install **R**, **RStudio**, and **R** packages into your laptops. Here is a list of softwares and packages to be installed in order,

- **R** available at <`https://cran.r-project.org/`>;
- **RStudio** available at <`https://www.rstudio.com/products/rstudio/`>;
- **R packages** `caret`, `dplyr`, `Matrix`, `missRanger`, `POCRE`, `ROCR`, `SIS`, `splitTools`, `xgboost`;
- **R** package `mixOmics` installed following the instruction at <`http://mixomics.org/install/`>.

1 Install R

1.1 Install R in Windows

1. Go to the website <`https://cran.r-project.org/`>;
2. Click "Download R for Windows";
3. Click "base" or " install R for the first time";
4. Click "Download R 4.2.0 for Windows";
5. Run the "R-4.2.0-win.exe" file;
6. Select "English", then click "Next", "Next", "Next", and read the "GNU GENERAL PUBLIC LICENSE";
7. Click "Next", "Next", "Next", "Next", "Next", and it begins to install R;
8. Click "Finish", and you will see an icon "R 4.2.0" on your desktop;
9. You can delete "R-4.2.0-win.exe" from your computer.

1.2 Install R in MacOS

1. Go to the website <`https://cran.r-project.org/`>;
2. Click "Download R for macOs";
3. Open and run the "R-4.2.0.pkg" file ;
4. Click "continue", "continue", "continue", and "agree";
5. Click "continue and "install";
6. Enter mac computer password in the pop up window;
7. Click on "Install Software", and it begins to install RStudio;
8. Click "close";
9. You can delete "R-4.2.0.pkg" from your computer.

2 Install RStudio

2.1 Install RStudio in Windows

Once R is installed, you can proceed to install **RStudio** to have a greatly improved environment to work with **R**.

1. Go to the website <`https://www.rstudio.com/products/rstudio/`>;
2. Click "DOWNLOAD RSTUDIO DESKTOP";
3. Click on the link for the windows version of **RStudio**;
4. Run the " RStudio-2022.02.3-492.exe" file;
5. Click "Next", "Next", "Install", and it begins to install **RStudio**;
6. Click "Finish", and you will see an icon "RStudio" on your desktop;
7. You can delete " RStudio-2022.02.3-492.exe" from your computer.

2.2 Install RStudio in MacOS

Once **R** is installed, you can proceed to install **RStudio** to have a greatly improved environment to work with **R**.

1. Go to the website <`https://www.rstudio.com/products/rstudio/`>;
2. Click "DOWNLOAD RSTUDIO FOR MAC";
3. Open and Run the "RStudio-2022.02.3-492.dmg" file;

4. Drag(copy) **RStudio** to Applications file;
5. Go to "Launchpad" to open Rstudio;
6. You can delete " RStudio-2022.02.3-492.dmg" from your computer.

3 Install Packages in R

There are two ways to install **R** packages. Here is the first way:

1. Launch **R** and type **install.packages("package_name")** in the **R** console. package_name is the actual name of the package you want to install;
2. In the "CRAN mirror" pop-up window (you will see this window if this is your first time to install a package), select a Mirror for the installation. You may choose a mirror which is closer to your geographic location (or whichever you would like);

Here is the second way:

1. Go to **R**, click "Packages", then click "Install package(s)...";
2. In the "CRAN mirror" pop-up window (you will see this window if this is your first time to install a package), select a Mirror for the installation. You may choose a mirror which is closer to your geographic location (or whichever you would like);
3. In the "Packages" pop-up window, select "package_name" and click "OK", "Yes", package_name is the actual name of the package you want to install;

Caution: You may not see the "CRAN mirror" pop-up window if you have installed some other packages before (so the CRAN mirror has already selected).

4 Install R Package mixOmics

Please visit <`http://mixomics.org/install/`>, and follow the instruction there to install the package `mixOmics`.

5 Setting Working Directory and Checking Packages

Once you launch **RStudio** you can set up your working directory by the following commands:

```
setwd ("my_dir")}
```

where `my_dir` is the path to your directory. You can also directly work through the menu `Session` of **RStudio** to set up your working directory:

`Session` → `Set Working Directory` → `Choose Directory`

You can test whether you have successfully install the **R** packages by running the following command:

```
library(my_package)
```

where `my_package` is replaced by the package you want to test. For example, you can run

```
library(POCRE)
```

If the package is not installed, RStudio will throw the following message:

```
Error in library(POCRE): there is no package called 'POCRE'.
```