# **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?



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- 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 live of ...

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



### A year in the live of ...

- to test: barebone, minimal reimplementation
  - waste of time
  - not well tested
  - hard to reproduce
  - slow
- to deploy: put their 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...

- The 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 communicatable!



#### **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



### 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,  $\lambda$ ) =  $\lambda * sum(x.^2)$
- 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

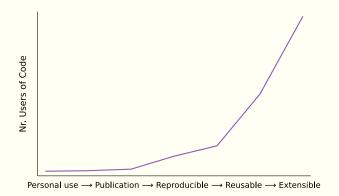


# **But why?**

convenience



### The leverage of extensible software



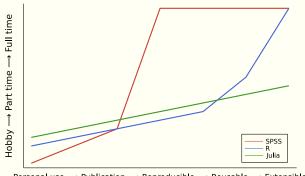


# How to improve convenience?

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



### **Time is limited**



Personal use  $\longrightarrow$  Publication  $\longrightarrow$  Reproducible  $\longrightarrow$  Reusable  $\longrightarrow$  Extensible



### **Documentation**

- Documentation for users
- Documentation for contributors/developers



### **User Interface**

- Frictionless
- Connected to prior knowledge

