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PROJECTS' WORKFLOW FOR REPRODUCIBILITY AND REPLICABILITY USING R

PART 2 – COMPUTATIONAL REPRODUCIBILITY

Second Rostock Open Science Workshop, MPIDR, Rostock 17-18 March 2025

Egor Kotov & Jonas Schöley







Reproducible analysis workflow





Reproducible analysis workflow



Complete computational environment











upytei



You are here

Lock R packages and specific versions



Reproducible analysis workflow



Complete computational environment









OS /users/u1/R/library (user installed R pkgs) /users/u1/R/library (base R packages)



/users/u1/projects/01/ (ordinary R project) /users/u1/R/library (user installed R pkgs)

Logos by respective copyright holders



























/bin/R/library (base R packages)



package installation

^{mac}

OS



















You are here

Lock R packages and specific versions



Reproducible analysis workflow

targets

Complete computational environment Uocker. SINGULARITYCE PPTAINER R Studio



tar_target(mtcars_data, mtcars),

```
tar_target(mpg_mean,
    mean(mtcars_data$mpg)),
```

tar_target(plot_mpg,
 ggplot2::qplot(mpg,data=mtcars_data))







```
library(targets)
tar dir({
tar script({
 library(targets)
 list(
   tar target(mtcars data,
     mtcars),
   tar target(mpg mean,
     mean(mtcars data$mpg)),
   tar target(plot mpg,
      ggplot2::qplot(mpg,data=mtcars data))
   ) }, ask = FALSE)
   tar visnetwork()
```





```
)}, ask = FALSE)
tar_visnetwork()
```





)}, ask = FALSE) tar_visnetwork()









```
)}, ask = FALSE)
tar_visnetwork()
```











targets: PROJECT STRUCTURE

library(targets)

```
list(
   tar_target(output1,
     function_1()),
```

```
tar_target(output2,
   function 2(input1 = output1)),
```

```
tar_target(output3,
   function_3(input1 = output1,
        input 2 = output2) ),
```



targets: PROJECT STRUCTURE

```
library(targets)
list(
  tar target(output1,
     function 1() ),
  tar target (output2,
     function 2(input1 = output1) ),
  tar target(output3,
     function 3(input1 = output1,
        input 2 = output2) ),
```

/rpoject01 - targets.R - R/ -01 scripts.R -02 scripts.R - . . . - targets/ - objects/



targets: PROJECT STRUCTURE library(targets) /rpoject01 - targets.R list(tar target (output1, - R/ function 1()), -01 scripts.R -02 scripts.R tar target (output2, function 2 (input1 = output1) - targets/ tar target (output3 - objects/ function 3(input1 = output1, input 2 = output(2)),



/rpoject01

targets: PROJECT STRUCTURE

library(targets)

ist(- targets.R
tar_target(output1,	$-\overline{R}/$
function_1()),	-01_scripts.R
tar_target(output2,	-02 scripts.R
$function_2(input1 = output1)),$	
<pre>tar_target(output3,</pre>	targets/
$function_3(input1 = output1,$	
input 2 = output2)),	



targets: COMPLEX WORKFLOW EXAMPLE





containers: ENVIRONMENT PRESERVATION

You are here


Accepted

40% OF ALL PACKAGES EVER IN CRAN GOT AT ONE POINT **ARCHIVED**

Times a package has been archived



40% OF ALL PACKAGES EVER IN CRAN GOT AT ONE POINT **ARCHIVED**



Times a package has been archived



Source: https://www.cranhaven.org/cran-archiving-stats.htm



renv: PACKAGE VERSION CONTROL

/bin/R/library (base R packages)

/users/**USER3**/projects/02/renv/library renv::restore() install required /users/USER3/home/.cache/renv/ package versions ...which is not always possible

ConsoleTerminal ×Background Jobs ×R A4.0 · ~/ > Sys.time(); remotes::install_version("comrades00"); Sys.time()[1] "2024-06-17 23:28:52 CEST"Downloading package from url: https://ftp.gwdg.de/pub/misc/cran//src/contrib/Archive/comradesoo/comradesoo_0.1.1.tar.gzThese packages have more recent versions available.It is recommended to update all of them.Which would you like to update?

remotes::install_version()

```
Console Terminal × Background Jobs ×
                                                                                          F
(R 4.4.0 · ~/ ∼∕
> Sys.time() ; remotes::install_version("comrades00") ; Sys.time()
[1] "2024-06-17 23:28:52 CEST"
Downloading package from url: https://ftp.gwdg.de/pub/misc/cran//src/contrib/Archive/c
omrades00/comrades00_0.1.1.tar.gz
These packages have more recent versions available.
It is recommended to update all of them.
which would you like to update?
 1: A]]
 2: CRAN packages only
 3: None
 4: rlang
                (1.1.3 \rightarrow 1.1.4) [CRAN]
 5: fastmap
             (1.1.1 \rightarrow 1.2.0) [CRAN]
            (1.0.8 \rightarrow 1.1.0) [CRAN]
 6: cachem
 7: xfun
                (0.44 \rightarrow 0.45) [CRAN]
 8: highr (0.10 -> 0.11 ) [CRAN]
9: evaluate (0.23 -> 0.24.0) [CRAN]
10: knitr
                (1.46 \rightarrow 1.47) [CRAN]
11: textshaping (0.3.7 \rightarrow 0.4.0) [CRAN]
12: DBI
                (1.2.2 -> 1.2.3 ) [CRAN]
Enter one or more numbers, or an empty line to skip updates: 3
```

Installing 11 packages: crosstalk, reshape2, foreach, plotly, ade4, TopDom, heatmap3, igraph, doParallel, mixtools, seqinr

```
Console Terminal × Background Jobs ×
                                                                                         P
R 4.4.0 · ~/ ~
> Sys.time() ; remotes::install_version("comrades00") ; Sys.time()
[1] "2024-06-17 23:28:52 CEST"
Downloading package from url: https://ftp.gwdg.de/pub/misc/cran//src/contrib/Archive/c
omrades00/comrades00_0.1.1.tar.gz
These packages have more recent versions available.
It is recommended to update all of them.
which would you like to update?
 1: A]]
 2: CRAN packages only
 3: None
 4: rlang
                (1.1.3 \rightarrow 1.1.4) [CRAN]
 5: fastmap
             (1.1.1 \rightarrow 1.2.0) [CRAN]
               (1.0.8 \rightarrow 1.1.0) [CRAN]
 6: cachem
 7: xfun
                (0.44 \rightarrow 0.45) [CRAN]
 8: highr (0.10 -> 0.11 ) [CRAN]
 9: evaluate (0.23 -> 0.24.0) [CRAN]
10: knitr
                (1.46 \rightarrow 1.47) [CRAN]
11: textshaping (0.3.7 \rightarrow 0.4.0) [CRAN]
12: DBI
                (1.2.2 \rightarrow 1.2.3) [CRAN]
Enter one or more numbers, or an empty line to skip updates: 3
Installing 11 packages: crosstalk, reshape2, foreach, plotly, ade4, TopDom, heatmap3,
igraph, doParallel, mixtools, seginr
Installing packages into 'C:/Users/kotov/AppData/Local/R/win-library/4.4'
(as 'lib' is unspecified)
trying URL 'https://ftp.gwdg.de/pub/misc/cran/src/contrib/crosstalk_1.2.1.tar.gz'
Content type 'application/octet-stream' length 297970 bytes (290 KB)
downloaded 290 KB
trving URL 'https://ftp.gwdg.de/pub/misc/cran/src/contrib/reshape2 1.4.4.tar.gz'
```



2.5 hours later of building from source the package is **NOT installed**



Installing archived packages and their dependencies using remotes::install_version()



Installing archived packages and their dependencies using remotes::install_version()

Running R (or Python) in **containers**

CONTAINERS FOR MORE CONSISTENT WORKFLOW



Image generated by Microsoft Image Creator powered by DALL-E 3

Kotov, E., and Denecke, E. (2024). Expanding the Lifespan of Software for Demographic Analysis with Containers: An Application of Spatial Sampling. The Denominator, Population Dynamics Lab. https://doi.org/10.6069/WY8K-D973







Hey, I want to run your code!





Hey, I want to run your code!



Sure, I'll send you my laptop #45 via DHL. Just give me a week to find which one it is.





Project_1_OS+Rstudio+R+Packages.zip

Image by DALL-E







WHAT ARE CONTAINERS? R Studio julia 🗬 **?** python ^{mac} jupyte ZIP R Studio julia 🗬 epython" ^{mac} jupyter

Logos by respective copyright holders



WHAT ARE CONTAINERS? R Studio julia 😱 **е**python™ ^{mac} jupyte ١, That would take a lot of time... ZIP R Studio julia 😱 **е**python™ ^{mac} jupytei

Logos by respective copyright holders





Ubuntu operating system (or another Linux)







R Studio RStudio or any other code editor



R or any other analytics software

Ubuntu operating system (or another Linux)







SOFTWARE TO BUILD AND RUN CONTAINERS



- Most popular, widely known
- Windows/macOS/Linux
- Many compatible alternative software



SOFTWARE TO BUILD AND RUN CONTAINERS



- Most popular, widely known
- Windows/macOS/Linux
- Many compatible alternative software

- Often used in academic HPCs
- Mostly Linux
- Can import Docker containers





SOFTWARE TO BUILD AND RUN CONTAINERS



- Most popular, widely known
- Windows/macOS/Linux
- Many compatible alternative software

- Often used in academic HPCs
- Mostly Linux
- Can import Docker containers





- Run small containers (1-2 GB memory)
- In the cloud, for free
- Based on Docker

RUNNING ANALYSIS IN A CONTAINER @ MYBINDER.ORG



Github-en	ioloxi@ro.sampii x +		
→ C II https	://github.com/e-kotov/grid-sample-containerized?tab=readme-ov-file	역 ☆ 🔲 🖨 incognit	
🖽 README 🕀	MIT license :=	No releases published	
Expand	ing Lifespan of Software for	Packages	
Demog	raphic Analysis with Containers: A Case	No packages published	
for a Sa	mpling Technique		
This repository with application	contains files for the article about using containers for reproducible research		
Files desc	ription		
File	Description		
Dockerfile	This text file defines which container image Binder needs to launch.		
install.R	This R script contains lines to install packages required for the analysis.		
main.Rmd	This is the file with the example code we will run inside the container once it is launched		

Kotov, E., and Denecke, E. (2024). Expanding the Lifespan of Software for Demographic Analysis with Containers: An Application of Spatial Sampling. The Denominator,

Population Dynamics Lab. https://doi.org/10.6069/WY8K-D973 || repo https://github.com/Population-Dynamics-Lab/grid-sample-containerized

RUNNING ANALYSIS IN A CONTAINER @ MYBINDER.ORG



😑 😑 🌒 🦷 GitHub - e-kotov/demogra	aphi × +			~
C S https://github.com/e	e-kotov/demographic-research.44-19-c	ontainerized?tab=readme-ov-file		I I 🔮 🗖 🕶 =
Product ~ Solutions ~	Resources 🗸 Open Source 🗸 E	Enterprise 🗸 Pricing		Q Sign in Sign up
🛱 e-kotov / demographic-r	research.44-19-containerize	d Public	¢	Notifications
<> Code ⊙ Issues \$\$ Pull r	requests 🕞 Actions 🖽 Projects	🛈 Security 🗠 Insights		
양 main - 양 1 Branch ⓒ 0	Tags	Q Go to file	<> Code +	About
🔵 e-kotov update regarding con	tainers preservation	ebaae7b · 3 days	ago 🕚 3 Commits	 ♂ doi.org/10.5281/zenodo.15024144 □ Readme
Dockerfile4build	commit all files, initia	al try	4 days ago	∽ Activity
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ata data	commit all files, initia	al try	4 days ago	양 0 forks
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nenv 🔁	commit all files, initia	al try	4 days ago	containerized
C .Rhistory	commit all files, initia	al try	4 days ago	Languages

Schöley, J., 2021. The centered ternary balance scheme: A technique to visualize surfaces of unbalanced three-part compositions. Demographic Research 44, 443–458.

https://doi.org/10.4054/DemRes.2021.44.19

Repo link: https://github.com/e-kotov/demographic-research.44-19-containerized

PRESERVING THE COMPUTATIONAL ENVIRONMENT

GitHub - e-kotov/demogra	aphi × +			~	
< > C % https://github.com/	e-kotov/demographic-research.44-19-containeriz	ed?tab=readme-ov-file		E 💖 🗖 🕶 =	
Product ~ Solutions ~	Resources V Open Source V Enterprise	e ~ Pricing		Q Sign in Sign up	
📮 e-kotov / demographic- ı	research.44-19-containerized Public		Ţ	Notifications	
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양 main 👻 양 1 Branch 📀 0	Tags	Q Go to file	<> Code -	About	
e-kotov update regarding con	tainers preservation	ebaae7b · 3 days ag	o 🕓 3 Commits	doi.org/10.5281/zenodo.15024144 Readme	
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Code	commit all files, initial try		4 days ago	☆ 0 stars	
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📄 media	update regarding containers p	reservation	3 days ago	Packages 1	
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renv	commit all files, initial try		4 days ago	containerized	
.Rhistory	commit all files, initial try		4 days ago	Languages	

Schöley, J., 2021. The centered ternary balance scheme: A technique to visualize surfaces of unbalanced three-part compositions. Demographic Research 44, 443–458. https://doi.org/10.4054/DemRes.2021.44.19

Repo link: https://github.com/e-kotov/demographic-research.44-19-containerized

PRESERVING THE COMPUTATIONAL ENVIRONMENT

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	Zenodo	•
	Planned intervention: On Tuesday March 18th 06:30 UTC Zenodo will be unavailable for 10-20 minutes to perform a storage cluster upgrade.	1
	Published March 14, 2025 Version v0.1	
	Docker and Apptainer container images for Schöley, J., 2021, Demographic Research 44, 443–458	
	Kotov, Egor (Producer) ¹ (b); Schöley, Jonas (Project leader) ¹ (b) Show affiliations	
	This repository contains R+RStudio computational environment preserved in Docker and Apptainer container images to reproduce the code in Schöley, J., 2021. The centered ternary balance scheme: A technique to visualize surfaces of unbalanced three-part compositions. Demographic Research 44, 443–458. https://doi.org/10.4054/DemRes.2021.44.19. These containerized environments contain all R package and system level dependencies required to reproduce the code and do not rely on any external online repositories to install anytning else at runtime.	
	The Docker image is also hosted in the GitHub Container registry at https://github.com/e-kotov/demographic-research.44-19-containerized/pkgs/container/demographic-research.44-19-containerized and the live preview in a web browser can be launched from the repository at https://github.com/e-kotov/demographic-research.44-19-	

Schöley, J., 2021. The centered ternary balance scheme: A technique to visualize surfaces of unbalanced three-part compositions. Demographic Research 44, 443–458. https://doi.org/10.4054/DemRes.2021.44.19 Repo link: https://github.com/e-kotov/demographic-research.44-19-containerized

PRESERVING THE COMPUTATIONAL ENVIRONMENT



Schöley, J., 2021. The centered ternary balance scheme: A technique to visualize surfaces of unbalanced three-part compositions. Demographic Research 44, 443–458. https://doi.org/10.4054/DemRes.2021.44.19

Repo link: https://github.com/e-kotov/demographic-research.44-19-containerized ; Logos by respective copyright holders

WITH CONTAINERS YOU ARE FREE TO RUN ANY SOFTWARE, NO NEED TO BOTHER YOUR IT





Image from The I.T Crowd C4 TV Show

For the record, this is not in any way representative of the IT team at MPIDR or GWDG HPC



WHERE TO GET CONTAINERS?

data science containers python jupyter



Icons and search bar by Google, but feel free to use other search engines



WHERE TO GET CONTAINERS?





WHERE TO GET CONTAINERS?





Vanilla R

- NUCKEI FTUJECC

The Rocker Project

Docker Containers for the R Environment

Getting Started

Home	Code of Conduct	Images 👻
The Rocker Ima	ages	_
VERSIONED STA	ск	
r-ver		
rstudio, tidyver	se, verse, geospatial	
binder		
shiny, shiny-ve	rse	
cuda, ml, ml-ve	rse	
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r-devel, drd, drp, r-devel-san, r-devel-ubsan-clang		
ADDITIONAL IM	AGES	






WHERE TO GET CONTAINERS?





















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kotov@demogr.mpg.de

Jonas Schöley

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