Extensible Software for Research

principles and an example in julia

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Contents

- Why should you care?
- How do you get there?

Research Software Personas

- research software engineers
- statistics researcher
- applied user

A day in the live of …

a statistics researcher

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

Now we need software

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

What's the fastest way to get there?

existing software

It would be nice if they could extend existing software

But ...

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

these hurdles are often too high!

A day in the live of …

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

- to deploy: put their code on github
  - bad user interface, no documentation
  - missing features
  - incompatible to existing software

My Experience

- from R $\rightarrow$ julia
- most R packages are very hard to extend
- most julia packages are very easy to extend

Culture

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

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!

Two modes of extension

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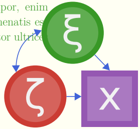


Why julia?

In Julia, everything has a type:

```
a = 1.0
typeof(a) # Float64

b = ”hello”
typeof(b) # String
```

Why julia?

You can define your own types:

```julia
struct ClockTime{T}
    time::T
end

my_time = ClockTime(5.0) # ClockTime{Float64}(5.0)
my_time.time # 5.0
```

Why julia?

A function is a collection of methods:

```
typeof(1.0) # Float64
typeof(1) # Int64

@code_llvm 6.0*7.0
@code_llvm 6*7

methods(*)
```

Why julia?

We can write our own addition:

```julia
import Base: +

function +(x::ClockTime{T}, y::ClockTime{T}) where{T}
    return ClockTime((x.time + y.time) % T(24))
end

my_time = ClockTime(11.2)
your_time = ClockTime(18.4)

our_time = my_time + your_time
```

Goal achieved

We have just written extensible code.

I have memory problems, and I only care about full hours.

```
my_time = ClockTime(UInt8(5))
your_time = ClockTime(UInt8(8))

our_time = my_time + your_time
```

Why julia?

I want to multiply sparse matrices of clock times

```julia
using SparseArrays

import Base: zero, *

function *(x::T, y::ClockTime{T}) where T
    return ClockTime((x * y.time) % T(24))
end

zero(x::ClockTime{T}) where T = ClockTime(zero(T))
zero(::Type{ClockTime{T}}) where T = ClockTime(zero(T))
```

Why julia?

Let’s define some matrices!

```
a = zeros(ClockTime{Float64}, 20, 20)

a[1,1] = ClockTime(5.0)
a[1,2] = ClockTime(11.673)
a[6,9] = ClockTime(17.23)
a[16,4] = ClockTime(20.87)

a_sparse = sparse(a)

b = zeros(20, 20)
b[3,9] = 1
b[6,9] = sqrt(2)
b[19,1] = π
b[4,5] = e

b_sparse = sparse(b)
```

Why julia?

```
using BenchmarkTools

@benchmark b_sparse*a_sparse

BenchmarkTools.Trial: 10000 samples with 199 evaluations.
 Range (min … max):  422.864 ns …  12.295 μs
 Time  (median):     453.877 ns
 Time  (mean ± σ):   566.627 ns ± 648.451 ns
Memory estimate: 2.22 KiB

@benchmark b*a

BenchmarkTools.Trial: 10000 samples with 1 evaluation.
 Range (min … max):  56.683 μs …  1.323 ms
 Time  (median):     57.111 μs
 Time  (mean ± σ):   59.411 μs ± 18.922 μs
 Memory estimate: 23.75 KiB
```

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

- 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.

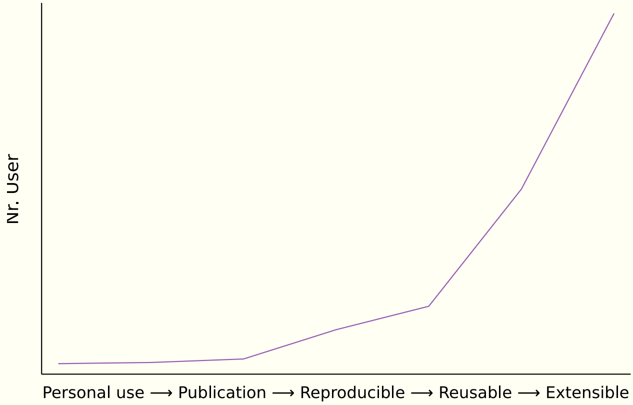
Why?

- 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

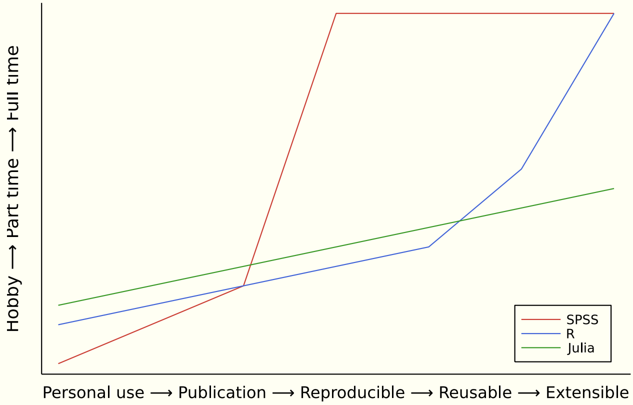
The leverage of convenience



How to improve convenience?

1. Extensible Software
2. Dokumentation
3. User Interface

Time is limited



Dokumentation

- Dokumentation for users
- Dokumentation for contributors/developers

User Interface

- Frictionless
- Connected to prior knowledge