Programming best practices

Agent-based modelling, Konstanz, 2024

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Plan

- This week, we will look at a few practices that have the potential to make your code better
- Here, "better" can mean:
  - more logical organization of code
  - better performance (faster running, and/or less memory consumption)
- In addition, we will wrap up the first half of the course and talk about any issues/challenges you may have run into

> **Note**
>
> Today's lecture requires the following Julia packages:
>
> - Agents
> - BenchmarkTools
> - Random
>
> It would be a good idea to install them now, if your system does not already have them.

- The "best practices" bit of today's session is broken down into three major topics:
  1. Abstract types, inheritance and multiple dispatch
  2. Benchmarking
  3. Random numbers

Abstract types and inheritance

- Some weeks ago, we defined a variational learner type which lives in an unstructured population
- Last week, we defined one that lives in a grid space

- Two possible strategies:

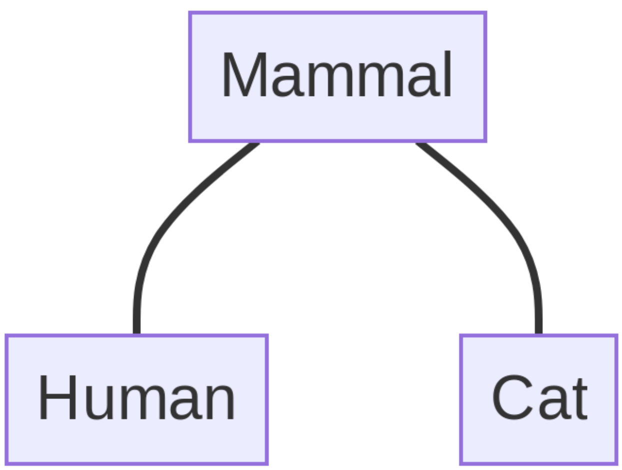
1. Name both types `VariationalLearner`

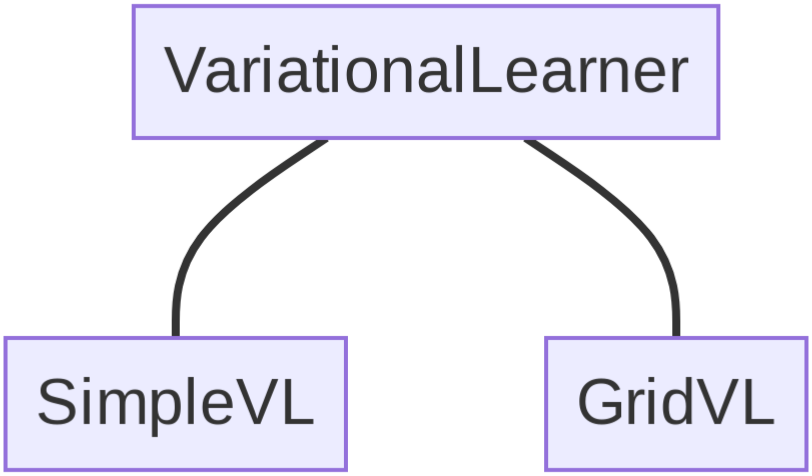
   - pro: we can reuse the functions we've written that take `VariationalLearner` objects as arguments, such as `speak`, `learn!` and `interact!`
   - con 1: we can't use both types in the same code
   - con 2: Julia does not deal well with type redefinitions, forcing a restart when moving from one definition to the other

2. Give the new type a new name, such as `GridVL`

   - pro: no complaints from Julia
   - con: we can't reuse our functions, since they're defined for `VariationalLearner` objects

- A neat solution to this problem is to start thinking about **type hierarchies**
- Intuitively: types can have hierarchical relationships, a bit like biological taxonomies



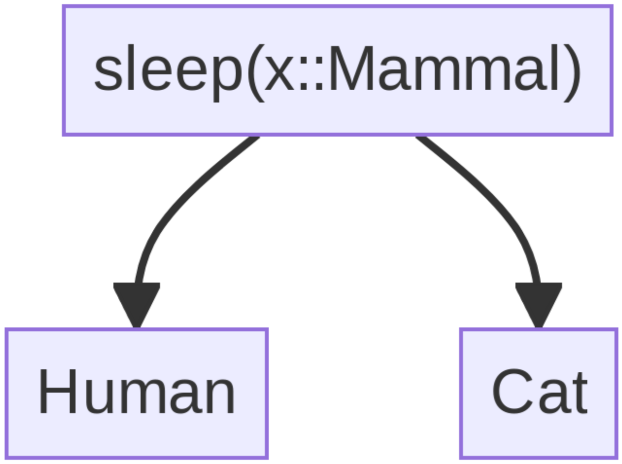


Important

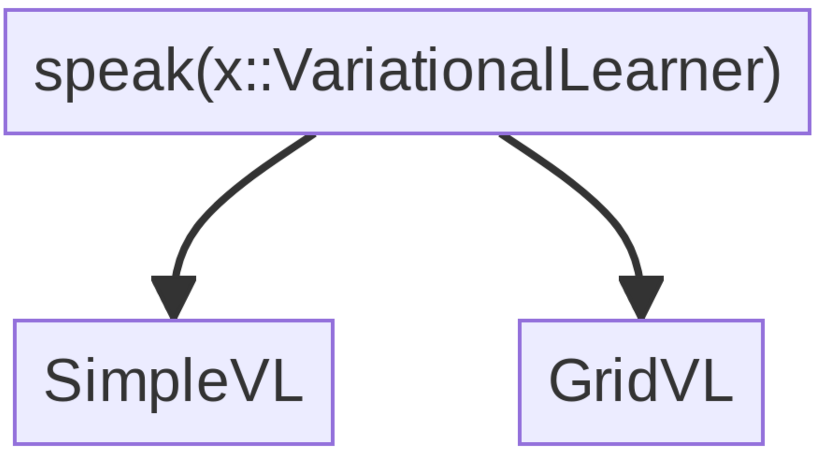
From now on, I will use `SimpleVL` to refer to our original `VariationalLearner`, i.e. the type that lives in an unstructured population.
`VariationalLearner` from now on will denote the **supertype** of all "variational learnery" things.

Abstract types and inheritance

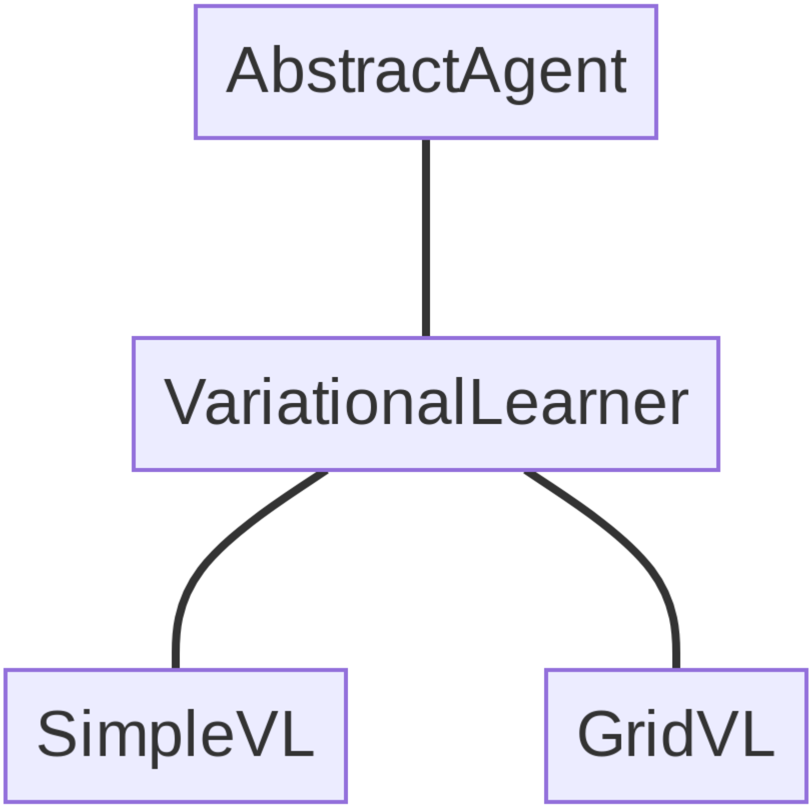
- The point of this is: a function can be defined for the supertype, whose subtypes then **inherit** that function
- E.g. we can define a `sleep` function for `Mammal`
- Both `Human` and `Cat` inherit this function, and so we don't need to define one for them separately



- Similarly, we can define `speak` for the supertype `VariationalLearner`
- Then both `SimpleVL` and `GridVL` have access to this function



- In Julia such "supertypes" are known as **abstract types**
- They have no fields; they only exist to define the type hierarchy
- Inheritance relations are defined using a special `<:` operator
- To use Agents.jl, our `VariationalLearner` abstract type itself needs to inherit from `AbstractAgent`




```
abstract type VariationalLearner <: AbstractAgent end

mutable struct SimpleVL <: VariationalLearner
  # code goes here...
end

@agent struct GridVL(GridAgent{2}) <: VariationalLearner
  # code goes here...
end

function speak(x::VariationalLearner)
  # code goes here...
end
```

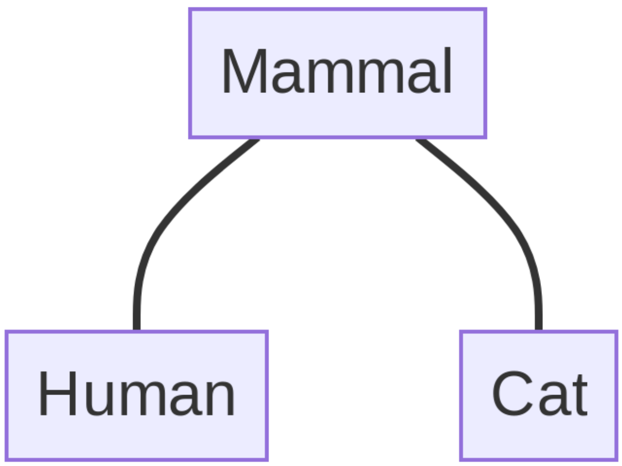
- We can now do things like:

```
bob = SimpleVL(0.1, 0.01, 0.4, 0.1)

speak(bob)
```

even though `speak` wasn't defined for `SimpleVL`

Multiple dispatch



- What if `Cat` needs to sleep differently from other `Mammals`?
- Easy: we simply define a function `sleep(x::Cat)`
- Other `Mammals` will use the default function `sleep(x::Mammal)`

- In Julia, this is called **multiple dispatch**
- One and the same function (here, `sleep`) can have multiple definitions depending on the argument's type
- These different definitions are known as **methods** of the function
- When figuring out which method to use, the compiler tries to apply the method that is deepest in the type hierarchy, moving upwards if such a definition isn't found
  - e.g. in our example calling `sleep` on `Human` will trigger the `sleep` method defined for `Mammal`, since no `sleep` method specific to `Human` has been defined

Our VL code so far

> Tip
>
> You can also download this code: VL.jl. To use:
>
> ```
> include("VL.jl")
> using .VL
> ```
>
> If VSCode complains about modules, simply delete the first and last lines of the file and include it like so:
>
> ```
> include("VL.jl")
> ```

```
module VL

# Agents.jl functionality
using Agents

# we need this package for the sample() function
using StatsBase

# we export the following types and functions
export VariationalLearner
export SimpleVL
export GridVL
export speak
export learn!
export interact!
export VL_step!


# abstract type
abstract type VariationalLearner <: AbstractAgent end

# variational learner type on a 2D grid
@agent struct GridVL(GridAgent{2}) <: VariationalLearner
  p::Float64      # prob. of using G1
  gamma::Float64  # learning rate
  P1::Float64     # prob. of L1 \ L2
  P2::Float64     # prob. of L2 \ L1
end
```

```julia
# "simple" variational learner in unstructured population
mutable struct SimpleVL <: VariationalLearner
  p::Float64      # prob. of using G1
  gamma::Float64  # learning rate
  P1::Float64     # prob. of L1 \ L2
  P2::Float64     # prob. of L2 \ L1
end

# makes variational learner x utter a string
function speak(x::VariationalLearner)
  g = sample(["G1", "G2"], Weights([x.p, 1 - x.p]))

  if g == "G1"
    return sample(["S1", "S12"], Weights([x.P1, 1 - x.P1]))
  else
    return sample(["S2", "S12"], Weights([x.P2, 1 - x.P2]))
  end
end

# makes variational learner x learn from input string s
function learn!(x::VariationalLearner, s::String)
  g = sample(["G1", "G2"], Weights([x.p, 1 - x.p]))

  if g == "G1" && s != "S2"
    x.p = x.p + x.gamma * (1 - x.p)
  elseif g == "G1" && s == "S2"
    x.p = x.p - x.gamma * x.p
  elseif g == "G2" && s != "S1"
    x.p = x.p - x.gamma * x.p
  elseif g == "G2" && s == "S1"
    x.p = x.p + x.gamma * (1 - x.p)
  end

  return x.p
end

# makes two variational learners interact, with one speaking
# and the other one learning
function interact!(x::VariationalLearner, y::VariationalLearner)
  s = speak(x)
  learn!(y, s)
end
```

```
# steps a model
function VL_step!(agent, model)
  interlocutor = random_nearby_agent(agent, model)
  interact!(interlocutor, agent)
end

end   # this closes the module
```

Benchmarking

- When working on larger simulations, it is often important to know how long some function takes to run
- It may also be important to know how much memory is consumed
- Both of these things can be measured using the `@benchmark` macro defined by BenchmarkTools.jl

- Example:

```
using BenchmarkTools

@benchmark sum(1:1_000_000_000)
```

```
BenchmarkTools.Trial: 10000 samples with 1000 evaluations.
 Range (min … max):   1.300 ns … 28.568 ns    GC (min … max): 0.00% … 0.00%
 Time  (median):      1.497 ns                GC (median):    0.00%
 Time  (mean ±  ):   1.538 ns ±  0.535 ns    GC (mean ±  ):  0.00% ± 0.00%



  1.3 ns         Histogram: frequency by time        1.98 ns <

 Memory estimate: 0 bytes, allocs estimate: 0.
```

All roads lead to Rome, but they're not all equally fast…

- Suppose we want to calculate the square root of all numbers between 0 and 100,000 and put them in an array
- One way of doing this:

```
result = []   # empty array
for x in 0:100_000
  append!(result, sqrt(x))   # put √x in array
end
```

```
@benchmark begin
  result = []   # empty array
  for x in 0:100_000
    append!(result, sqrt(x))   # put √x in array
  end
end
```

```
BenchmarkTools.Trial: 3370 samples with 1 evaluation.
 Range (min … max):  1.166 ms …   5.402 ms   GC (min … max): 0.00% …  0.00%
 Time  (median):     1.333 ms                GC (median):    0.00%
 Time  (mean ± ):   1.481 ms ± 509.888  s   GC (mean ± ):  8.66% ± 14.22%



  1.17 ms      Histogram: log(frequency) by time      4.11 ms <

 Memory estimate: 3.35 MiB, allocs estimate: 100012.
```

- Another way:

```
result = zeros(100_000 + 1)
for x in 0:100_000
  result[x+1] = sqrt(x)   # put √x in array
end
```

```
@benchmark begin
  result = zeros(100_000 + 1)
  for x in 0:100_000
    result[x+1] = sqrt(x)   # put √x in array
  end
end
```

```
BenchmarkTools.Trial: 10000 samples with 1 evaluation.
 Range (min … max):   99.881  s … 714.503  s   GC (min … max): 0.00% … 47.34%
 Time  (median):     102.953  s                GC (median):    0.00%
 Time  (mean ± ):   110.683  s ±  41.915  s   GC (mean ± ):  4.14% ±  8.85%
```

```
  99.9  s       Histogram: log(frequency) by time        384  s <

 Memory estimate: 781.36 KiB, allocs estimate: 2.
```

- A third possibility:

```
result = [sqrt(x) for x in 0:100_000]
```

```
@benchmark result = [sqrt(x) for x in 0:100_000]
```

```
BenchmarkTools.Trial: 10000 samples with 1 evaluation.
 Range (min … max):  77.961  s … 645.886  s   GC (min … max): 0.00% … 49.10%
 Time  (median):     79.247  s                GC (median):    0.00%
 Time  (mean ±  ):   84.362  s ±  28.078  s   GC (mean ±  ):  3.25% ±  8.20%

  78  s          Histogram: log(frequency) by time       248  s <

 Memory estimate: 781.36 KiB, allocs estimate: 2.
```

- A fourth way:

```
result = sqrt.(0:100_000)
```

```
@benchmark result = sqrt.(0:100_000)
```

```
BenchmarkTools.Trial: 10000 samples with 1 evaluation.
 Range (min … max):  78.122  s … 666.327  s   GC (min … max): 0.00% … 49.06%
 Time  (median):     79.081  s                GC (median):    0.00%
 Time  (mean ±  ):   84.377  s ±  29.139  s   GC (mean ±  ):  3.43% ±  8.37%

  78.1  s       Histogram: log(frequency) by time       255  s <

 Memory estimate: 781.36 KiB, allocs estimate: 2.
```

Summing up the findings

Procedure	Median time	Mem. estimate
Growing an array	~1.4 ms	~3.4 MiB
Adding to 0-array	~0.1 ms	~0.8 MiB
Array comprehension	~80 μs	~0.8 MiB
Broadcasting	~80 μs	~0.8 MiB

- Lesson: try to avoid growing (and shrinking!) arrays whenever possible
- Of course, sometimes this is practically unavoidable (such as when adding and removing agents from a population)
- Another lesson: if procedure X gets repeated very many times in a simulation, try to make X as efficient as possible
  - Procedures which are only carried out once or a few times (such as initializing a population) don't matter so much

Random numbers

- In the first lecture, we talked about the importance of (pseudo)random numbers in ABM simulations
- E.g. whenever an agent needs to be sampled randomly, the computer needs to generate a random number
- There are two important issues here:
  1. Reproducibility – how to obtain the same sequence of "random" numbers if this is desired
  2. Consistency – making sure that whenever a random number is drawn, it is drawn using the same generator (i.e. from the same sequence)

Reproducibility

- Recall: a PRNG (pseudorandom number generator) generates a **deterministic** sequence which appears random
- The sequence is generated from an initial **seed** number
- If you change the seed, you obtain different sequences
- Normally, when Julia is started, the PRNG is seeded with a different seed every time
  - Hence, you obtain different sequences

Reproducibility: illustration

- To illustrate this, suppose you want to toss a coin 10 times. This is easy:

```
rand(["heads", "tails"], 10)
```

```
10-element Vector{String}:
 "tails"
 "tails"
 "tails"
 "heads"
 "tails"
 "heads"
 "heads"
 "tails"
 "tails"
 "heads"
```

- Now restart Julia and execute the same thing. You will get a different result:

```
# here, restart Julia...

rand(["heads", "tails"], 10)
```

```
10-element Vector{String}:
 "tails"
 "tails"
 "heads"
 "heads"
 "heads"
 "heads"
 "tails"
 "tails"
 "tails"
 "heads"
```

- If you want to make sure the exact same sample is obtained, you can seed the PRNG manually after startup
- For example, seed with the number 123:

```julia
using Random
Random.seed!(123)

rand(["heads", "tails"], 10)
```

```
10-element Vector{String}:
 "tails"
 "tails"
 "tails"
 "heads"
 "tails"
 "heads"
 "heads"
 "tails"
 "tails"
 "heads"
```

Reproducibility

- Why would you do this? Wasn't randomness kind of the point?
- Suppose someone (e.g. your supervisor, or an article reviewer) wants to check that your code actually produces the results you have reported
- Using a manually seeded PRNG makes this possible

Consistency

- It is possible to have multiple PRNGs running simultaneously in the same code
- This is rarely desired, but may happen by mistake…
- For example, when you call `StandardABM`, Agents.jl will set up a new PRNG by default
- If your own functions (such as `speak` or `learn!`) utilize a different PRNG, you may run into problems
  - For one, it will be difficult to ensure reproducibility
- To avoid this, pass `Random.default_rng()` as an argument to `StandardABM` when creating your model:

```julia
using Agents
using Random
include("VL.jl")
using .VL
```

```julia
Random.seed!(123)

space = GridSpace((10, 10))

model = StandardABM(GridVL, space; agent_step! = VL_step!,
                    rng = Random.default_rng())
```

Reminder: not all agents are humans!

https://youtu.be/UzgMw3SJn2s

Looking ahead

- Homework:
    1. **Keep thinking about your project!**
    2. Read Smaldino (2023), chapter 10
- The following two weeks constitute a break for us: the first one is the lecture-free period, the second one is consolidation week ("Vertiefungswoche")
- After this break, you need to
    1. have a project team (or have decided to work on your own)
    2. have at least an initial idea about your project topic
- If you struggle, I'm happy to help! You can always write me an email, and/or come to see me in my office.

Smaldino, Paul E. 2023. *Modeling Social Behavior: Mathematical and Agent-Based Models of Social Dynamics and Cultural Evolution*. Princeton, NJ: Princeton University Press.