Enabling painless reuse of shared research data and code: a case study on computational reproducibility

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**Agenda**

- Short introduction (5 mins)
- Talk #1 (20 mins):
  - Enabling Painless Reuse of Shared Research Data and Code in data repository Dataverse, by Ana Trisovic
- Talk #2 (20 mins):
  - Enabling Painless Reuse of Shared Research Data and Code for HPC-driven computational reproducibility of research, by Qian Zhang
- Q&A and open discussion (15 mins)
Acknowledgements

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Enabling Painless Reuse of Shared Research Data and Code in data repository Dataverse

Ana Trisovic,
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Agenda of this talk

- Introduction
- Quality of shared data & code
  - How do we ensure it?
- Code execution experiments
  - What happens when we automatically re-execute R or Python code?
  - What are the most common errors?
- Painless research reproducibility and reuse
  - Toward enabling painless reproducibility and reuse in Dataverse
Introduction

- "Reproducibility (computational) is obtaining consistent results using the same input data, computational steps, methods and code"
- "Replicability is obtaining consistent results across studies aimed at answering the same scientific questions, each of which has obtained its own data"

Introduction

- Enabling research reproducibility and reuse in practice:
  - Researchers collect, create, process, analyze and interpret data
  - They publish their findings through journal publication
  - They share their data and code (when possible) typically through data repositories
  - Researchers often face numerous degrees of freedom and lack of guidance when sharing data, which later hinder reproducibility and reuse

Figure credit: NTU Libraries
Introduction

- Dataverse is a free and open-source software platform to archive, share, and cite research data
- 60 institutions around the globe run Dataverse instances as their data repository
Introduction

Political Analysis is the official journal of the Society for Political Methodology. We publish articles that provide original and significant methodology, including both quantitative and qualitative methodological approaches.

1 to 10 of 421 Results

- Replication Data for: Generalized full matching
  - Sávija, Fredrik; Higgins, Michael; Sekhon, Jasjeet, 2020. "Replication Data for: https://doi.org/10.7910/DVN/1XK00D, Harvard Dataverse, V1
  - Replication code for simulation and application presented in the paper.
Introduction
Quality of shared research data & code

- Data quality is determined by its **fitness-for-use** for a given community. Data accuracy, precision, consistency, and completeness are valued across all user communities.
- Before data is published and disseminated, there is a **high potential** in developing its documentation that can improve its fitness for future use.
- After data is deposited, measuring reuse is one way to understand researchers' perceived quality of data products.
  - For example, Harvard Dataverse measures dataset view, downloads, and citations.
Computational metrics: research code completeness

- Necessary component for reproducibility:
  - Input data
  - Research code
  - Code dependencies (libraries, system dependencies, etc.)
  - Research workflow (i.e., a sequence of analysis steps)
  - Other (computational infrastructure, OS, contextual information etc.)
The experiment is implemented on **AWS Batch**

- A replication dataset contains: R (or Python) code, data and documentation
- Allocated time to run each R file is 1 hour (we also ran experiments with 10 minutes per R file)
- We studied over 2091 datasets, containing over 8178 R files.
How do datasets with R code look like?
How do datasets with R code look like?
How do datasets with R code look like?

Distribution of average file name lengths

Replication package contains documentation (readme or instructions)?

- Yes: 57.96% (1212)
- No: 42.04% (879)
Execution of R code

Without code cleaning:

Re-execution rate with R3.6 and no code cleaning

- Success: 14.76% (577)
- Error: 85.03% (3323)
- Time Limit Exceeded: 0.20% (8)
Execution of R code

Without code cleaning:

Re-execution rate with R3.6 and no code cleaning

- Error: 85.03% (3323)
- Success: 14.76% (577)
- Time Limit Exceeded: 0.20% (8)

With code cleaning:

Re-execution rate with R3.6 & code cleaning

- Error: 74.56% (4441)
- Success: 20.94% (1247)
- Time Limit Exceeded: 4.50% (268)
## Execution of R code: errors

<table>
<thead>
<tr>
<th></th>
<th>Without code cleaning:</th>
<th>With code cleaning:</th>
</tr>
</thead>
<tbody>
<tr>
<td>library</td>
<td>60%</td>
<td>25%</td>
</tr>
<tr>
<td>setwd</td>
<td>12%</td>
<td>0%</td>
</tr>
<tr>
<td>TLE</td>
<td>1%</td>
<td>15%</td>
</tr>
<tr>
<td>file</td>
<td>10%</td>
<td>10%</td>
</tr>
<tr>
<td>other</td>
<td>17%</td>
<td>50%</td>
</tr>
</tbody>
</table>
Execution rate of R 3.4 (with code cleaning) files per year of publishing
Execution rate per Dataverse journal

Re-execution rate per journal Dataverse

- The Journal of Politics: 29.1% (505) Success, 37.7% (393) TLE, 34.8% (276) Error
- American Journal of Political Science (AJPS): 29.9% (344) Success, 34.8% (296) TLE, 36.3% (231) Error
- Political Analysis: 26.3% (228) Success, 36.0% (186) TLE, 23.1% (106) Error
- American Political Science Review: 31.6% (188) Success, 21.8% (67) TLE, 22.7% (68) Error
- British Journal of Political Science: 24.5% (50) Success, 32.4% (65) TLE, 43.1% (85) Error
- Political Science Research and Methods (PSRM): 36.0% (132) Success, 21.8% (67) TLE, 22.7% (68) Error
- Political Behavior: 24.5% (50) Success, 32.4% (65) TLE, 43.1% (85) Error
- International Studies Quarterly: 24.5% (50) Success, 32.4% (65) TLE, 43.1% (85) Error
- Review of Economics and Statistics: 24.5% (50) Success, 32.4% (65) TLE, 43.1% (85) Error
- Research & Politics: 24.5% (50) Success, 32.4% (65) TLE, 43.1% (85) Error
- International Interactions (II): 24.5% (50) Success, 32.4% (65) TLE, 43.1% (85) Error
Next steps

- We are analyzing re-execution rate for 3 different versions of R (3.2, 3.6 and 4.0)
  - With varied allocated time for execution (up to 1h per file)
  - Manuscript in preparation
- Also we want to prevent common execution mistakes before depositing code in Dataverse, possibly with an automatic CI (continuous integration)
Execution of Python code with code cleaning

Re-execution rate of Python files using Python 2.7

- Error: 75.84% (292)
- Success: 23.64% (91)
- TLE: 0.52% (2)

Re-execution rate of Python files using Python 3.5

- Error: 76.88% (296)
- Success: 22.86% (88)
- TLE: 0.26% (1)

Errors: ImportError, SyntaxError

TLE = time limit exceeded
Datasets with Python code

Packages contain documentation (readme, codebook or instructions file)?

- Yes: 68.48% (63)
- No: 31.52% (29)
Datasets with Python code

Packages contain documentation (readme, codebook or instructions file)?

- Yes: 68.48% (63)
- No: 31.52% (29)

<table>
<thead>
<tr>
<th>File</th>
<th>Count (out of 92)</th>
</tr>
</thead>
<tbody>
<tr>
<td>environment.yml</td>
<td>0</td>
</tr>
<tr>
<td>requirements.txt</td>
<td>6</td>
</tr>
<tr>
<td>Dockerfile</td>
<td>0</td>
</tr>
</tbody>
</table>
Enabling reproducibility and painless reuse

- Container technology (or encapsulation) provides a way to virtualize an OS in a lightweight way and capture data, software and its dependencies
  - It is often used on the cloud
- Containers are becoming popular for preserving research data & code, as they can facilitate research reproducibility and reuse.
  - They are one of the best solutions to enable reproducibility
- There are different types of containers and they can describe research processes in a variety of computing infrastructures
Use of containers in research

- Many new tools encapsulate research data and code in a container “behind the scenes”, which capture computational environment that can be shared, reproduced and reused.

- Examples:
  - Code Ocean
  - Whole Tale
  - Renku
  - ReproZip
  - Stencila
  - ...
Reproducibility platforms vs. data repositories

- **Reproducibility platforms support**
  - Research portability, reproducibility and reuse
  - However research data and code are not normally findable in data search engines, and there is no commitment for long-term preservation

- **Data repositories often support**
  - Findability through the use of standard metadata
  - Standardized persistent citation
  - Long-term accessibility of data and code
  - Troubles with enabling reproducibility
Dataverse approach

- Dataverse data repository aims to improve reproducibility of deposited research data & code by developing new functionality to capture containers
  - Ongoing integration with reproducibility platforms Code Ocean, Whole Tale, Renku and Binder, that would allow encapsulated data & code to be exported (deposited) in Dataverse
Dataverse approach

- Dataverse data repository aims to improve reproducibility of deposited research data & code by developing new functionality to capture containers
  - Ongoing integration with reproducibility platforms Code Ocean, Whole Tale, Renku and Binder, that would allow encapsulated data & code to be exported (deposited) in Dataverse
  - Any user should be able to preserve their container based artifacts regardless of their use of the reproducibility platforms.
Outlook

- How to enable painless reuse of shared research data and code?
  - Avoiding common mistakes
  - Including virtual environments in shared code
  - Better metadata to capture ever-more complicated computing infrastructures
Talk #2

Enabling Painless Reuse of Shared Research Data and Code for HPC-driven computational reproducibility of research

Qian Zhang
Agenda of this talk

- What is HPC-driven:
  - computational research?
  - computational reproducibility?
  - Why is it important?
- HPC-driven computational reproducibility: A case study
  - Challenges & Opportunities
- Painless HPC-driven research reproducibility and reuse
- Outlook
What is the HPC-driven computational research?

- *Not theoretical*: deductive mathematics
- *Not experimental*: empirical statistical analysis
- **Computational**: large-scale simulations / data-intensive computational science
  - **Big data**
  - High performance computing (HPC): Computational power, application of supercomputers, parallel computing
  - **Software & code** is persuasive in modern digital research landscape
What is the HPC-driven computational reproducibility?

- Same research results
  - Different team
  - Same experimental setup
    - Same artifacts
    - Same measurement procedure
  - *Same/different* operating conditions
Why does the HPC-driven computational reproducibility?

▸ “Reproducibility is a Process, not an Achievement” (Lin & Zhang, 2020)
▸ To root out the error
▸ Help to “frame the agenda of digital curation” (Stodden, V., 2011. Reproducible Research: A Digital Curation Agenda)
▸ Central to scientific communication
HPC-driven computational reproducibility: A case study in Astrophysics

- We attempted to reproduce a study:
  - IllinoisGRMHD: an open-source, user-friendly GRMHD code for dynamical spacetimes (Etienne et al., 2015)
HPC-driven reproducibility setup

- Link to the code: [IllinoisGRMHD](http://math.wvu.edu/~zetienne/ILGRMHD)
- “Instructions for downloading, compiling, and using IllinoisGRMHD may be found here: http://math.wvu.edu/~zetienne/ILGRMHD/"
- HPC resources: XSEDE
  - Stampede2's Skylake (SKX) @Texas Advanced Computing Center (TACC) & Comet @San Diego Supercomputer Center (SDSC)
- Download ⇒ compile ⇒ customize the parameter file ⇒ execute ⇒ post-analysis
Preliminary results of the reproducibility case study

Illinois GRMHD: $\Delta \rho_c(t)$ Convergence to Zero
- LR $\times (\Delta x_{HR}/\Delta x_{LR})^2$
- MR $\times (\Delta x_{HR}/\Delta x_{MR})^2$
- HR

Conv. Order

$\Delta \rho_c(t)$

$t/t_{dyn}$

{LR, MR} Conv. Order
{MR, HR} Conv. Order

Figure in the paper

Reproducibility experiment result
Observations & lessons learned

- Insufficient data/code
  - Lack of documentation
  - Computational model compilation/execution errors
    - Unstopabble hardware upgrade
    - Link rot, software incompatibilities
  - Missing key parameter (file)
Observations & lessons learned (cont.)

- Installation issues
  - If installed on local laptops
    - Have to be clean slate
  - If installed on local institutional cluster platform
    - ⇒ Setup issues (next slide)
- ⇒ Provide instruction on installation
  - Documentation
  - Checklist

- Issues when submitting jobs (shell script) to queuing system
  - ⇒ Provide Human-readable info.
Next step (in progress)

- **Develop generic setup template to configure a new machine**
  - Machine definition
  - Option list: Compilers, Compilation and linking flags, Debugging, Optimisation, Profiling, OpenMP, Warnings, ExternalLibraries (HDF5, MPI, Others)
  - Submission script
  - Run script

- **Provide template & examples**
  - XSEDE
  - Compute Canada
  - Perimeter Institute for Theoretical Physics
  - AWS
Why are HPC-driven research reproducibility and reuse so difficult?
Why are HPC-driven research reproducibility and reuse so difficult?

- Model
  - Model/code availability/ease of use
  - Platform/system availability
  - Where/how was this run?
  - Model re-usability (setup, etc.)
- Human efforts
- Data
  - Simulation inputs
  - Output usability
Why are HPC-driven research reproducibility and reuse so difficult (cont.)?

▸ Accessibility
  ▹ Conformance to open or established standards
  ▹ Archival accessibility
  ▹ Longevity of the technology

▸ Cost
  ▹ Computational cost
  ▹ Storage cost
Opportunities of HPC-driven research: reproducibility and reuse

- Ensure **transparency, reproducibility** and **reusability** of research results
- Provide effective **communication** of research outputs (publication, data and code) and advanced research computing resources
- Promote enhanced **access** to research outputs and resources
  - Policies and strategies
  - Network and collaborative initiatives
  - Research infrastructures
  - Research software as a primary output of research
Opportunities of HPC-driven research reproducibility and reuse (cont.)

- Develop standards for reproducibility **badges**
  - NISO’s Draft Recommended Practice for Reproducibility Badging and Definitions
  - ACM Artifact Review and Badging Version 1.1 - August 24, 2020

- **Tools & platforms** for supporting computational science
  - Dissemination/reproducibility platforms (code ocean, Whole Tale)
  - Workflow tracking (Kurator)
  - Better documentation (Jupyter notebook)

- Practices & guidelines
- Training opportunities
Painless HPC-driven research reproducibility and reuse

- Accessioning, stabilizing, evaluating & describing digital objects
- Documenting and making documentation available
- Sharing resources
  - Data (& documentation) collected & used in analysis
  - Data output result(s) (& documentation) produced by analysis
  - Software (& documentation) in source code& human - readable formats
  - Software/hardware dependencies (technical details, system/software environments)
  - Computational research workflow and provenance
  - Software program(s) dependencies for replicating published results
  - Journal article
- Providing access
Outlook

▸ Extensive re-use of data and code will become the norm
▸ Researcher competitiveness will be re-defined with multi-facet metrics
▸ Cultural change
  ▸ Policy from publishers and funders
  ▸ Author
Takeaways

▸ “Reproducibility is a Process, not an Achievement”
▸ Research community’s recommendations on good practices
▸ Greater clarity and guidance on dissemination of computational claims
▸ Code dissemination in data repositories:
  ▶ Avoiding common mistakes by testing code in a clean environment
  ▶ Including virtual environments in shared code
  ▶ Better metadata to capture ever-more complicated computing infrastructures
Q & A

Questions for the audience
Questions for the audience

- How were your experiences with research reproducibility and reuse? What difficulties have you encountered?
- How do you disseminate data and code at your institution (or research field)? How do you document them?
Thank you for your attention!