Extensible Software for Research



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Contents

Principles of Extensible Research Software

Application: StructuralEquationModels.jl





- work with a specific type of model
 - regression, structural equation models, deep learning, ...



- work with a specific type of model
 - regression, structural equation models, deep learning, ...
- have an idea



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 - regression, structural equation models, deep learning, ...
- have an idea
- test it



- work with a specific type of model
 - regression, structural equation models, deep learning, ...
- have an idea
- test it
- make it available to applied researchers



- **▶** to test → prototype
- to make it available → distribute



- ightharpoonup to test \rightarrow prototype
- to make it available → distribute

What's the fastest way to get there?



- **▶** to test → prototype
- to make it available → distribute

What's the fastest way to get there?

We are already working with existing software.



- ightharpoonup to test \rightarrow prototype
- to make it available → distribute

What's the fastest way to get there?

We are already working with existing software.

It would be nice if we could extend existing software!





understand 1000s of lines of code



- **understand** 1000s of lines of code
- make changes, possibly breaking stuff



- understand 1000s of lines of code
- make changes, possibly breaking stuff
- get maintainers to adopt our changes



- understand 1000s of lines of code
- make changes, possibly breaking stuff
- get maintainers to adopt our changes

These hurdles are often too high!





A year in the life of ...

- > to test: minimal reimplementation
 - waste of time
 - not well tested
 - hard to reproduce
 - slow



A year in the life of ...

- to test: minimal reimplementation
 - waste of time
 - not well tested
 - hard to reproduce
 - slow
- to deploy: put code on github
 - bad user interface, no documentation
 - missing features
 - incompatible to existing software



My Experience

▶ from R → **julia**



Culture

- care about extensibility
- developer documentation
- assume their code is read



An Example

Let's make a thought experiment...

- encyclopedia
 - add an entry
 - some syntactical requirements 300-400 words, alphabetical, ...
- book
 - a draft already exists
 - add something everywhere it is applicable



An Example

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Software Design

Not all research articles can be encyclopedias, but maybe all research software can be...



Software Design

You need to be able to add new features...

- without understanding existing code
- without changing existing code
- syntactical requirements need to be clear and easy communicable!



The Benefits

- Applied Researchers
 - user interface
 - better documentation
 - faster availability of new features
 - less bugs
 - higher performance
- Statistical Researchers
 - no re-implementation → less time-consuming
 - more users
 - no software engineering skills needed
- Maintainers
 - changes are easier to integrate



Less Abstract



A few days in a methods researchers life

- Do you have any ideas why this does not converge?
- Staring puzzled at the theory (should work?!).
- Staring very puzzled at the implementation in C++.
- Rinse and repeat for a couple of days and researchers.



An hour in our life

- **▶** Look at the formula: $ridge(x, \lambda) = \lambda \sum_{i=1}^{p} x^2$
- Implement in Julia: ridge(x, λ) = $\lambda * sum(x.^2)$
- add 30 lines of API (formal requirements)
- Enjoy.



Two hours in our life

Simulation in Juila works (converges as it should)



Two hours in our life

- Simulation in Juila works (converges as it should)
- Original simulation takes weeks on a dedicated workstation.
- Original simulation freezes our cluster due to poor parallelization.
- Simulation in Julia takes 2 hours on my laptop.



Why?

- Some investments in extensibility
- division of labor:
 - optimizing linear algebra is done by Intel
 - numerical optimization is done by dedicated experts
 - differentiation is automated
- modern infrastructure



But why?

convenience

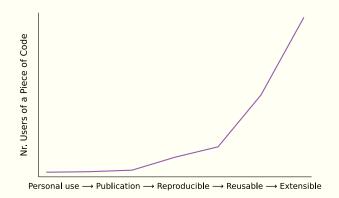


How to improve convenience?

- 1. Extensible Software
- 2. Documentation
- 3. User Interface

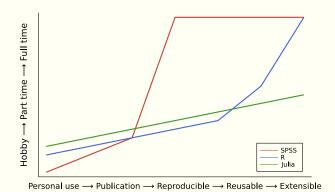


The leverage of extensible software





Time is limited





Documentation

- Documentation for users
- Documentation for contributors/developers



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- Documentation is not always called documentation (e.g. papers/talks/blog posts)



Documentation

- Documentation for users
- Documentation for contributors/developers
- Documentation is not always called documentation (e.g. papers/talks/blog posts)
- Code itself is the best developer documentation



User Interface

- Frictionless
- Connected to prior knowledge



More Concrete



Structural Equation Models.jl

