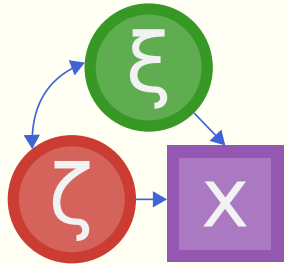
Extensible Software for Research

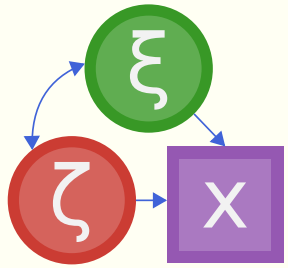


Maximilian Ernst

Aaron Peikert

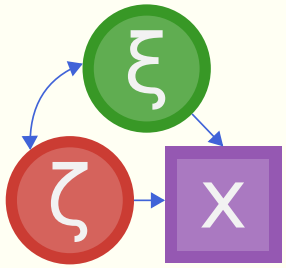
Contents

- Principles of Extensible Research Software
- Application: StructuralEquationModels.jl



A day in the life of …

a statistical methods researcher



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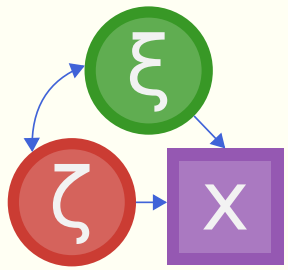
- work with a specific type of model
  - regression, structural equation models, deep learning, …



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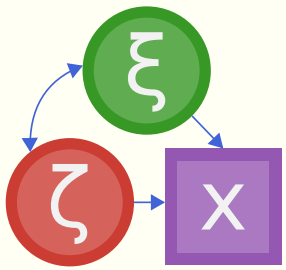

A day in the life of …

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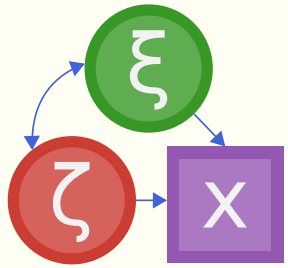
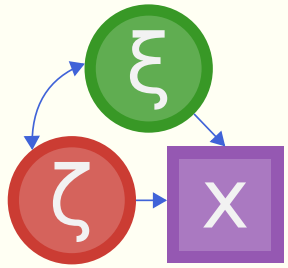
- work with a specific type of model
  - regression, structural equation models, deep learning, …
- have an idea
- test it



A day in the life of …

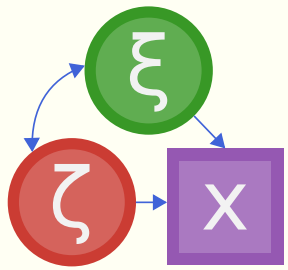
a statistical methods researcher

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



We need to write Software

- to test $\rightarrow$ prototype
- to make it available $\rightarrow$ distribute



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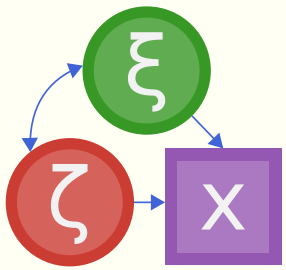
What's the fastest way to get there?



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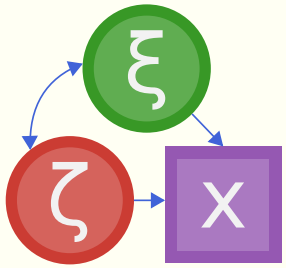
We are already working with existing software.



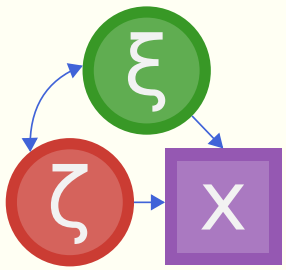
We need to write Software

- to test $\rightarrow$ prototype
- to make it available $\rightarrow$ distribute

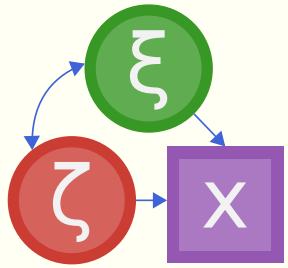
What's the fastest way to get there?

We are already working with existing software.

It would be nice if we could extend existing software!

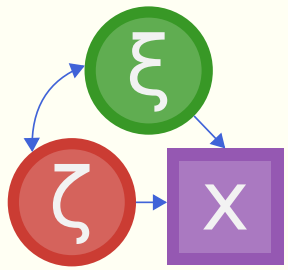


But …



But …

- **understand** 1000s of lines of code



But …

- **understand** 1000s of lines of code
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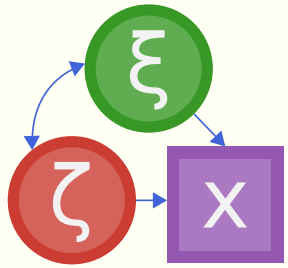

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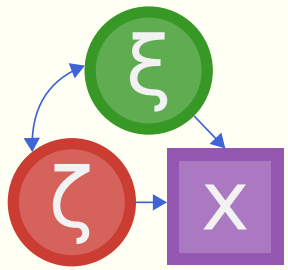

But …

- **understand** 1000s of lines of code
- make **changes**, possibly breaking stuff
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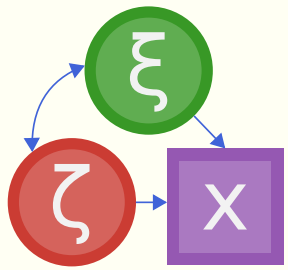
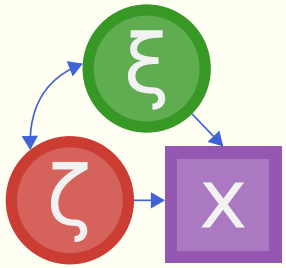
These hurdles are often too high!

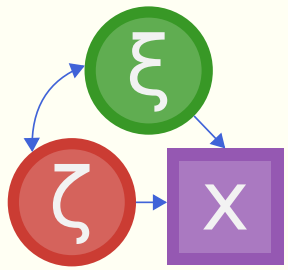


A day in the life of …



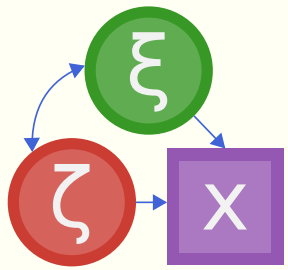
A year in the life of …

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



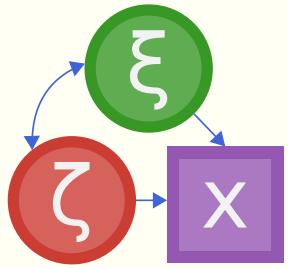
A year in the life of …

- 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



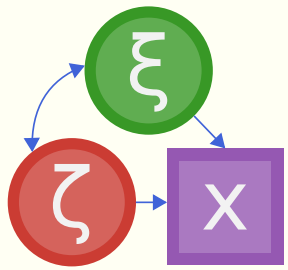
My Experience

- from R → julia



Culture

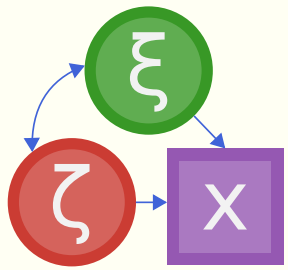
- care about extensibility
- developer documentation
- assume their code is read



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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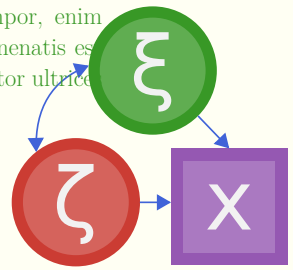
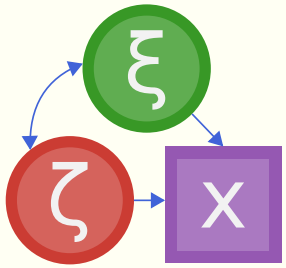


Software Design

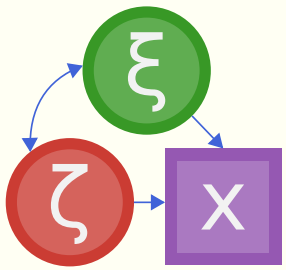
Not all research articles can be encyclopedias, but maybe all research software can be...



Software Design

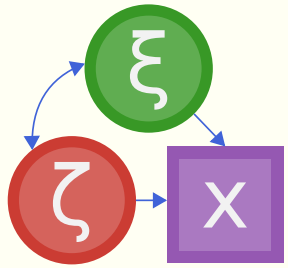
You need to be able to add new features...

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

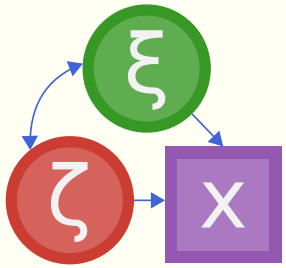


The Benefits

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

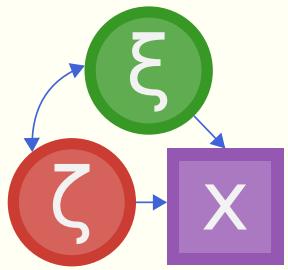


Less Abstract



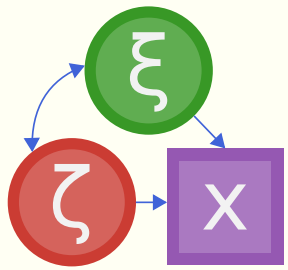
A few days in a methods researchers life

- 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.



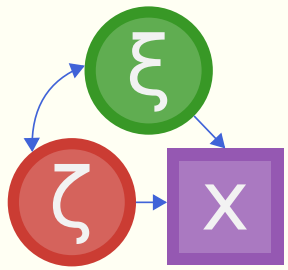
An hour in our life

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



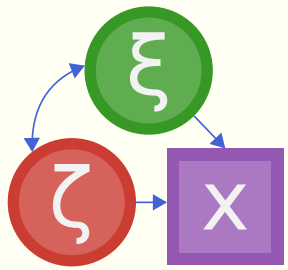
Two hours in our life

- Simulation in Juila works (converges as it should)



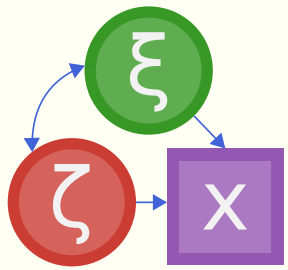
Two hours in our life

- 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.



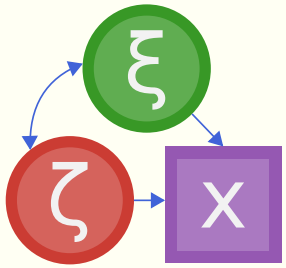
Why?

- 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



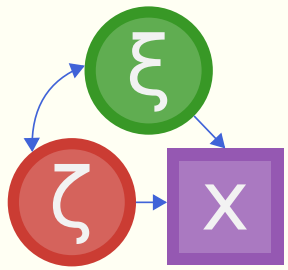
But why?

convenience

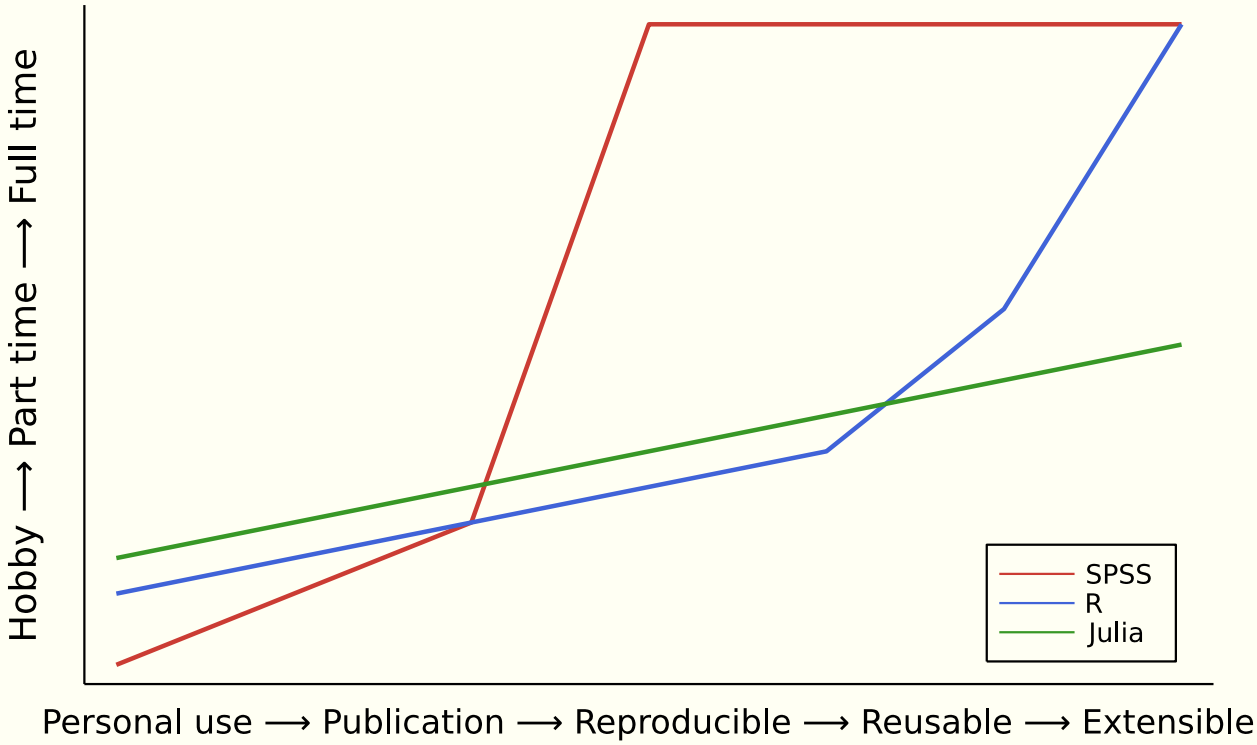


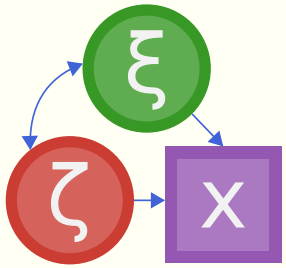
How to improve convenience?

1. Extensible Software
2. Documentation
3. User Interface

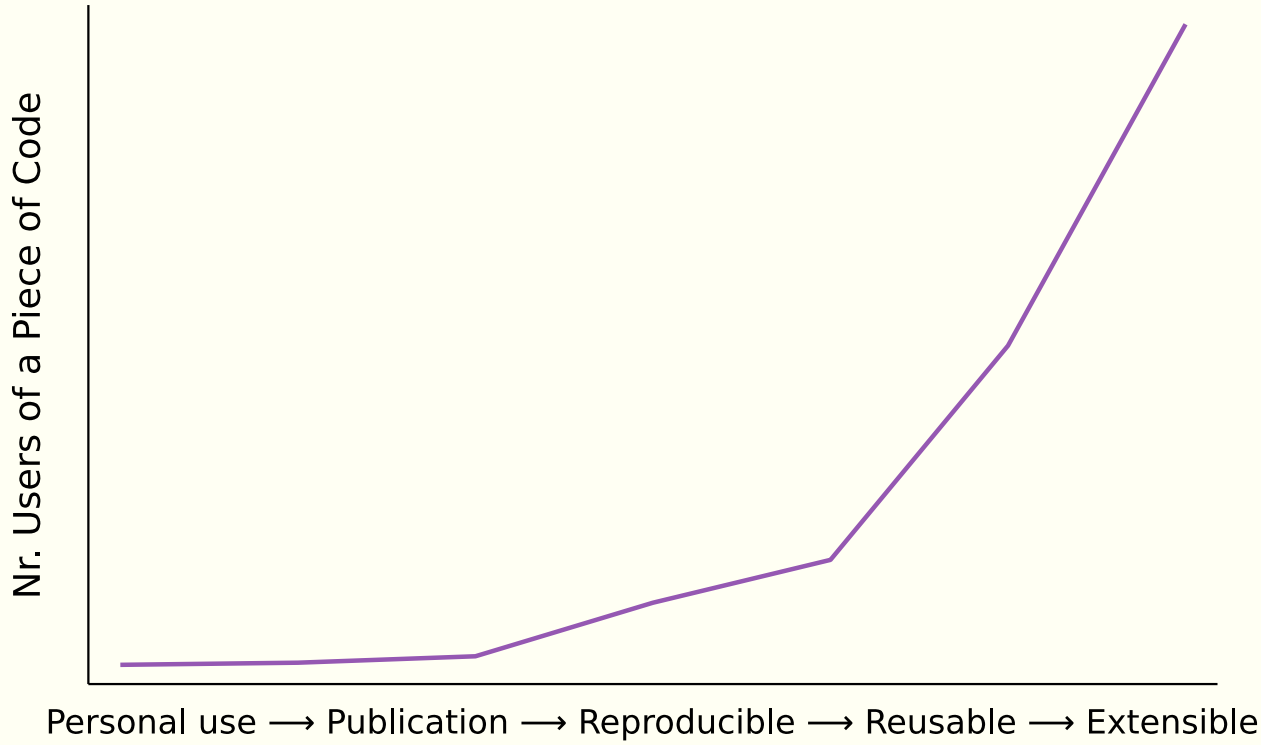


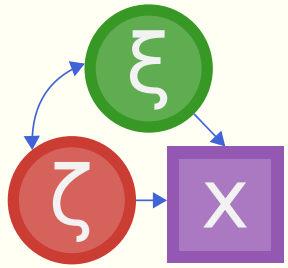
Time is limited





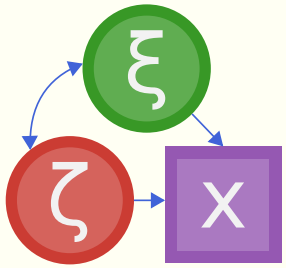
The leverage of extensible software





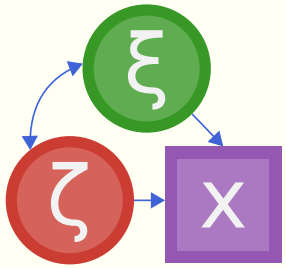
Documentation

- Documentation for users
- Documentation for contributors/developers



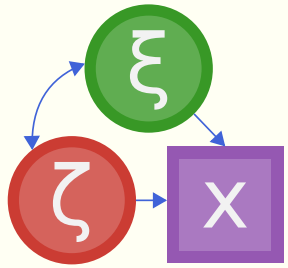
Documentation

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



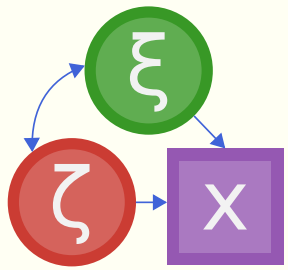
Documentation

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

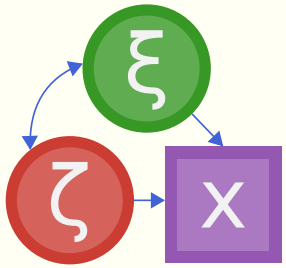


User Interface

- Frictionless
- Connected to prior knowledge



Less Abstract



StructuralEquationModels.jl