repliMAT: A Guide to Reproducible MATLAB

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Welcome!

Welcome to repliMAT!

:construction: This book is very much under development :construction:

This is a resource for learning and teaching about developing reproducible and sustainable code in the MATLAB programming language.

Here you will find content, exercises and videos intended to either be followed alone or with a group, or taught as part of a workshop.

The materials are primarily aimed at researchers and their specific demands, but should be applicable to all uses of MATLAB.

How to use this guide

This guide is split into two main parts: a reference guide and a set of exercises.

The intention is for the reference guide (begin here) to act as a place to learn about the reasoning behind concepts in reproducible MATLAB project design, as well as somewhere to come back to as a reference when working on your own project.

The exercises are a worked-through set of examples that can either be taught as part of a workshop or followed on your own.

The third part of these two main parts (:roll_eyes:) is the extra credit section, containing concepts that aren't absolutely essential for reproducibility, but are considered good/excellent practice in programming.

Contributing

Contributions to the replimaterials are welcomed! Please follow the guidance below prior to making contributions to ensure that your kind efforts do not go to waste.

The project's source code and development is managed at its GitHub repository. There are a few ways to contribute, depending on whether you want to make changes to the source code or not.

In all interactions, please abide by the code of conduct

Issues

Open a new issue to describe a bug, error or to request changes.

Contributing code

If contributing source code changes to the project please follow the following workflow:

- 1. Make a fork of the repository on GitHub.
- 2. Clone your fork to your local machine and make a new branch with a name relevant to the task you're working on.
- 3. Make some changes and ensure that the pages render as expected by following the instructions in the README to render the materials.
- 4. Commit those changes with meaningful commit messages.
- 5. Push your branch to GitHub and open a pull request against the upstream repository's main branch.
- 6. In the pull request description, please reference the issue that you are resolving.
- 7. Someone will review your pull request and hopefully it will be merged! :tada:

1 Introduction

1.1 What is research reproducibility?

According to The Turing Way's definitions¹, the term *reproducibility* refers to performing the *same* analysis on the *same* data for the *same* result. Other terms such as replicability and generalisability are used to refer to using different analyses or different data. This may not be your definition, but it's the one meant here and derived from the research done by the authors of The Turing Way (an exemplary guide to reproducible research software).

Research that is reproducible has many benefits, it:

- is easier to validate (perhaps even *possible* to validate),
- has more long-term validity,
- is more extensible,
- reduces repetition,
- decreases likelihood of losing methodology,

among many others.

Code is great for research reproducibility in lots of ways. Code describes a proceduralised sequence of operations to some data, with (arguably) zero ambiguity - great! That's just what we need for research. Where appropriate, code is an excellent solution to capturing and reproducing the steps taken to go from some raw data/input to some research conclusions.

However, in practice it isn't always as easy as that. So this guide aims to provide researchers who code with the tools they need to make their MATLAB-based research (more) reproducible.

1.2 Open Research & Reproducibility

Open research is the idea that the entire research lifecycle should be transparent for all to see. As an approach, open research continues to grow and many funders now stipulate that the research that they fund must follow open principles including the open availability of publications, data and code. How does this fit in with reproducibility? I would argue that if you are required to make your code available, whether that's for a publication, thesis or just to share it with a colleague, it would be a good thing for the code to actually work, and for it

to be relatively easy to make it do so. It's commonplace in research to obtain some code and spend a significant period of time attempting to run it successfully, let alone validating that it produces something accurate. Therefore reproducibility is an important component of open research, though it need not be complicated.

1.3 Is it worth the effort?

There's no denying that learning and implementing the approaches required to enable reproducible research is *yet another* thing to do. As researchers we already have so many different skills to master: domain expertise, writing, graphic design, experimental design, public speaking, statistics. The list goes on. So why should we *voluntarily* make our programming practices even more involved than they already are. Many of us don't even *like* programming, so can't we just get the job done?

Yes and no. As mentioned above, many funders and publishers require open research practices, so as far as I'm concerned, the code should actually work when we share it. Understandably, people are often resistant to making their practices even more complicated. The culture still hasn't really shifted to expecting fully reproducible research code. However, I would give most researchers the benefit of the doubt and assume that most want their work to be verifiably correct.

Moreso than just being "the right thing to do" - making one's research more reproducible has all sorts of benefits. Let's expand on the benefits mentioned above. If we want to check that our work is correct, being able to send it to a colleague who can then actually make it run is a huge advantage. I'm sure we've all been in the situation where someone sends a zip file of code with no instructions and we spend ages trying to make it work. Reproducible research saves us and our colleagues and collaborators time by simplifying this process, allowing us to actually get on with the research we're interested in. If we publish some work and people are able to make it work, they're more likely to build upon it and cite our work. This accelerates research and gets us the recognition we deserve. Importantly, when we come back to our work in the future, we may actually understand what we did and be able to build upon it ourselves. Imagine that!

1.4 Why MATLAB?

Why is MATLAB a tool that we should care about when it comes to reproducible practices? Because MATLAB is a popular language in research.

That's it.

Whatever your technical opinion of a language, or whether it is proprietary or open source, for all sorts of reasons, MATLAB is used by a lot of researchers. It has a relatively long history as being a tool with a lot of useful mathematical and analytical features, is relatively user friendly and a large number of universities have a license.

But, possibly because it's a proprietary language, most of the guidance and documentation comes from the organisation that develops it, MathWorks.

In comparison to other programming languages currently popular in research such as Python & R, the availability of guidance around reproducibility is relatively limited.

So that's why this guide has been developed, to allow those researchers who currently use MATLAB to make their research more reproducible and easier to share.

Not because I think MATLAB is the best, or the worst. I just think that all research should aim to be as reproducible as possible and that you should use the best tool for the job, even if that's just the one that you currently know.

Many researchers using MATLAB have said to me:

I know I should rewrite this in python so that I can share it.

But realistically, the likelihood is that you'll just move on to your next project. The demands and incentives of the research world mean that investigating a new thing carries much more value than refining an existing project to a higher standard.

So let's make the projects we're working on **now** as good as they can be.

Part I Writing cleaner code

Whilst this is primarily a guide to writing more *reproducible* MATLAB, I would argue that writing *cleaner* code is an important step. It can make your code easier to read and follow (for you as well as others) - making it simpler to spot errors and mistakes, as well as for others to make contributions and improve or build upon your code.

We'll explain this in several steps:

- variables
- functions
- codebase organisation (it's not just the programming that helps)
- how to document your code.

One significant reference here is the book "The Elements of MATLAB Style" by Richard Johnson² which acts as the *de facto* community standard for style when it comes to programming in MATLAB. As well as the book itself, there are several resources based on it that have the core elements of its teachings on code style in MATLAB:

- cheat sheet available from MATLAB file exhange much better than reading the actual book
- updates to the book also on file exchange

The cheat sheet is also reproduced on this site here for ease of searching and for quick reference.

With any programming language, it pays to disavow yourself of any *opinions* that you may have and save yourself the time of thinking about how to write your code by just following the standard practices of the community. Your code may **run** perfectly well. You may think that a certain way of function-naming is slightly better. But if we all stick to the same standards, we all have an easier time of reading each other's code and don't have to waste time arguing (yes, this is something that people argue about.)

2 Variables

3 Functions

4 Project Organisation

5 Documentation

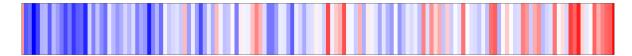
Part II Reproducibility

6 Projects

Part III

Exercises

Introduction



In this series of exercises, we're going to work with some research code which may be typical of what many of us would write and walk through how to transform this into a significantly more reproducible project.

We'll work with some publicly available data on surface temperatures in the USA from the late 19th to the early 21st century and create some interesting visualisations.

To start with, the project will hopefully look similar to what many of us would develop in our work, but it may not be as reproducible as it could be. By the end, we should have a project that we can easily share with anyone who can run it and generate the same results, and even use the code with different data.

How to work with these exercises

You'll either need a recent copy of MATLAB installed on your computer, or you can follow the links alongside the exercises to open the examples in MATLAB online.

To get hold of the code and use it on your own computer, you can use git to "clone" the code from GitHub, or just download it. Instructions are in the "Getting started" section.

7 Getting Started

7.1 Technical setup

You'll need an installation of MATLAB, preferably a recent version (i.e. in the last year or so). Where a specific version is needed, or doesn't work with an example, it should be indicated alongside the exercise. See Section 7.1.1 below for more info on versions.

Follow the instructions on MathWorks.com to install.

No specific toolboxes are required.

Note There is no guarantee that anything in these materials will work with Octave. In fact it probably won't. But let us know if you try!

7.1.1 MATLAB versions

A new version of MATLAB is released twice a year. The version numbers are comprised of the letter 'R' followed by the calendar year and 'a' if it's the first release in the year and 'b' for the second. e.g. R2022b. Each version has improvements from the last and makes changes. It's a good idea to be using the most recent version of MATLAB in most cases.

7.2 How to use these materials

7.2.1 Where to start

Anywhere you like! Hopefully the structure of the exercises included here means that you can dip in to any point that takes your fancy.

7.2.2 Prerequisites

These materials assume that you're already familiar with the basics of programming in MAT-LAB. Variables, arrays, loops, reading in data and making plots *etc*.

Part IV Extra Credit

 $: construction: \ \textit{Nothing here yet!} \ \textit{Check back later.} : construction:$

8 Testing

9 Version Control

Code Style Cheat Sheet {.appendix, .unnumbered}

This is a reproduction of the MATLAB Style Guidelines Cheat Sheet compiled by Jason Nicholson and Edited by Richard Johnson from the book $The\ Elements\ of\ MATLAB\ Style^2$.

Matlab Style Guidelines Cheat Sheet (https://www.mathworks.com/matlabcentral/fileexchange/45047-matlab-style-guidelines-cheat-sheet), MATLAB Central File Exchange. Retrieved February 5, 2024.

Reproduced here within this book for ease of use by its readers.

Naming Conventions

Variables

- Variable names should be mixed case starting with lower case: velocity, angularAcceleration.
- Variables with a large scope should have meaningful names. Variables with a small scope can have short names:

```
- Small scope: x, y, z
```

- Large scope: velocity, acceleration
- The prefix n should be used for variables representing the number of objects: nFiles, nCars, nLines
- Use a convention on pluralization consistently: point, pointArray
- Variables representing a single entity number can be suffixed by No: tableNo, employeeNo
- Iterator variables should be named or prefixed with i, j, k etc. e.g. iFiles, jColumns
- For nested loops, the iterator should be alphabetical order and helpful names e.g.

- Avoid negated boolean variable names: isNotFound instead use isFound
- Acronyms, even if normally uppercase, should be mixed or lower case. Use: html, isUsaSpecific
- Avoid using a keyword or special value name. Just don't do it.

Constants

- Named constants should be all uppercase using underscore to separate words: MAX_ITERATIONS, COLOR_RED
- Constants can be prefixed by a common type name: COLOR_RED, COLOR_GREEN, COLOR_BLUE

Structures

- Structure names should be mixed case and begin with a capital letter: Car, DumpTruck
- Do not include the name of the structure in the field name. Use Segment.length. Avoid Segment.segmentLength

Functions

- The names of functions should document their use.
- Names of functions should be written in lower or mixed case: width(), computeTotalWidth()
- Functions should have meaningful names. Use computeTotalWidth. Avoid compwid.
- Functions with single output can be named for the output: shearStress() standardError()
- Functions with no output argument or which only return a handle should be named after what they do: plotfft()
- Reserve the prefix get/set for accessing an object or property: getobj(), setappdata()
- Reserve the prefix compute for methods where something is computed: computeSumOfResiduals(), computeSpread()
- Reserve the prefix find for methods where something is looked up: findOldestRecord()
- Reserve the prefix initialize for instantiating an object or concept: initializeProblemState()
- Reserve the prefix is for boolean functions: isCrazy, isNuts, isOffHisRocker
- Use complement names for complement operations: get/set, add/remove, create/destroy, start/stop, insert/delete, increment/decrement, old/new, begin/end, first/last, up/down, min/max, next/previous, open/close, show/hide, suspend/resume, etc.
- Avoid unintentional shadowing of function names. Use the which -all or exist tools to check for shadowing.

General

- Abbreviations in names should be avoided. Use computeArrivalTime. Avoid comparr.
- Consider making names pronounceable.
- All names should be written in English.

Files and Organization

M-Files

- Modularize code. Use small well designed pieces to make the whole.
- Write functions that are easy to test.
- Make interaction clear. Use inputs and outputs rather than global variables.
- Replace long lists of arguments with structures.
- Partitioning. All sub-functions and most functions should do one thing very well.
- Use existing functions rather than custom coded functions when possible.
- Move blocks of code used in multiple m-files to functions.
- Use sub-functions when a function is only called by one other function.
- Write test scripts for every function.

Input/Output

- Make input and output modules for large functions.
- Format output for easy use. For humans, make it human readable. For machines, make it parsable.

Statements

Variables and constants

- Variables should not be reused unless required by memory limitations.
- Related variables of the same type can be declared in a common statement. Unrelated variables should not be declared in the same statement:

```
persistent x, y, z
```

- Document important variables in comments near the start of the file.
- Document constants with end of line comments:

```
THRESHOLD = 10; % Max noise level
```

Global Variables

- Minimize use of global variables and constants.
- Consider using a function instead of a global constant.

Loops

• Variables used in loops should be initialized immediately before the loop.

```
result = zeros(nDays,1);
for iDay = 1:nDays
    result(iDay) = foo(iDay);
end
```

- Minimize the use of break and continue in loops.
- The end lines in nested loops can have comments to clarify the code block.

```
for index=1:2
   if index==1
        dosomething(index);
        ...
   end % End if
end % End for
```

Conditionals

• Avoid complicated conditional expressions. Use temporary logical variables instead.

```
isValid = (v >= lowerLimit) & (v <= upperLimit);
isNew = ismember(v, valueArray);</pre>
```

- Avoid the conditional expression if 0.
- An if-else sequence should include the else condition.
- The usual case should be put in the if-part and the exception in the else-part of an if-else statement.
- A switch statement should include the otherwise condition.
- Use a switch sequence if the variable is a string.
- Use a switch statement in place of many if-elseif-else statements when possible.

General

- Avoid cryptic code. You should be able to look at it a month from now and know what it does.
- Use parentheses for clarity even if not need because of operator precedence.
- Minimize the use of numbers in expressions. Use a named constant instead.
- Always use a zero before the decimal point: THRESHOLD = 0.5
- Make floating point comparisons with caution.

Layout, Comments, and Documentation

Layout

- Contents should be kept within the first 80 columns.
- Lines should be split after commas, spaces, and operators.
- Align a continued line with the beginning of the expression on the previous line:

```
totalSum = a + b + c ...
d + e;
```

- Basic indentation should be 4 spaces.
- In general, a line of code should contain only one executable statement.
- Short single statement if, for, or while statements can be written on one line:

```
if(condition), statement; end
```

White Space

- Surround =, &, and | by spaces.
- Follow commas by a space.
- Keywords should be followed by a space.
- Blocks of code should be separated by three blank lines or a section break.
- Use code alignment wherever it enhances readability.

Comments

- Comments cannot justify poorly written code.
- Comments should agree with the code but not restate the code.
- Comments should have the same indentation as the statement(s) referenced.
- Traditional function header comments should support help and lookfor:
 - help prints the first continuous block of comments.
 - lookfor searches the 1st comment line of all m-files on the path.

- Function headers should discuss any special requirements for the input/output argument and describe any side effects of the function.
- Write the function name using correct case in the function header comments.

function runEverything

% runEverything runs all mfiles in its folder

- Put any copyright lines and change history after the function header with a blank line in between.
- All comments should be in English.

Documentation

- Write header comments with text markup to provide user documentation. Include sections that correspond to a help page: syntax, description, example, and see also.
- Consider writing the documentation first to better define inputs, outputs and functionality.
- Consider using a source control tool such as SVN or GIT. If you do not use a source control tool, document changes by adding change history comments after the function header or near the top of the script.

References

- 1. The Turing Way Community. The Turing Way: A handbook for reproducible, ethical and collaborative research. (2022) doi:10.5281/zenodo.3233853.
- 2. Johnson, R. K. The elements of MATLAB style. (Cambridge University Press, 2010).

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