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# Computerphysik

## Vorlesung — Programmiertechniken 3

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Sommersemester 2019

**Website:** <http://www.thp.uni-koeln.de/trebst/Lectures/2019-CompPhys.shtml> (<http://www.thp.uni-koeln.de/trebst/Lectures/2019-CompPhys.shtml>)

## 0. Erinnerung

### Schleifen

```
In [6]: for i in 1:10  
        println(i)  
        end
```

```
1  
2  
3  
4  
5  
6  
7  
8  
9  
10
```

```
In [7]: i = 1
while i <= 10
    println(i)
    i += 1
end
```

```
1
2
3
4
5
6
7
8
9
10
```

## Verzweigungen

```
In [9]: v = 11

if v > 10
    println("Die Variable ist größer als 10.")
elseif v < 5
    println("Die Variable ist kleiner als 5.")
else
    println("Die Variable ist irgendwo dazwischen.")
end
```

Die Variable ist größer als 10.

## Arrays

```
In [10]: a = [5, 1, 8, 9, 3, 7]
```

```
Out[10]: 6-element Array{Int64,1}:
 5
 1
 8
 9
 3
 7
```

```
In [11]: a[3]
```

```
Out[11]: 8
```

```
In [12]: a[3] = 0
```

```
Out[12]: 0
```

In [13]: a

```
Out[13]: 6-element Array{Int64,1}:  
 5  
 1  
 0  
 9  
 3  
 7
```

In [14]: a[100]

```
BoundsError: attempt to access 6-element Array{Int64,1} at index [100]
```

```
Stacktrace:
```

```
[1] getindex(::Array{Int64,1}, ::Int64) at .\array.jl:729  
[2] top-level scope at In[14]:1
```

In [15]: length(a)

```
Out[15]: 6
```

```
In [1]: ?length
```

```
search: length
```

```
Out[1]: length(collection) -> Integer
```

Return the number of elements in the collection.

Use [lastindex](#) [\(@ref\)](#) to get the last valid index of an indexable collection.

## Examples

```
julia> length(1:5)
```

```
5
```

```
julia> length([1, 2, 3, 4])
```

```
4
```

```
julia> length([1 2; 3 4])
```

```
4
```

```
length(A::AbstractArray)
```

Return the number of elements in the array, defaults to `prod(size(A))`.

## Examples

```
julia> length([1, 2, 3, 4])
```

```
4
```

```
julia> length([1 2; 3 4])
```

```
4
```

```
length(s::AbstractString) -> Int
```

```
length(s::AbstractString, i::Integer, j::Integer) -> Int
```

The number of characters in string `s` from indices `i` through `j`. This is computed as the number of code unit indices from `i` to `j` which are valid character indices. With only a single string argument, this computes the number of characters in the entire string. With `i` and `j` arguments it computes the number of indices between `i` and `j` inclusive that are valid indices in the string `s`. In addition to in-bounds values, `i` may take the out-of-bounds value `ncodeunits(s) + 1` and `j` may take the out-of-bounds value `0`.

See also: [isvalid](#) [\(@ref\)](#), [ncodeunits](#) [\(@ref\)](#), [lastindex](#) [\(@ref\)](#), [thisind](#) [\(@ref\)](#), [nextind](#) [\(@ref\)](#), [prevind](#) [\(@ref\)](#).

## Examples

```
julia> length("jμΛIα")  
5
```

```
In [17]: size(a)
```

```
Out[17]: (6,)
```

```
In [20]: Y = rand(2,4,8)
```

```
Out[20]: 2×4×8 Array{Float64,3}:  
[:, :, 1] =  
 0.152435  0.979689  0.0074239  0.420801  
 0.354892  0.150715  0.39802   0.564168  
  
[:, :, 2] =  
 0.618326  0.546292  0.561061  0.122623  
 0.476645  0.131552  0.920055  0.241142  
  
[:, :, 3] =  
 0.952622  0.994377  0.783856  0.856578  
 0.683555  0.737067  0.144527  0.793784  
  
[:, :, 4] =  
 0.828183  0.57101   0.995672  0.589804  
 0.961323  0.0506661 0.272348  0.563574  
  
[:, :, 5] =  
 0.261386  0.466898  0.899692  0.030649  
 0.753715  0.185559  0.48811  0.743139  
  
[:, :, 6] =  
 0.736457  0.263446  0.51642  0.0545521  
 0.773255  0.647353  0.152371 0.354608  
  
[:, :, 7] =  
 0.670055  0.797061  0.298981  0.391179  
 0.301899  0.83288  0.0433871 0.172567  
  
[:, :, 8] =  
 0.761125  0.995194  0.676004  0.459685  
 0.234348  0.507026  0.111185  0.740016
```

```
In [21]: size(Y)
```

```
Out[21]: (2, 4, 8)
```

```
In [18]: X = rand(2,2)
```

```
Out[18]: 2×2 Array{Float64,2}:  
 0.409139  0.590969  
 0.776841  0.329583
```

```
In [19]: size(X)
```

```
Out[19]: (2, 2)
```

```
In [22]: M = rand(2,2)
```

```
Out[22]: 2x2 Array{Float64,2}:  
 0.739909  0.0670009  
 0.997385  0.708088
```

```
In [23]: M * X # Matrix Multiplikation
```

```
Out[23]: 2x2 Array{Float64,2}:  
 0.354775  0.459345  
 0.958141  0.822797
```

```
In [24]: M .* X # Elementweise Multiplikation
```

```
Out[24]: 2x2 Array{Float64,2}:  
 0.302726  0.0395955  
 0.77481   0.233374
```

## Funktionen

```
In [25]: quadrat(x) = x^2
```

```
Out[25]: quadrat (generic function with 1 method)
```

```
In [26]: quadrat(3)
```

```
Out[26]: 9
```

```
In [27]: x = range(-2, stop=2, length=100)
```

```
Out[27]: -2.0:0.04040404040404041:2.0
```

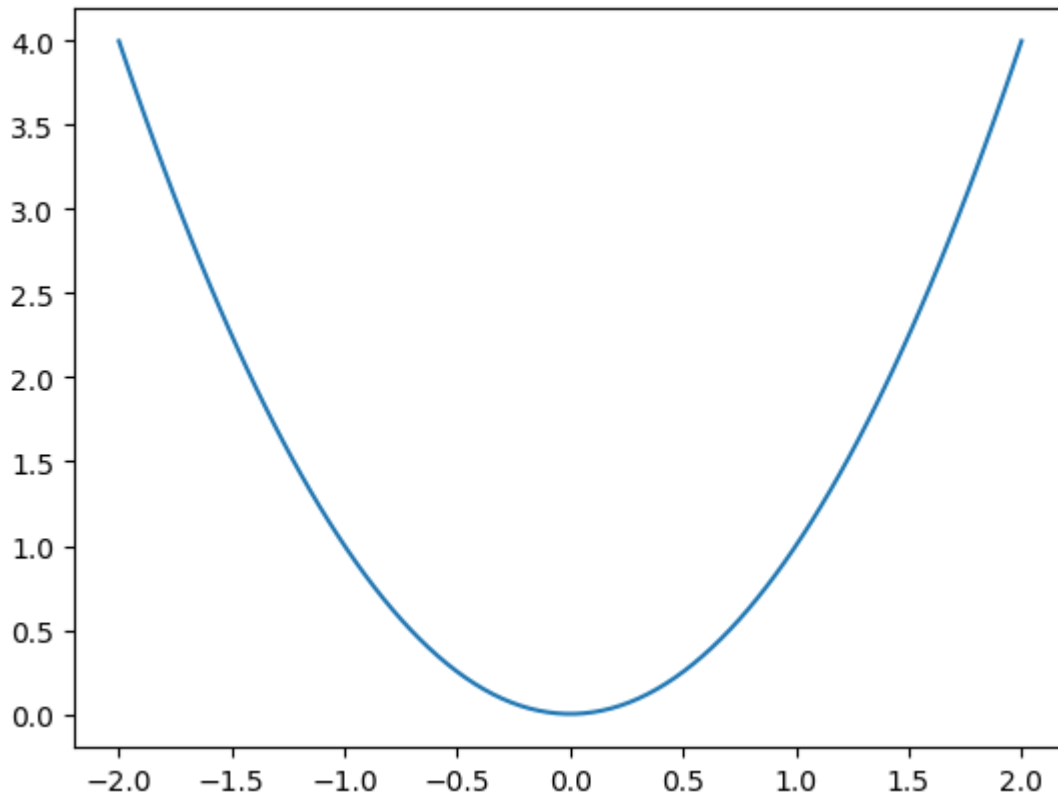
```
In [30]: y = quadrat.(x)
```

```
Out[30]: 100-element Array{Float64,1}:
 4.0
 3.8400163248648096
 3.683297622691562
 3.5298438934802574
 3.379655137230895
 3.232731353943475
 3.089072543617998
 2.9486787062544635
 2.8115498418528717
 2.6776859504132235
 2.5470870319355168
 2.419753086419753
 2.295684113865932
 ⋮
 2.419753086419753
 2.5470870319355168
 2.6776859504132235
 2.8115498418528717
 2.9486787062544635
 3.089072543617998
 3.232731353943475
 3.379655137230895
 3.5298438934802574
 3.683297622691562
 3.8400163248648096
 4.0
```

## Plots

```
In [29]: using PyPlot
```

```
In [31]: plot(x,y)
```



```
Out[31]: 1-element Array{PyCall.PyObject,1}:  
PyObject <matplotlib.lines.Line2D object at 0x000000002284400>
```

```
In [ ]:
```

# 1. Funktionen (cont'd)

## Mehrzeilige Funktionen

```
In [32]: shortfunc(x) = 2x + 3
```

```
Out[32]: shortfunc (generic function with 1 method)
```

```
In [33]: shortfunc(2)
```

```
Out[33]: 7
```

```
In [34]: function shortfunc2(x)  
          2x + 3  
end
```

```
Out[34]: shortfunc2 (generic function with 1 method)
```



```
In [35]: shortfunc2(2)
```

```
Out[35]: 7
```

```
In [36]: function longfunc(x)
          a = 2x
          a + 3
        end
```

```
Out[36]: longfunc (generic function with 1 method)
```

```
In [37]: longfunc(2)
```

```
Out[37]: 7
```

Eine Funktion *returned* automatisch den Wert der letzten Zeile. Oft ist es besser explizit anzugeben, was zurückgegeben wird.

```
In [38]: function longfunc2(x)
          a = 2x
          return a + 3
        end
```

```
Out[38]: longfunc2 (generic function with 1 method)
```

```
In [39]: longfunc2(2)
```

```
Out[39]: 7
```

```
In [40]: function longfunc3(x)
          a = 2x
          return a + 3
          4 + 4
        end
```

```
Out[40]: longfunc3 (generic function with 1 method)
```

```
In [41]: longfunc3(2)
```

```
Out[41]: 7
```

```
In [ ]: function machtwasanderes(x)
          if x > 10
            println("x > 10")
            return 1
          else
            println("x <= 10")
            return 0
          end
        end
```

## Mehrere Rückgabewerte

```
In [42]: function longfunc_multiple(x)
          a = 2x
          b = a + 3
          return a, b
        end
```

Out[42]: longfunc\_multiple (generic function with 1 method)

```
In [43]: longfunc_multiple(2)
```

Out[43]: (4, 7)

```
In [44]: a, b = longfunc_multiple(2)
```

Out[44]: (4, 7)

```
In [45]: a
```

Out[45]: 4

```
In [46]: b
```

Out[46]: 7

```
In [47]: c = longfunc_multiple(2)
```

Out[47]: (4, 7)

```
In [48]: c[1]
```

Out[48]: 4

```
In [49]: c[2]
```

Out[49]: 7

```
In [50]: d, e = longfunc_multiple(3)
```

Out[50]: (6, 9)

### Globale und lokale Variablen

Eine Funktion sollte *autonom* sein und nur mit den Eingabeparametern arbeiten.

```
In [51]: function f(x)
          2x + 3
        end
```

Out[51]: f (generic function with 1 method)

```
In [52]: f(5)
```

```
Out[52]: 13
```

```
In [53]: # Schlecht!!!!!!!!!!!!
```

```
x = 2

function f()
    2x + 3
end

f()
```

```
Out[53]: 7
```

### Übung: Elemente in einem Array vertauschen

```
In [54]: function swap(a, i, j)
           tmp = a[i]
           a[i] = a[j]
           a[j] = tmp
           return a
       end
```

```
Out[54]: swap (generic function with 1 method)
```

```
In [55]: a = collect(1:10)
```

```
Out[55]: 10-element Array{Int64,1}:
```

```
 1
 2
 3
 4
 5
 6
 7
 8
 9
10
```

```
In [56]: swap(a, 6, 10)
```

```
Out[56]: 10-element Array{Int64,1}:
 1
 2
 3
 4
 5
10
 7
 8
 9
 6
```

```
In [57]: a
```

```
Out[57]: 10-element Array{Int64,1}:
 1
 2
 3
 4
 5
10
 7
 8
 9
 6
```

In Julia gibt es die Konvention, dass Funktionen die mindestens eines ihrer Funktionsargumente modifizieren, mit einem Ausrufezeichen am Ende versehen werden.

```
In [58]: function swap!(a, i, j)
           tmp = a[i]
           a[i] = a[j]
           a[j] = tmp
           return a
       end
```

```
Out[58]: swap! (generic function with 1 method)
```

```
In [59]: swap!(a, 2,3)
```

```
Out[59]: 10-element Array{Int64,1}:
 1
 3
 2
 4
 5
10
 7
 8
 9
 6
```

```
In [60]: a
```

```
Out[60]: 10-element Array{Int64,1}:  
 1  
 3  
 2  
 4  
 5  
10  
 7  
 8  
 9  
 6
```

```
In [61]: issorted(a)
```

```
Out[61]: false
```

```
In [62]: sort(a)
```

```
Out[62]: 10-element Array{Int64,1}:  
 1  
 2  
 3  
 4  
 5  
 6  
 7  
 8  
 9  
10
```

```
In [63]: a
```

```
Out[63]: 10-element Array{Int64,1}:  
 1  
 3  
 2  
 4  
 5  
10  
 7  
 8  
 9  
 6
```

```
In [64]: sort!(a)
```

```
Out[64]: 10-element Array{Int64,1}:
 1
 2
 3
 4
 5
 6
 7
 8
 9
10
```

```
In [65]: a
```

```
Out[65]: 10-element Array{Int64,1}:
 1
 2
 3
 4
 5
 6
 7
 8
 9
10
```

```
In [70]: a = rand(2,2)
```

```
Out[70]: 2x2 Array{Float64,2}:
 0.080248  0.76882
 0.416823  0.0826709
```

```
In [71]: b = a
```

```
Out[71]: 2x2 Array{Float64,2}:
 0.080248  0.76882
 0.416823  0.0826709
```

```
In [72]: b[1] = 123
```

```
Out[72]: 123
```

```
In [73]: b
```

```
Out[73]: 2x2 Array{Float64,2}:
123.0      0.76882
 0.416823  0.0826709
```

In [74]: a

Out[74]: 2x2 Array{Float64,2}:  
123.0 0.76882  
0.416823 0.0826709

```
In [66]: function swap(b, i, j)
          a = copy(b)
          tmp = a[i]
          a[i] = a[j]
          a[j] = tmp
          return a
        end
```

Out[66]: swap (generic function with 1 method)

In [67]: a

Out[67]: 10-element Array{Int64,1}:  
1  
2  
3  
4  
5  
6  
7  
8  
9  
10

In [68]: swap(a, 3, 7)

Out[68]: 10-element Array{Int64,1}:  
1  
2  
7  
4  
5  
6  
3  
8  
9  
10

In [69]:

```
a
```

Out[69]: 10-element Array{Int64,1}:

```
1  
2  
3  
4  
5  
6  
7  
8  
9  
10
```

## 2. Selbst sortieren: BubbleSort

"Größte Elemente steigen nacheinander ans Ende des Arrays auf"

In [78]: `collect(1:10) # start:ende`

Out[78]: 10-element Array{Int64,1}:

```
1  
2  
3  
4  
5  
6  
7  
8  
9  
10
```



```
In [79]: collect(1:0.1:10) # start:schrittweite:ende
```

```
Out[79]: 91-element Array{Float64,1}:
 1.0
 1.1
 1.2
 1.3
 1.4
 1.5
 1.6
 1.7
 1.8
 1.9
 2.0
 2.1
 2.2
  ⋮
 8.9
 9.0
 9.1
 9.2
 9.3
 9.4
 9.5
 9.6
 9.7
 9.8
 9.9
10.0
```

```
In [80]: collect(10:-1:1)
```

```
Out[80]: 10-element Array{Int64,1}:
10
 9
 8
 7
 6
 5
 4
 3
 2
 1
```

```
In [94]: function bubblesort!(a)
          N = length(a)

          for rechts in N:-1:2
              for i in 1:(rechts-1)
                  if a[i] > a[i+1] # wenn links größer als rechts
                      swap!(a, i, i+1)
                  end
              end
          end

          return a
      end
```

Out[94]: bubblesort! (generic function with 1 method)

```
In [82]: a = rand(1:10, 10)
```

```
Out[82]: 10-element Array{Int64,1}:
 2
 3
 2
 6
 8
10
 2
 3
 4
10
```

```
In [84]: rand(["hallo", "köln", "wasauchimmer"], 7)
```

```
Out[84]: 7-element Array{String,1}:
 "köln"
 "wasauchimmer"
 "hallo"
 "wasauchimmer"
 "hallo"
 "wasauchimmer"
 "köln"
```

```
In [95]: a = rand(1:10, 10)
```

```
Out[95]: 10-element Array{Int64,1}:
 9
 8
 1
 4
10
 4
 5
 3
10
 7
```

```
In [96]: bubblesort!(a)
```

```
Out[96]: 10-element Array{Int64,1}:  
 1  
 3  
 4  
 4  
 5  
 7  
 8  
 9  
10  
10
```

```
In [97]: a
```

```
Out[97]: 10-element Array{Int64,1}:  
 1  
 3  
 4  
 4  
 5  
 7  
 8  
 9  
10  
10
```

## Visualisierung

```

In [98]: using PyPlot, Random

function show_bubble_schritt(n)
    a = shuffle(1:n)

    pygui(true)
    fig = figure()
    title("Bubble-Schritt")
    for rechts = length(a):-1:length(a)
        # bubble-Schritt
        for i in 1:rechts-1
            if a[i]>a[i+1]
                swap!(a, i, i+1)
            end
            fig.clear()
            bar(1:length(a), a)
            m, mind = findmax(a)
            bar(mind, m, color="red")
            sleep(0.001)
        end
    end
    pygui(false)
    nothing
end

function show_bubble_sort(n)
    a = shuffle(1:n)

    pygui(true)
    fig = figure()
    title("Bubble-Sort")
    for rechts = length(a):-1:2
        # bubble-Schritt
        for i in 1:rechts-1
            if a[i]>a[i+1]
                swap!(a, i, i+1)
            end
        end
        fig.clear()
        bar(1:length(a), a)
        m, mind = findmax(a[1:rechts])
        bar(mind, m, color="red")
        sleep(0.001)
    end
    pygui(false)
    nothing
end

```

Out[98]: show\_bubble\_sort (generic function with 1 method)

```
In [100]: show_bubble_schritt(40)
```

```
In [101]: show_bubble_sort(40)
```

### 3. Timing und Komplexität

```
In [6]: b = rand(50000);
```

```
In [7]: @time bubblesort!(b);
```

4.237893 seconds (26.33 k allocations: 1.333 MiB, 0.08% gc time)

```
In [8]: function benchmark_bubblesort()
    number_count = [0.0]
    elapsed_time = [0.0]

    for i in 1:16
        b = rand(2^i)
        t = @elapsed bubblesort!(b)
        println(2^i, "\t", t)
        push!(number_count, 2^i)
        push!(elapsed_time, t)
    end

    return number_count, elapsed_time
end
```

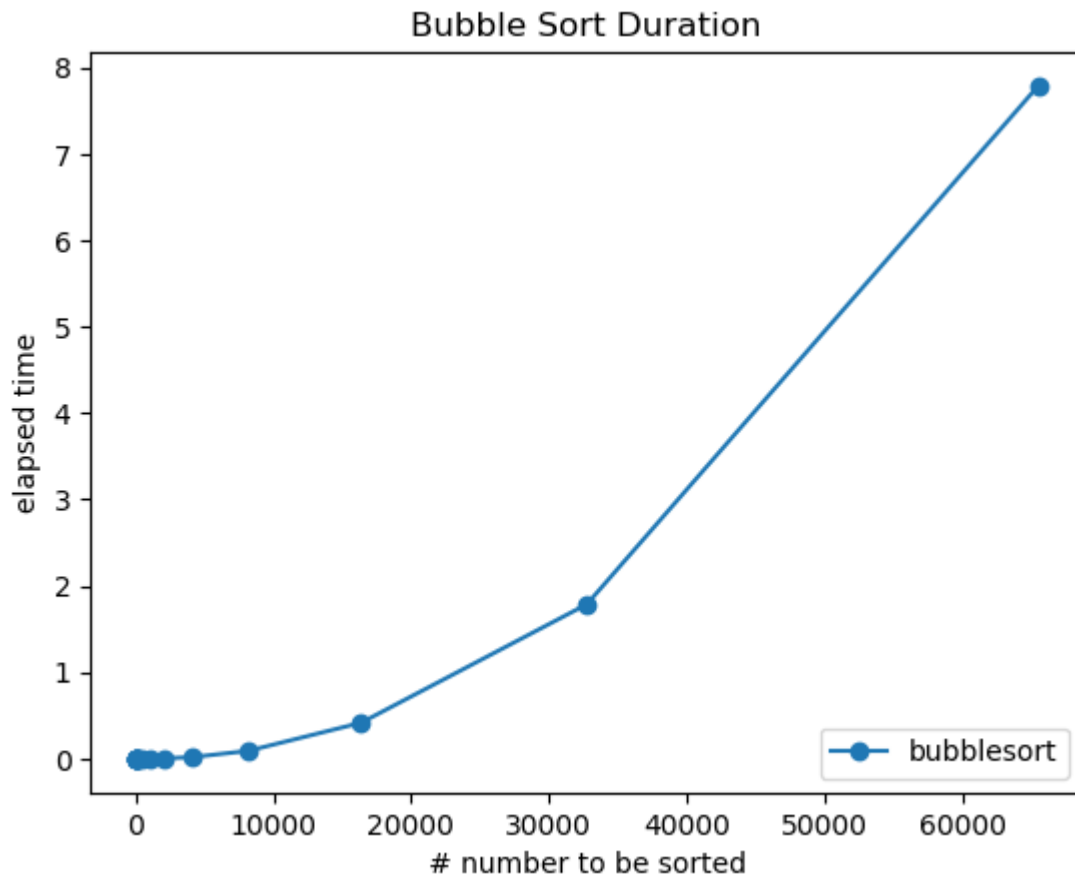
Out[8]: benchmark\_bubblesort (generic function with 1 method)

```
In [9]: number_count, elapsed_time = benchmark_bubblesort();
```

2	4.99e-7
4	4.0e-7
8	2.99e-7
16	6.0e-7
32	1.599e-6
64	5.899e-6
128	1.67e-5
256	0.000196
512	0.0002221
1024	0.0008542
2048	0.003413601
4096	0.0172408
8192	0.090724101
16384	0.416059101
32768	1.7874153
65536	7.7880827

In [10]: using PyPlot

```
plot(number_count, elapsed_time, marker="o", label="bubblesort");  
legend(loc=4);  
xlabel("# number to be sorted");  
ylabel("elapsed time");  
title("Bubble Sort Duration")
```

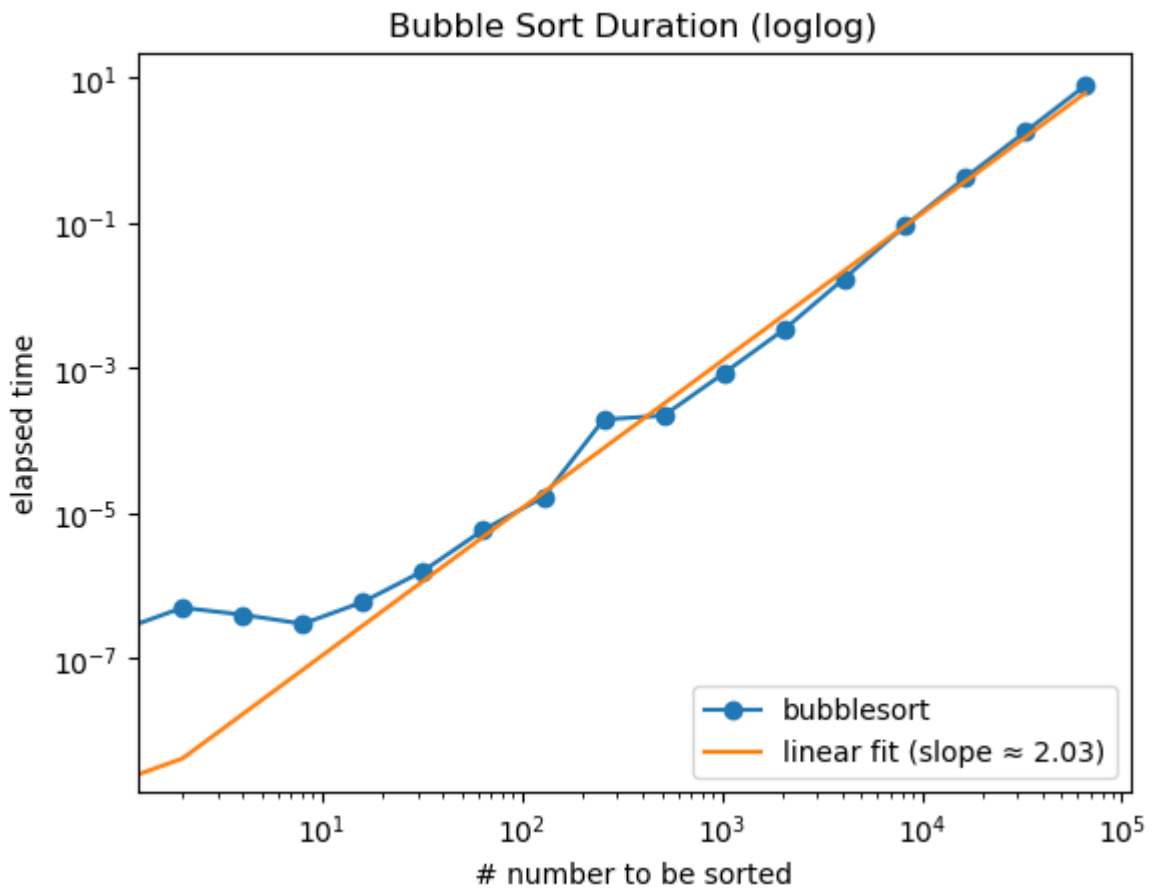


Out[10]: PyObject Text(0.5, 1.0, 'Bubble Sort Duration')

In [11]: **using** PyPlot, Polynomials

```
# fit straight line in loglog space (ignoring first couple of datapoints)
p = polyfit(log.(number_count[7:end]), log.(elapsed_time[7:end]), 1)
m = p.a[2]

plot(number_count, elapsed_time, marker="o", label="bubblesort");
plot(number_count, exp.(p.(log.(number_count))), label="linear fit (slope = $(rou
legend(loc=4);
xscale("log")
yscale("log")
xlabel("# number to be sorted");
ylabel("elapsed time");
title("Bubble Sort Duration (loglog)");
```



**Komplexität (asymptotisches Verhalten): BubbleSort  $\in \mathcal{O}(n^2)$**

O-Notation: [https://de.wikipedia.org/wiki/Landau-Symbole#Beispiele\\_und\\_Notation](https://de.wikipedia.org/wiki/Landau-Symbole#Beispiele_und_Notation)  
[https://de.wikipedia.org/wiki/Landau-Symbole#Beispiele\\_und\\_Notation](https://de.wikipedia.org/wiki/Landau-Symbole#Beispiele_und_Notation)

**Vergleich mit Julias sort !**

```
In [12]: function benchmark_juliasort()
          number_count = [0.0]
          elapsed_time = [0.0]

          for i in 1:16
              b = rand(2^i)
              t = @elapsed sort!(b)
              println(2^i, "\t", t)
              push!(number_count, 2^i)
              push!(elapsed_time, t)
          end

          return number_count, elapsed_time
        end
```

Out[12]: benchmark\_juliasort (generic function with 1 method)

```
In [13]: number_count, elapsed_time = benchmark_juliasort();
```

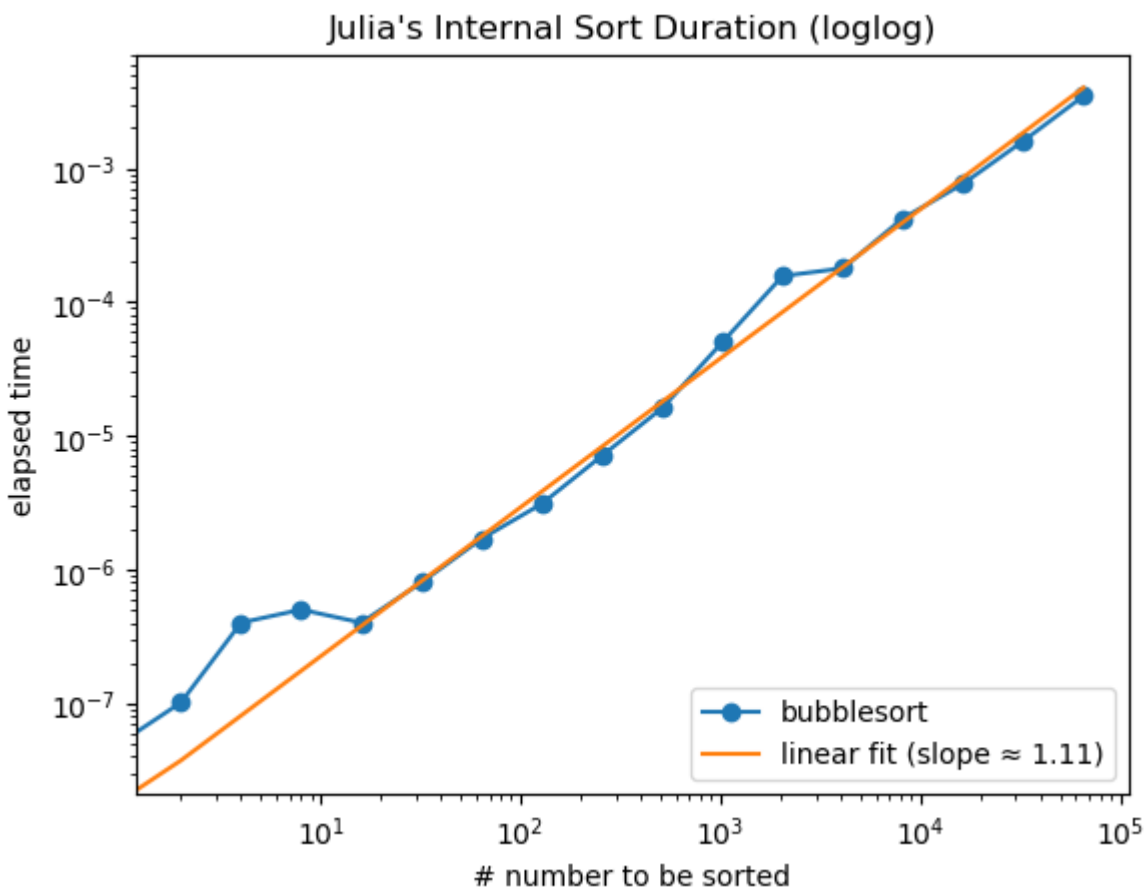
```
2      1.01e-7
4      4.0e-7
8      5.01e-7
16     4.0e-7
32     8.0e-7
64     1.699e-6
128    3.101e-6
256    7.099e-6
512    1.61e-5
1024   5.01e-5
2048   0.000156601
4096   0.000178901
8192   0.000422901
16384  0.000766699
32768  0.0016012
65536  0.003472799
```



In [14]: **using** PyPlot, Polynomials

```
# fit straight line in loglog space (ignoring first couple of datapoints)
p = polyfit(log.(number_count[7:end]), log.(elapsed_time[7:end]), 1)
m = p.a[2]

plot(number_count, elapsed_time, marker="o", label="bubblesort");
plot(number_count, exp.(p.(log.(number_count))), label="linear fit (slope = $(rou
legend(loc=4);
xscale("log")
yscale("log")
xlabel("# number to be sorted");
ylabel("elapsed time");
title("Julia's Internal Sort Duration (loglog)");
```



Übersicht der Komplexität verschiedener Sortierverfahren:

<https://de.wikipedia.org/wiki/Sortierverfahren> (<https://de.wikipedia.org/wiki/Sortierverfahren>)

**Randnotiz:** Die Macros `@time` und `@elapsed` sind hilfreich, sollten jedoch meistens vermieden werden, da Nebeneffekte das Messergebnis verzerren können. Führen Sie beispielsweise `@time sort(rand(1000))`; zweimal aus und beobachten Sie, wie sich das Ergebnis ändert.

Es ist stattdessen empfehlenswert auf `@btime` und `@belapsed` aus dem Paket [BenchmarkTools.jl](https://github.com/JuliaCI/BenchmarkTools.jl) (<https://github.com/JuliaCI/BenchmarkTools.jl>) verwenden.

```
In [15]: @time sort(rand(1000));
```

```
0.004349 seconds (6.02 k allocations: 336.401 KiB)
```

```
In [16]: @time sort(rand(1000));
```

```
0.000041 seconds (6 allocations: 16.031 KiB)
```

```
In [ ]: ] add BenchmarkTools
```

```
In [17]: using BenchmarkTools
```

```
In [18]: @btime sort(rand(1000));
```

```
30.499 μs (2 allocations: 15.88 KiB)
```

```
In [19]: @btime sort(rand(1000));
```

```
31.800 μs (2 allocations: 15.88 KiB)
```