PROGRAMA DE PÓS-GRADUAÇÃO EM INFORMÁTICA
UNIVERSIDADE FEDERAL DO RIO DE JANEIRO

Introduction to Data Science

MODULE I – PART 3

REPRODUCIBILITY IN PYTHON

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Reproducible Experiment in CS

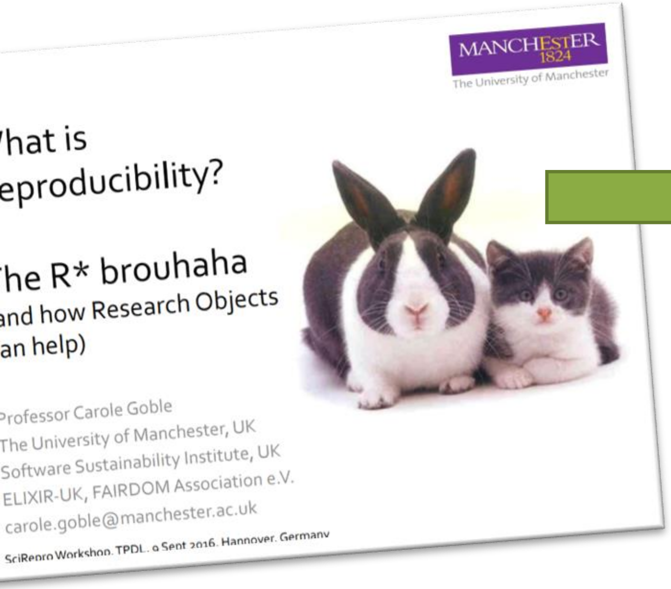
"An experiment composed by a sequence of steps **S** that has been developed at time **T**, on environment (hardware and OS) **E**, and on data **D** ***is reproducible if*** it can be executed with a sequence of steps **S'** (different or the same as S) at time **T' > T,** on environment **E'** (different or the same as E), and on data **D'** (different or the same as D) with **consistent results** (R and R' consistent)".

This definition includes both **exact reproducibility (repeatability)** and **approximate reproducibility**

- **Exact Reproducibility** requires reproducing the exact same result
  - $S' = S$ and $E' = E$ and $D' = D \Rightarrow \mathbf{R = R'}$
- **Approximate Reproducibility** involves producing similar results as the original ones
  - $S' \neq S$ or $E' \neq E$ or $D' \neq D \Rightarrow \mathbf{R \sim R'}$

FREIRE, J.; CHIRIGATI, F. Provenance and the Different Flavors of Computational Reproducibility. IEEE Data Engineering Bulletin. V. 41:15-26, 2018.

1P5R



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The University of Manchester
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eproducibility?
'he R* brouhaha
and how Research Objects
an help)
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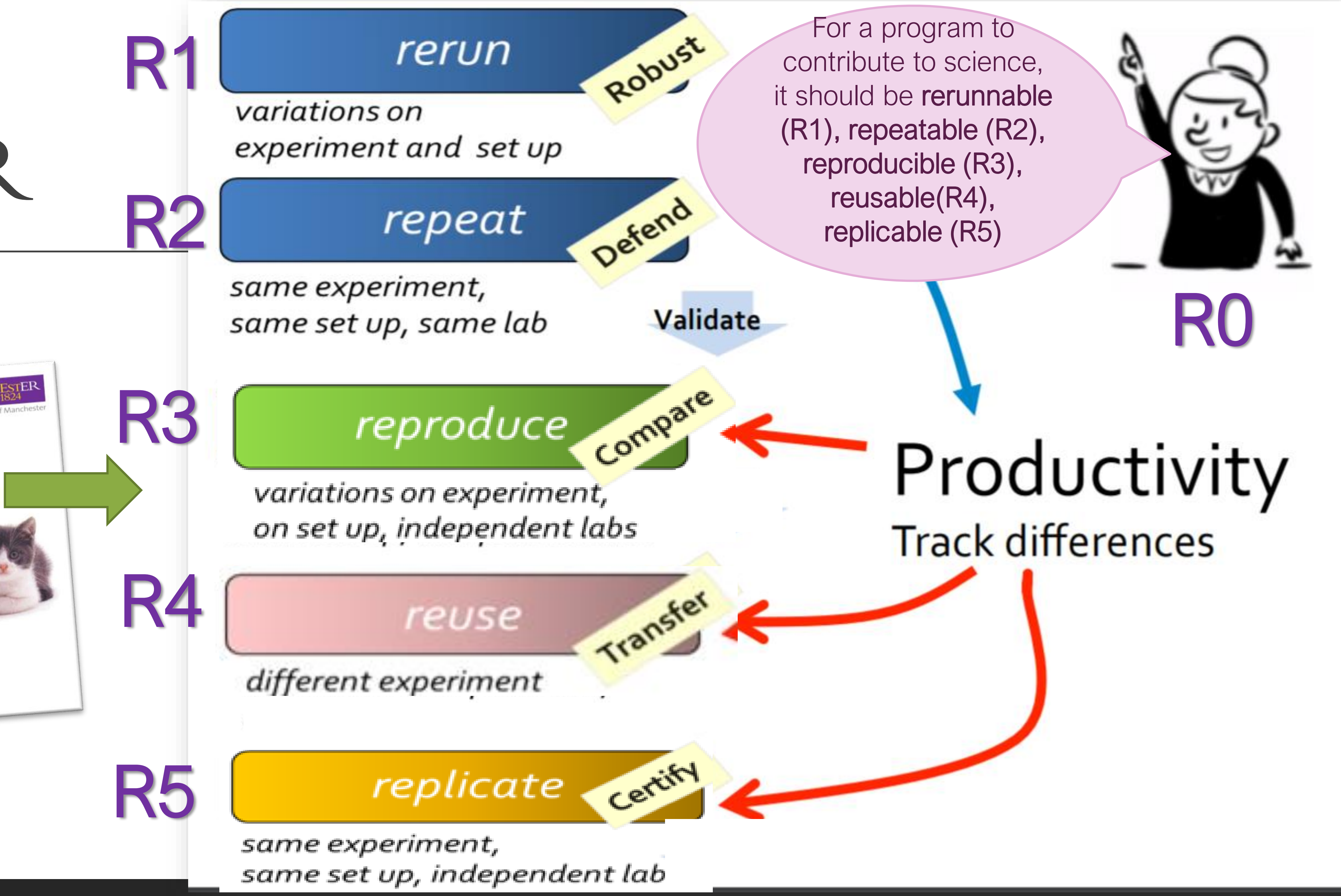


R1
rerun
Robust
variations on
experiment and set up
R2
repeat
Defend
same experiment,
same set up, same lab
Validate
R3
reproduce
Compare
variations on experiment,
on set up, independent labs
R4
reuse
Transfer
different experiment
R5
replicate
Certify
same experiment,
same set up, independent lab
For a program to contribute to science, it should be rerunnable (R1), repeatable (R2), reproducible (R3), reusable(R4), replicable (R5)
R0
Productivity
Track differences

R0 – Random Walk

Environment info is unknown. Does it work on any Python version?

```
In [23]:  # Random walk (R0: worst you can do)
          import random

          x = 0
          for i in xrange(10):
              step = random.choice([-1,+1])
              x += step
              print x,

---------------------------------------------------------------------------
NameError                                 Traceback (most recent call last)
<ipython-input-23-ff098a3b5866> in <module>
      3
      4 x = 0
----> 5 for i in xrange(10):
      6     step = random.choice([-1,+1])
      7     x += step

NameError: name 'xrange' is not defined
```

Python 2

```
In [21]:  # Random walk (R0: worst you can do)
          import random

          x = 0
          for i in range(10):
              step = random.choice([-1,+1])
              x += step
              print (x),

-1
0
1
2
1
2
3
2
1
0
```

Python 3

Benureau, F., Rougier, (2018) N. Re-run, Repeat, Reproduce, Reuse, Replicate: Transforming Code into Scientific Contributions. Frontiers in Neuroinformatics. V.11, article 69.

R1 – Re-runnable

Environment Info. Scientist is responsible for keeping this info!

```
In [25]:
# Random walk (R1: re-runnable)
# Tested with Python 3
import random

x =  0
walk = []
for i in range(10):
    step = random.choice([-1,+1])
    x += step
    walk.append(x)

print(walk)
```

```
[1, 0, -1, 0, -1, -2, -3, -2, -1, 0]
```

Re-runnable code should describe—with enough details to be recreated—an execution environment in which it is executable.
It is far from being either obvious or easy.

R2 - Repeatable

In [30]:

```
# Random walk (R2: repeatable)
# Tested with Python 3
import random

random.seed(1) # RNG initialization

x =  0
walk = []
for i in range(10):
    step = random.choice([-1,+1])
    x += step
    walk.append(x)

print(walk)
# Saving output to disk
with open('results-R2.txt', 'w') as fd:
    fd.write(str(walk))
```

```
[-1, -2, -1, -2, -1, 0, 1, 2, 1, 0]
```

A repeatable code is one that can be rerun and that produces the same result on successive runs

- Program needs to be **deterministic**
- Control **the initialization of pseudo-random** number generators

Previous results need to be available (it is possible to compare with current results)

- S'= S and E'~ E and D'= D and R = R'

R2 - Repeatable

```
In [30]:
# Random walk (R2: repeatable)
# Tested with Python 3
import random

random.seed(1) # RNG initialization

x =  0
walk = []
for i in range(10):
    step = random.choice([-1,+1])
    x += step
    walk.append(x)

print(walk)
# Saving output to disk
with open('results-R2.txt', 'w') as fd:
    fd.write(str(walk))
```

```
[-1, -2, -1, -2, -1, 0, 1, 2, 1, 0]
```

initialization of Randon Seed!

- Verifying the qualitative aspects of the results and the conclusions that are made are not tied to a specific initialization of the pseudo-random generator is an integral part of any scientific undertaking in computational Science

- This is usually done by repeating the simulations multiple times with different seeds

Due to a **change** that occurred in the **pseudo-random number generator** between Python 3.2 and Python 3.3, executing this code in Python 3.3 **WILL NOT** generate the same results when compared to the Python 3.2 execution.

R2 - Repeatable

```
In [30]:
# Random walk (R2: repeatable)
# Tested with Python 3
import random

random.seed(1) # RNG initialization

x =  0
walk = []
for i in range(10):
    step = random.choice([-1,+1])
    x += step
    walk.append(x)

print(walk)
# Saving output to disk
with open('results-R2.txt', 'w') as fd:
    fd.write(str(walk))
```

```
[-1, -2, -1, -2, -1, 0, 1, 2, 1, 0]
```

Repeatable Random Walk Example is not reproducible!

- Executed with **Python 2.7–3.2**, the code will produce the sequence

  −1, 0, 1, 0, −1, −2, −1, 0, −1, −2

- But with **Python 3.3–3.6**, it will produce

  −1, −2, −1, −2, −1, 0, 1, 2, 1, 0

- **With future versions of the language, it may change still**

R2 - Repeatable

Repeatable Random Walk Example is not reproducible!

```
In [30]:
# Random walk (R2: repeatable)
# Tested with Python 3
import random

random.seed(1) # RNG initialization

x =  0
walk = []
for i in range(10):
    step = random.choice([-1,+1])
    x += step
    walk.append(x)

print(walk)
# Saving output to disk
with open('results-R2.txt', 'w') as fd:
    fd.write(str(walk))
```

```
[-1, -2, -1, -2, -1, 0, 1, 2, 1, 0]
```

Save output to allow comparing different runs

R3 – Reproducible

Use notepad to keep track of code versions

Test for reproducibility

Record environment
with output data

```
In [43]: # Copyright (c) 2017 N.P. Rougier and F.C.Y. Benureau
         # Adapted by Serra
         # Release under the Windows 10
         # Tested with 64 bit (AMD64)
         import sys, subprocess, datetime, random

         def compute_walk():
             x = 0
             walk = []
             for i in range(10):
                 if random.uniform(-1, +1) > 0:
                     x += 1
                 else:
                     x -= 1
                 walk.append(x)
             return walk

         # If repository is dirty, don't run anything
         if subprocess.call(("notepad", "diff-index",
                             "--quiet", "HEAD")):
             print("Repository is dirty, please commit first")
             sys.exit(1)

         # Get git hash if any
         hash_cmd = ("notepad", "rev-parse", "HEAD")
         revision = subprocess.check_output(hash_cmd)

         # Unit test
         random.seed(42)
         assert compute_walk() == [1,0,-1,-2,-1,0,1,0,-1,-2]

         # Random walk for 10 steps
         seed = 1
         random.seed(seed)
         walk = compute_walk()

         # Display & save results
         print(walk)
         results = {
             "data"     : walk,
             "seed"     : seed,
             "timestamp": str(datetime.datetime.utcnow()),
             "revision" : revision,
             "system"   : sys.version}
         with open("results-R3.txt", "w") as fd:
             fd.write(str(results))

[-1, 0, 1, 0, -1, -2, -1, 0, -1, -2]
```

R4 - Reusability

In [45]:

```
import sys, subprocess, datetime, random

def compute_walk(count, x0=0, step=1, seed=0):
    """Random walk
       count: number of steps
       x0   : initial position (default 0)
       step : step size (default 1)
       seed : seed for the initialization of the
         random generator (default 0)
    """
    random.seed(seed)
    x = x0
    walk = []
    for i in range(count):
        if random.uniform(-1, +1) > 0:
            x += 1
        else:
            x -= 1
        walk.append(x)
    return walk

def compute_results(count, x0=0, step=1, seed=0):
    """Compute a walk and return it with context"""
    # If repository is dirty, don't do anything
    if subprocess.call(("notepad", "diff-index",
                        "--quiet", "HEAD")):
        print("Repository is dirty, please commit")
        sys.exit(1)
```

```
    # Get git hash if any
    hash_cmd = ("notepad", "rev-parse", "HEAD")
    revision = subprocess.check_output(hash_cmd)

    # Compute results
    walk = compute_walk(count=count, x0=x0,
                        step=step, seed=seed)
    return {
        "data"       : walk,
        "parameters": {"count": count, "x0": x0,
                       "step": step, "seed": seed},
        "timestamp" : str(datetime.datetime.utcnow()),
        "revision"  : revision,
        "system"    : sys.version}

if __name__ == "__main__":
    # Unit test checking reproducibility
    # (will fail with Python<=3.2)
    assert (compute_walk(10, 0, 1, 42) ==
        [1,0,-1,-2,-1,0,1,0,-1,-2])

    # Simulation parameters
    count, x0, seed = 10, 0, 1
    results = compute_results(count, x0=x0, seed=seed)

    # Save & display results
    with open("results-R4.txt", "w") as fd:
        fd.write(str(results))
    print(results["data"])
```

```
[-1, 0, 1, 0, -1, -2, -1, 0, -1, -2]
```

R4 - Reusability

Making your program **reusable** means it can be **easily used**, and **modified**, by you and other people, **inside and outside your lab**

The easier it is to use your code, the lower the threshold is for other to study, modify and extend it

- This implies it should be **well documented**

Scientists constantly face the constraint of time

- if a model is **available, documented,** and can be installed, run, and **understood** all in a few hours, it will be preferred over another that would require weeks to reach the same stage

A **reproducible** and **reusable** code offers a platform both verifiable and easy-to-use, fostering the development of derivative works by other researchers on solid foundations •

Those derivative works **contribute to the impact of your original contribution (citations!!)**

R4 – Reusability - Tips

Avoid hardcoded or magic numbers

- **Magic numbers** are those present directly in the source code (no name, no semantics)
- **Hardcoded values** are variables that cannot be changed through an argument or a parameter configuration file
  - Example: R3 Random Walk, the seed is hardcoded, and the number of steps is a magic number

Code behavior should not be changed by commenting/uncommenting code

- Instead, it should be **explicitly set through parameters** that are accessible to the end user
- This improves reproducibility in two ways
  - it allows those conditions to be recorded as parameters in the result files, and
  - it allows to define separate scripts to run or configuration files to load to produce each of the figures of the published paper

R5 - Replicability

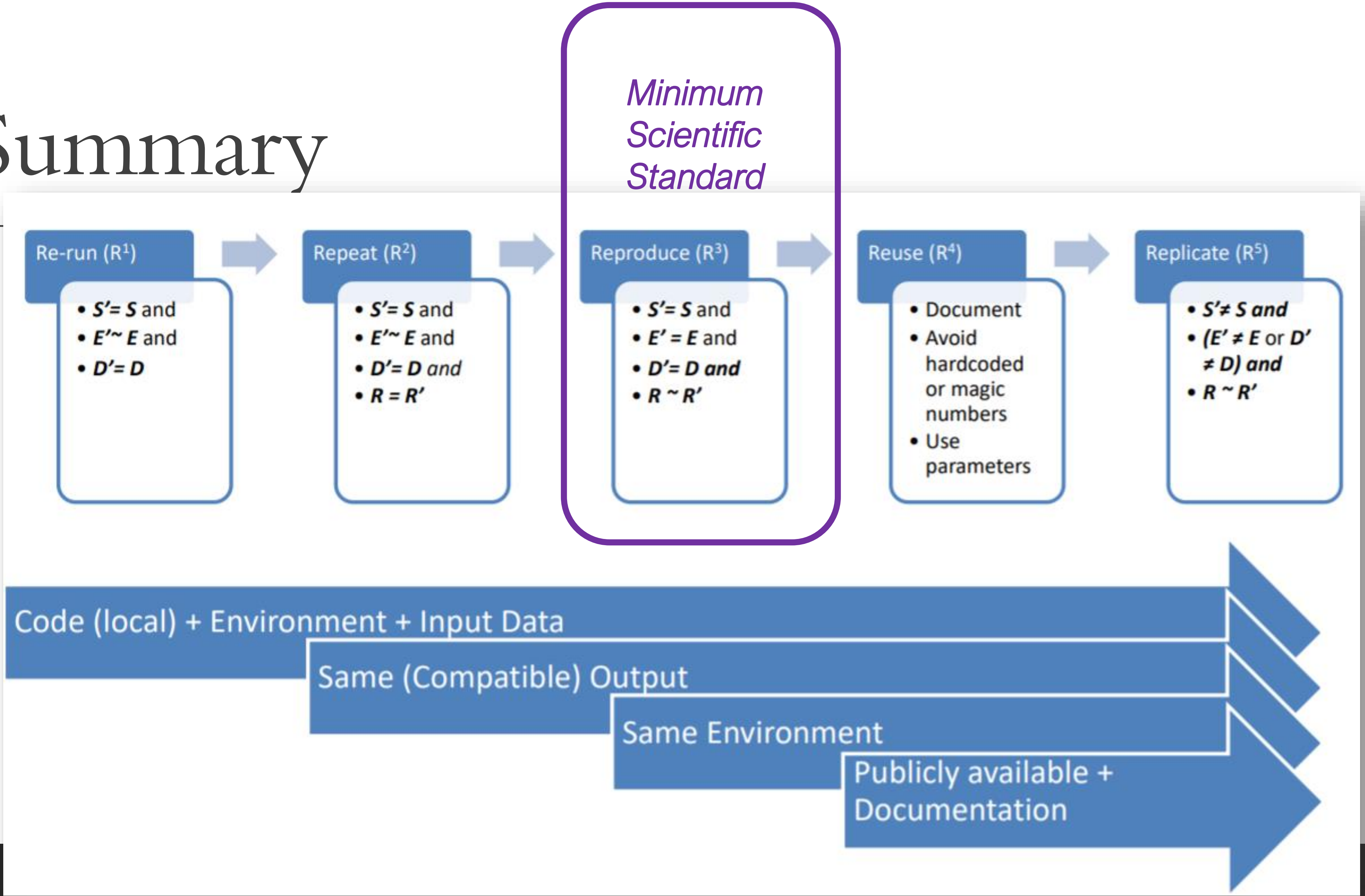
Replicating implies **writing a new code** matching the conceptual description of the article, in order to obtain the same **(compatible) results**

- S'≠ S and (E' ≠ E or D' ≠ D) ⇒ R ~ R'

Replication affords **robustness** to the results

- if the original code contain an error, a different codebase creates the possibility that this error will not be repeated
- Every paper is a mistake if a parameter is forgotten
- Replication efforts use the paper first, and then the reproducible code that comes along with it whenever the paper falls short of being precise enough

Summary



Braganholo, 2019

Introduction

Latest Release build passing coverage 90% Code Health wheel yes python 3.6 | 3.7 | 3.8 | 3.9 license MIT

A library for W3C Provenance Data Model supporting PROV-O (RDF), PROV-XML, PROV-JSON import/export

- Free software: MIT license
- Documentation: http://prov.readthedocs.io/.
- Python 3 only.

https://github.com/trungdong/prov

Features

- An implementation of the W3C PROV Data Model in Python.
- In-memory classes for PROV assertions, which can then be output as PROV-N
- Serialization and deserialization support: PROV-O (RDF), PROV-XML and PROV-JSON.
- Exporting PROV documents into various graphical formats (e.g. PDF, PNG, SVG).
- Convert a PROV document to a Networkx MultiDiGraph and back.

Uses

See a short tutorial for using this package.

This package is used extensively by ProvStore, a free online repository

jupyter nbviewer JUPYTER FAQ

notebooks / PROV Tutorial.ipynb

Support JSON, XML and RDF

PROV Python Library - A Short Tutorial

The PROV Python library is an implementation of the Provenance Data Model by the World Wide Web Consortium. This tutorial shows how to use the library to:

- create provenance statements in Python;
- export the provenance to PROV-N, PROV-JSON, and graphical representations like PNG, SVG, PDF; and
- store and retrieve provenance on ProvStore.

Installation

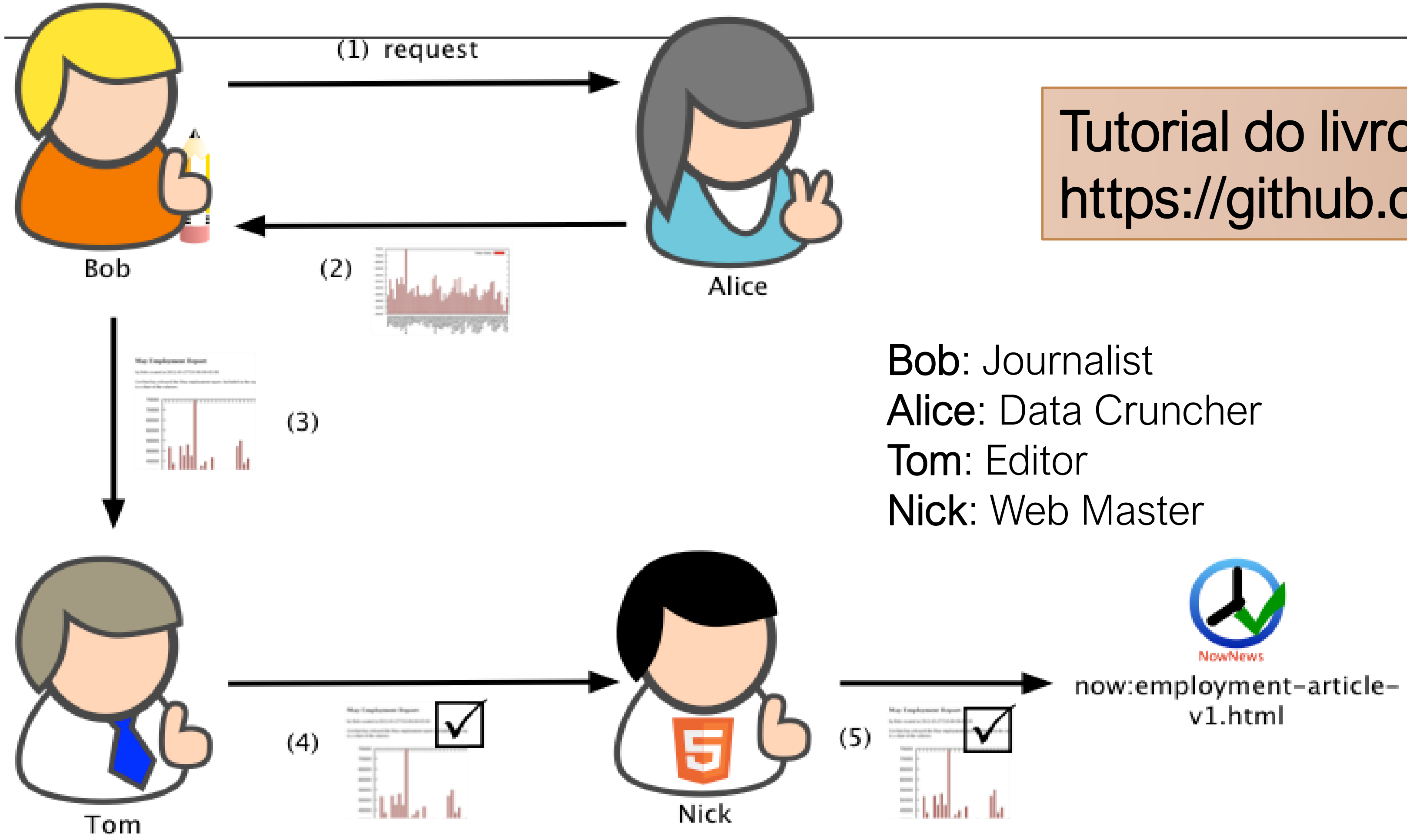
To install the prov library using pip with support for graphical exports:

```
pip install prov[dot]
```

Note: We recommend using virtualenv (and the excellent companion virtualenvwrapper) to avoid package version conflicts.

Tutorial do livro:
https://github.com/trungdong/prov

Running Example: NowNews



Tutorial do livro:
https://github.com/trungdong/prov

Bob: Journalist
Alice: Data Cruncher
Tom: Editor
Nick: Web Master

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provenance 0.14.1

```
pip install provenance
```

Latest version

Released: Dec 2, 2020

Provenance and caching library for functions, built for creating lightweight machine learning pipelines.

https://pypi.org/project/provenance/

Navigation

- Project description
- Release history
- Download files

Project links

- Homepage

Project description

pypi v0.14.1 conda-forge v0.14.1 build error docs passing

`provenance` is a Python library for function-level caching and provenance that aids in creating Parsimonious Pythonic Pipelines™. By wrapping functions in the `provenance` decorator computed results are cached across various tiered stores (disk, S3, SFTP) and provenance (i.e. lineage) information is tracked and stored in an artifact repository. A central artifact repository can be used to enable production pipelines, team collaboration, and reproducible results. The library is general purpose but was built with machine learning pipelines in mind. By leveraging the fantastic joblib library object serialization is optimized for `numpy` and other PyData libraries.

What that means in practice is that you can easily keep track of how artifacts (models, features, or any object or file) are created, where they are used, and have a central place to store and share these artifacts. This basic plumbing is required (or at least desired!) in any machine learning pipeline and project. `provenance` can be used standalone along with a build server to run pipelines or in conjunction with more advanced workflow systems (e.g. Airflow, Luigi).

References

Benureau, F., Rougier, N. Re-run, Repeat, Reproduce, Reuse, Replicate: Transforming Code into Scientific Contributions. Frontiers in Neuroinformatics. V.11, article 69, 2018.

Freire, J.; Chirigati, F. Provenance and the Different Flavors of Computational Reproducibility. IEEE Data Engineering Bulletin. V. 41:15-26, 2018.

Goble, C. What is reproducibility? The Rbrouhaha, In:First International Workshop on Reproducible Open Science (Hannover), 2016.

Goble, C. http://repscience2016.research-infrastructures.eu/img/CaroleGoble-ReproScience2016v2.pdf