Reprocessing Selevsek Data With Skyline Batch

This tutorial covers how to use Skyline Batch to import and run five configurations using the Selevsek 2015 data.

If you have not already downloaded Skyline, Skyline Batch, the Skyline Batch configuration file (Selevsek.bcfg), and the R script (install_R_packages.R), you can find and download them here:

https://panoramaweb.org/dia-selevsek15.url

Setting Up R

Check if you have a "C:\Program Files\R\ R-4.0.3" folder. If you do not, go to:

Index of /bin/windows/base/old/4.0.3 (r-project.org)

*Note: You can use an R-4.0.3 installation located somewhere else on your computer. However, you will have to add your R directory to Skyline Batch.

Install R-4.0.3 from the R-4.0.3-win.exe link. When it is done downloading, the setup installer will open.

- Click the **Next** button until you see a green Installing progress bar.
- Click the **Finish** button.

Go to the Rtools website:

Building R for Windows (r-project.org)

- Click on "Rtools35.exe" to begin downloading the correct version of Rtools.
- Click the **Next** button until you reach **Install** to accept the default settings.
- Click the **Install** button.
- Click the **Finish** button.

If you do not have Rstudio, download it here:

Download the RStudio IDE – Rstudio

- Install it, accepting the default settings.
- Open RStudio.
- Go to **Tools** and click **Global Options**.
- Select the **General** tab on the left-hand side.
- Check if **R version** is showing R-4.0.3
 - If it is:
 - Click OK
 - If it is not:

- Click Change
- Select **R-4.0.3**
- Click **OK** twice
- Restart RStudio

You are now ready to start downloading packages in R-4.0.3

- In RStudio, click **File** > **Open File**
- Navigate to your downloads folder and double-click on "install_R_packages.R" to open it.
- Select line 2, then click the **Run** toolbar button. (Ctrl-Enter)

You should see this output if the download was successful:

package 'gplots' successfully unpacked and MD5 sums checked package 'dplyr' successfully unpacked and MD5 sums checked

• Select lines 4-5, then click the **Run** toolbar button. (Ctrl-Enter)

You should see this output if the download was successful:

package 'BiocManager' successfully unpacked and MD5 sums checked package 'MSstats' successfully unpacked and MD5 sums checked

Opening Configurations

• Navigate to your Downloads folder and double-click on "Selevsek.bcfg" to open it.

This will open Skyline Batch and start importing the configurations. You will see a dialog asking for a root folder:

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Configuration		Modified	Status	Start Time	Run Time		Add	
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	🏦 Open Co	onfigurations				×	Share	
	Preparing to	import configurations	from Selevsek.b	cfg		-		
		ify a root folder for the limarsh\Downloads	configurations:					
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		-	configurations:	ОК	Cance	4		
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		-	configurations:	OK	Cance	4		

- Click the folder explorer (...) button and create a "Selevsek" folder on a drive with at least 134GB of free space.
- Click **OK**.

This will save the configuration file inside the Selevsek folder and import the configurations. You will see the imported configurations in the configuration list:

Skyline Batch 21.1.0.312					-		2
nfigurations Log							
aved configurations:							
Configuration Selevsek-reps Selevsek-lowcv Selevsek-all Selevsek-lowcv (MSstats) Selevsek-all (MSstats)	Modified 11/7/2021 11/7/2021 11/7/2021 11/7/2021 11/7/2021	Status	Start Time	Run Time]]]]]]]]]]]]]]]]]]]	Add Edit Copy Import Share	

Running the Configurations

The first three configurations are checked, meaning they will be run when the run button is clicked.

• Click the **Run All Steps** button.

Skyline Batch brings you to the **Log** tab to show the output of running the configurations. It will download files, import data, and export reports for all three configurations.

When the configuration has finished running, it will display a **Completed** status in the main window. Wait until the Skyline Batch run has completed.

To run the MSstats processing, we can run the MSstats configurations from the "R scripts only" step.

- Uncheck all the configurations.
- Check the (MSstats) configurations.

The configurations should now look like this:

Configuration
Selevsek-reps
Selevsek-lowcv
Selevsek-all
Selevsek-lowcv (MSstats)
Selevsek-all (MSstats)

• Click the downward arrow next to Run all steps to expand the run options



• Click **R** scripts only.

This will run the MSstats scripts for Selevsek-all (MSstats) and Selevsek-lowcv (MSstats).

When the Skyline Batch has finished running, view the output files by clicking on a configuration to select it, and using the following buttons:

- Opens the Skyline template document
- Dens the Skyline results document
- Copens the analysis folder

If you want to learn more about Skyline Batch, visit the documentation at:

SkylineBatchDocumentation.pdf