

Notes 5: Efficiency

Chris Paciorek

2025-02-04

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Introduction

This document is the fifth of a set of notes, this document focusing on writing efficient Julia code. The notes are not meant to be particularly complete in terms of useful functions (Google and LLMs can now provide that quite well), but rather to introduce the language and consider key programming concepts in the context of Julia.

Given that, the document heavily relies on demos, with interpretation in some cases left to the reader.

Timing

Being able to time code is critical for understanding and improving efficiency.

Compilation time

With Julia, we need to pay particular attention to the effect of just-in-time (JIT) compilation on timing. The first time a function is called with specific set of argument types, Julia will compile the method that is invoked. We generally don't want to time the compilation, only the run time, assuming the function will be run repeatedly with a given set of argument types.

`@time` is a macro that will time some code. However, it's better to use `@btime` from `BenchmarkTools` as that will run the code multiple times and will make sure not to count the compilation time.

```
function myexp!(x)
    for i in 1:length(x)
        x[i] = exp(x[i])
    end
end

n = Int(1e7)
y = rand(n);
@time myexp!(y) ## Compilation time included.
```

0.075221 seconds (2.62 k allocations: 178.000 KiB, 10.40% compilation time)

```
y = rand(n);
@time myexp!(y) ## Compilation time not included.
```

0.069284 seconds

```
using BenchmarkTools
```

```
y = rand(n);
@btime myexp!(y)
```

59.500 ms (0 allocations: 0 bytes)

⚠ Exercise

How long does that loop take in R or Python? What about a vectorized solution in R or Python?

We can time a block of code, but I'm not sure what Julia does in terms of JIT for code that is not in functions. You may discover more in working on the fourth problem of PS2.

```
@btime begin
y = 3
z = 7
end
```

1.299 ns (0 allocations: 0 bytes)

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Profiling

Profiling involves timing each step in a set of code. One can use the `Profile` module to do this in Julia.

One thing to keep in mind when profiling is whether the timing for nested function calls is included in the timing of the function that makes the nested function calls.

```

using Profile

function ols_slow(y::Vector{<:Number}, X::Matrix{<:Number})
    xtx = X'X;
    xty = X'y;
    xtxinverse = inv(xtx); ## This is an inefficient approach.
    return xtxinverse * xty
end

n = Int(1e4)
p = 2000
y = randn(n);
X = randn((n,p));

## Run once to avoid profiling JIT compilation.
coefs = ols_slow(y, X);

```

Directly interpreting the Profile output can be difficult. In this case, if we ran the following code, we'd see very long, hard-to-interpret information.

```

@profile coefs = ols_slow(y, X)
Profile.print()

```

Instead let's try a visualization. There are other Julia packages for visualizing profiler output. Some might be better than this. (I tried `ProfileView` and liked `StatProfilerHTML` better.)

```

using ProfileView
@profview ols_slow(y, X)

using StatProfilerHTML
@profilehtml ols_slow(y, X)

```

`@profilehtml` produces [this output](statprof/index.html), which can in some ways be hard to interpret, but the color-coded division between `inv`, *and* gives us an idea of where time is being spent. That output might not show up fully in the links - you might need to run the code above yourself.

Pre-allocation

In R (also with numpy arrays in Python), it's a bad idea to iteratively increase the size of an object, such as doing this:

```

n <- 5000
x <- 1
for(i in 2:n)
    x <- c(x, i)

```

Python lists [handle this much better](#) by allocating increasingly large additional amounts of memory

as the object grows when using `.append()`.

Let's consider this in Julia.

```
function fun_prealloc(n)
    x = zeros(n);
    for i in 1:n
        x[i] = i;
    end
    return x
end

function fun_grow(n)
    x = Float64[];
    for i in 1:n
        push!(x, i);
    end
    return x
end

using BenchmarkTools

n = 100000000
@btime x1 = fun_prealloc(n);
```

331.161 ms (2 allocations: 762.94 MiB)

```
@btime x2 = fun_grow(n);
```

1.679 s (23 allocations: 1019.60 MiB)

That indicates that it's better to pre-allocate memory in Julia, but the time does not seem to grow as order of n^2 as it does in R or with numpy arrays. So that suggests Julia is growing the array in a smart fashion.

We can verify that by looking at the memory allocation information returned by `@btime`.

For `fun_prealloc`, we see an allocation of ~800 MB, consistent with allocating an array of 100 million 8 byte floats. (It turns out the "second" allocation occurs because we are running `@btime` in the global scope).

For `fun_grow`, we see 23 allocations of ~1 GB, consistent with Julia growing the array in a smart fashion but with some additional memory allocation.

If the array were reallocated each time it grew by one, we'd allocate and copy $1+2+\dots+n = n(n+1)/2$ numbers in total over the course of the computation (but not all at once), which would take a lot of time.

Vectorization

As we've seen, the [vectorized](#) versions of functions have a dot after the function name (or before an operator).

```
x = ["spam", 2.0, 5, [10, 20]]  
length(x)
```

```
4
```

```
length.(x)
```

```
4-element Vector{Int64}:
```

```
4
```

```
1
```

```
1
```

```
2
```

```
map(length, x)
```

```
4-element Vector{Int64}:
```

```
4
```

```
1
```

```
1
```

```
2
```

```
x = [2.1, 3.1, 5.3, 7.9]  
x .+ 10
```

```
4-element Vector{Float64}:
```

```
12.1
```

```
13.1
```

```
15.3
```

```
17.9
```

```
x + x
```

```
4-element Vector{Float64}:
```

```
4.2
```

```
6.2
```

```
10.6
```

```
15.8
```

```
x .> 5.0
```

```
4-element BitVector:
```

```
0
```

```
0
```

```
1
```

```
1
```

```
x == 3.1
```

```
4-element BitVector:
```

```
0
1
0
0
```

Unlike in Python or R, it shouldn't matter for efficiency if you use a vectorized function or write a loop, because with Julia's just-in-time compilation, the compiled code should be similar. (This assumes your code is inside a function.) So the main appeal of vectorization is code clarity and ease of writing the code.

We can automatically use the dot vectorization with functions we write:

```
function plus3(x)
    return x + 3
end
```

```
plus3.(x)
```

```
4-element Vector{Float64}:
```

```
5.1
6.1
8.3
10.9
```

This invokes `broadcast(plus3, args...)`.

Broadcasting will happen over multiple arguments if more than one argument is an array.

Consider the difference between the following vectorized calls:

```
x = randn(5)
= 10;
y1 = x .+ .* randn.()
y2 = x .+ .* randn()
print((y1 - x) / )
print((y2 - x) / )
```

```
[0.4170656514220214, -0.8850493432768529, 0.1260295830134405, -0.22061211497134475, -0.19497228825436]
```

That's perhaps a bit surprising given one might think that because the multiplication is done first, the `.* randn.()` might produce a scalar, as it does if you just run `.* randn.()` on its own.

Loop fusion

If one runs a vectorized calculation that involves multiple steps in a language like R or Python, there are some inefficiencies.

Consider this computation:

```
x = tan(x) + 3*sin(x)
```

If run as vectorized code in a language like R or Python, it's much faster than using a loop, but it does have some downsides.

- First, it will use additional memory (temporary arrays will be created to store `tan(x)`, `sin(x)`, `3*sin(x)`). (We can consider what the abstract syntax tree would be for that calculation.)
- Second, multiple for loops will have to get executed when the vectorized code is run, looping over the elements of `x` to calculate `tan(x)`, `sin(x)`, etc. (For example in R or Python/numpy, multiple for loops would get run in the underlying C code.)

In contrast, running via a for loop (in R or Python or Julia) avoids the temporary arrays and involves a single loop:

```
for i in 1:length(x)
    x[i] = tan(x[i]) + 3*sin(x[i])
end
```

Thankfully, Julia “fuses” the loops of vectorized code automatically when one uses the dot syntax for vectorization, so one shouldn't suffer from the downsides of vectorization. One could of course use a loop in Julia, and it should be fast, but it's more code to write and harder to read.

Memory allocation with loop fusion

Let's look at memory allocation when putting the code into a function:

```
function mymath(x)
    return tan(x) + 3*sin(x)
end

function mymathloop(x)
    for i in 1:length(x)
        x[i] = tan(x[i]) + 3*sin(x[i])
    end
    return x
end

n = 100000000;
x = rand(n);

@btime y = mymath.(x);
```

```
2.525 s (3 allocations: 762.94 MiB)
```

```
@btime y = mymathloop(x);
```

```
3.066 s (0 allocations: 0 bytes)
```

Note that it appears only 800 MB (~760 MiB; ~0.95 MiB = 1 MB) are allocated (for the output) in the (presumably) fused operation, rather than multiples of 800 MB for various temporary arrays that one might expect to be created.

And in the loop, there is no allocation. We might expect some allocation of scalars, but those are probably handled differently than allocating memory for arrays off the [heap](#). I’ve seen some information for how Julia handles allocation of space for immutable objects (including scalars and strings), but I haven’t had a chance to absorb that.

Cases without loop fusion

We can do addition or subtraction of two arrays or multiplication/division with array and scalar without the “dot” vectorization. However, as seen with the additional memory allocation here, the loop fusion is not done.

```
function mymath2(x)
    return 3*x+x/7
end

@btime y = mymath2(x);
```

1.065 s (6 allocations: 2.24 GiB)

In contrast, here we see only the allocation for the output object.

```
@btime y = mymath2.(x);
```

454.403 ms (3 allocations: 762.94 MiB)

Cache-aware programming and array storage

Julia stores the values in a matrix contiguously column by column (and analogously for higher-dimensional arrays).

We should therefore access matrix elements within a column rather than within a row. Why is that?

Memory access and the cache

When a value is retrieved from main memory into the CPU cache, a block of values will be retrieved, and those will generally include the values in the same column but (for large enough arrays) not all the values in the same row. If subsequent operations work on values from that column, the values won’t need to be moved into the cache. (This is called a “cache hit”).

Let’s first see if it makes a difference when using Julia’s built-in `sum` function, which can do the reduction operation on various dimensions of the array.

```
using Random
using BenchmarkTools

nr = 800000;
nc = 100;
A = randn(nr, nc); # long matrix
tA = randn(nc, nr); # wide matrix
```



```
function sum_by_column(X)
    return sum(X, dims=1)
end

function sum_by_row(X)
    return sum(X, dims=2)
end

@btime tmp = sum_by_column(A);
```

39.221 ms (1 allocation: 896 bytes)

```
@btime tmp = sum_by_row(tA);
```

43.396 ms (5 allocations: 976 bytes)

There's little difference.

Are we wrong about how the cache works? Probably not; rather it's probably that Julia's `sum()` is set up to take advantage of how the cache works by being careful about the order of operations used to sum the rows or columns.

Exercise

How could you program the for loops involved in row-wise summation to be efficient when a matrix is stored column-major given how caching work? If you retrieve the data by column, how do you get the row sums?

In contrast, if we manually loop over rows or columns, we do see a big (almost order-of-magnitude) difference.

```
@btime tmp = [sum(A[:,col]) for col in 1:size(A,2)];
```

135.859 ms (405 allocations: 610.36 MiB)

```
@btime tmp = [sum(A[row,:]) for row in 1:size(A,1)];
```

778.063 ms (4798474 allocations: 750.71 MiB)

So while one lesson is to code with the cache in mind, another is to use built-in functions that are probably written for efficiency.

Exercise

In your own work, can you think of an algorithm and associated data structures where one has to retrieve a lot of data and one would want to think about cache hits and misses? In general the idea is that if you retrieve a value, try to make use of the nearby values at that same time, rather than retrieving the nearby values later on in the computation.

Store values contiguously in memory

If we are storing an array of all the same type of values, these can be stored contiguously. That's not the case with abstract types.

For example, here `Real` values can vary in size.

```
a = Real[]
sizeof(a)
push!(a, 3.5)
sizeof(a)
push!(a, Int16(2))
sizeof(a[2])
sizeof(a)
```

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And we see that having an array of Reals is bad for performance. As part of this notice the additional allocation.

```
using LinearAlgebra
n = 100;
A = rand(n, n);
@btime tmp = A'A; # Equivalent to A' * A or transpose(A) * A.
```

45.131 s (3 allocations: 78.19 KiB)

100×100 Matrix{Float64}:

31.3434	28.2991	23.3785	22.2482	...	22.8816	23.144	25.6776	23.1401
28.2991	40.381	26.3591	28.3626		25.8735	27.3842	29.9671	26.2799
23.3785	26.3591	32.6379	23.8486		25.1776	23.2087	27.3518	23.6795
22.2482	28.3626	23.8486	31.2422		22.1873	23.8796	25.6417	22.2948
24.3474	29.1835	26.0694	26.0089		25.9571	28.0218	28.0398	23.3216
24.2326	28.4558	26.0709	25.0149	...	25.407	27.7716	28.9334	24.154
24.4235	27.5001	24.3027	24.3611		24.7207	25.1982	26.7347	25.5547
22.6136	26.6354	25.0601	23.7247		26.0032	22.8209	25.973	23.3979
25.0136	28.6411	23.6948	23.5412		24.0284	24.2705	28.0546	25.2663
22.4926	26.0361	25.136	23.4652		23.6698	24.1082	27.5221	21.1363
21.0514	25.0219	21.9994	22.6873	...	22.9995	23.0049	25.1662	23.2241
24.9928	27.1519	24.073	23.8966		23.7997	24.0047	27.19	23.5732
27.7282	28.9997	27.4725	25.8123		26.6285	26.9111	28.3441	25.1172
23.3272	27.7131	24.4456	22.9734		22.1652	25.582	26.7593	22.6326
23.9461	29.2237	25.4995	25.3786		24.2368	27.2959	27.5395	25.5569
23.9127	27.8013	26.6871	24.2284	...	26.1844	27.3045	28.2586	26.2357
25.0488	27.6548	24.1603	22.9998		25.6098	24.2775	26.4557	23.6312
25.884	30.9974	27.4021	26.2885		26.5123	27.2523	29.6701	26.254
25.3851	27.0305	25.8697	23.3191		25.1691	24.5485	27.5205	25.2234
24.5266	29.1042	26.2418	25.2955		23.7441	26.1753	26.3628	24.2068
23.3792	27.1223	24.3354	23.7604	...	22.5078	26.2251	27.2906	23.7979

22.8816	25.8735	25.1776	22.1873	32.8427	22.7119	26.4834	22.0585
23.144	27.3842	23.2087	23.8796	22.7119	32.9915	25.9671	23.43
25.6776	29.9671	27.3518	25.6417	26.4834	25.9671	36.366	24.7744
23.1401	26.2799	23.6795	22.2948	22.0585	23.43	24.7744	29.8628

```
rA = convert{Array{Real}, A};
@btime tmp = rA'rA;
```

41.008 ms (2030004 allocations: 31.05 MiB)

Lookup speed

If we have code that needs to retrieve a lot of values from a data structure, it's worth knowing the situations in which we can expect that lookup to be fast.

Lookup in arrays is fast ($O(1)$; i.e., not varying with the size of the array) because of the “random access” aspect of RAM (random access memory).

```
n=Int(1e7);

x = randn(n);
ind = Int(n/2);
@btime x[ind];
```

19.613 ns (1 allocation: 16 bytes)

```
y = rand(10);
@btime y[5];
```

19.994 ns (1 allocation: 16 bytes)

Next, lookup in a Julia dictionary is fast $O(1)$ because dictionaries using hashing (like Python dictionaries and R environments).

```
function makedict(n)
    d=Dict{String,Int}()
    for i in 1:n
        push!(d, string(i) => i)
    end
    return d
end

## Make a large dictionary, with keys equal to strings representing integers.
d = makedict(n);
indstring = string(ind);
@btime d[indstring];
```

42.118 ns (1 allocation: 16 bytes)

Finally, let's consider tuples. Lookup by index is quite slow, which is surprising as I was expecting it to be similar to lookup in the array, as I think the tuple in this case has values stored contiguously.

```
xt = Tuple(x);  
@btime xt[ind];
```

49.232 ms (1 allocation: 16 bytes)

For named tuples, I'm not sure how realistic this is, since it would probably be a pain to create a large named tuple. But we see that lookup by name is slow, even though we are using a smaller tuple than the array and dictionary above.

```
## Set up a named tuple (this is very slow for large array, so use a subset).  
dsub = makedict(100000);  
xsub = x[1:100000];  
names = Symbol.('x' .* keys(dsub)); # For this construction of tuple, the keys need to be symbols.  
xtnamed = (;zip(names, xsub)...);  
@btime xtnamed.x50000;
```

60.583 s (1 allocation: 16 bytes)

Developing a perspective on speed

Note that while all the individual operations above are fast in absolute terms for a single lookup, for simple operations, we generally want them to be really fast (e.g., order of nanoseconds) because we'll generally be doing a lot of such operations for any sizeable overall computation.

Performance tips

The Julia manual has an [extensive section on performance](#).

We won't dive too deeply into all the complexity, but here are a few key tips, which mainly relate to writing in a way that is aware of the JIT compilation that will happen:

- Code for which performance is important should be inside a function, as this allows for JIT compilation.
- Avoid use of global variables that don't have a type, as that is hard to optimize since the type could change.
- The use of immutable objects can improve performance.
- Have functions always return the same type and avoid changing (or unknown) variable types within a function.