

# Scientific Computing and (Big) Data Analysis with Julia

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#### julialang.org



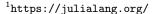
Julia is dynamically typed, feels like a scripting

Julia was designed for high performance, Julia

High Performance Computing & Dynamic

- Julia was designed for high performance. Julia programs automatically compile to efficient native code via LLVM, and support multiple platforms (Windows, MacOS, Linux, etc.).
- Julia is dynamically typed, feels like a scripting language, and has good support for interactive use, but can also optionally be separately compiled<sup>1</sup>.



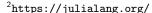




Composable & Open Source

- Julia uses multiple dispatch as a paradigm, making it easy to express many object-oriented and functional programming patterns. The talk on the Unreasonable Effectiveness of Multiple Dispatch explains why it works so well.
- Julia is an open source project with over 1,000 contributors. It is made available under the MIT license. The source code is available on GitHub<sup>2</sup>.







### Compilation to Binary

Julia code is compiled into binary executable via LLVM (Low-Level Virtual Machine).

```
julia> @code_native 2 - 5
        .text
        .file
        .qlobl
               "julia_-_199"
        .p2align
                "julia_-_199",@function
        push
                rbp
        mov
                rax, rdi
                rbp, rsp
        mov
        sub
                rax, rsi
        pop
                rbp
        ret
Lfunc end0:
        .size
                "julia_-_199", .Lfunc_end0-"julia_-_199"
        .section
                         ".note.GNU-stack", "", @progbits
```



First things first!

### helloworld.jl file

```
println("Hello, world!")
```

```
julia > include("helloworld.jl")
Hello, world!
```



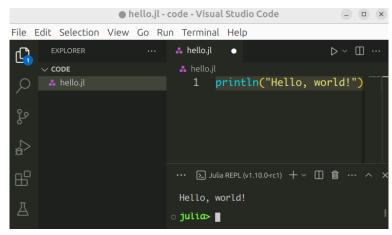


Welcome!





The editor: Visual Studio Code







**Basics** 

Variables have types (Int, Float, Bool, String, etc.)

```
julia > a = 3
3
julia > b = 3.14159265
3.14159265
julia > typeof(a)
Int64
julia > typeof(b)
Float64
```





### **Basics**

Vectors and Matrices are first-class citizens (no need for external libs)

```
julia> v = [1, 42, -8, 10]
4-element Vector{Int64}:
1
42
-8
10
```





# Julia Programming Language Basics

```
julia > hcat(zeros(5), ones(5), 1:5, 5:(-1):1)
5x4 Matrix{Float64}:
0.0 1.0 1.0 5.0
0.0 1.0 2.0 4.0
0.0 1.0 3.0 3.0
0.0 1.0 4.0 2.0
0.0 1.0 5.0 1.0
```





#### **Basics**

```
julia > m = zeros(5, 3)
5x3 Matrix{Float64}:
0.0 0.0
         0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
julia> size(m)
(5, 3)
```



Installing packages

```
julia> using Pkg
julia> Pkg.add("JMcDM")
```

```
julia > ]
@v1.10) pkg > add JMcDM
```





Importing Data



Importing Data

```
julia> using Latexify
julia> latexify(mydata, env = :table) |> println
```

```
1 2
2 4
3 5
4 -1
5 2
```



if/elseif/else

```
function numberofrealroots(delta)
  if delta > 0
     return 2
  elseif delta == 0
     return 1
  else
     return 0
  end
```



Pattern Matching



# Julia Programming Language Basics

### For loops are single threaded by design

```
results = zeros(10)

for i in 1:10
    results[i] = dosomethingwith(i)
end
```





# Julia Programming Language Basics

## Using multiple threads<sup>3</sup>

```
using Base.Threads
results = zeros(10)

@threads for i in 1:10
    results[i] = dosomethingwith(i)
end
```



Functions are first-class citizens

```
function apply(f, x)
  return f(x)
end

julia> apply(abs, -10)
10
```

- Functions can take functions as arguments.
- Functions can return functions as values.





Multiple Dispatch

```
struct Point2D
    x::Float64
    y::Float64
end
```

- Structs are user-defined concrete data types.
- An object instance can be created like Point2D(1, 2).
- Object fields can be accessed like p.x and p.y.





Multiple Dispatch

```
julia > Point2D(1, 2) + Point2D(4, 5)
Point2D(5.0, 7.0)
```

- Operator + is overloaded for the type Point2D.
- Now, both 2 + 2 and p1 + p2 are legal Julia codes where p1 and p2 are in type of Point2D.



Multiple Dispatch

```
function Base.:*(p::Point2D, other::Point2D)::Float64
   return p.x * other.x + p.y * other.x
end
```

```
julia> Point2D(1, 2) * Point2D(4, 5)
12.0
```

- The operator \* is overloaded for the type Point2D.
- \* now operates like the dot product of vectors in linear algebra.





The formulation

$$y = \beta_0 + \beta_1 x + \varepsilon \tag{1}$$

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x \tag{2}$$

$$\hat{\boldsymbol{\beta}} = (X'X)^{-1}X'y \tag{3}$$





### Sample Data

$$X = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \\ 1 & 5 \end{bmatrix}, y = \begin{bmatrix} 2 \\ 5 \\ 5 \\ 8 \\ 12 \end{bmatrix}$$
 (4)





The Matrix Solution

```
using LinearAlgebra

x = [1, 2, 3, 4, 5]
y = [2, 5, 5, 8, 12]
X = hcat(ones(5), x)
betahats = inv(X'X)X'y
println(betahats)
```

```
julia > include("reg-matrix.jl")
[-0.5, 2.3]
```



Pseudo Inverse - Numerical Fit

```
x = [1, 2, 3, 4, 5]
y = [2, 5, 5, 8, 12]
betahats = hcat(ones(5), x) \ y
println(betahats)
```

```
julia> include("reg-simple.jl")
[-0.5, 2.3]
```



### The GLM package

```
using GLM
x = [1, 2, 3, 4, 5]
y = [2, 5, 5, 8, 12]
result = lm(hcat(ones(5), x), y)
println(result)
```

### The GLM package - Results

```
julia > include ("reg-glm.jl")
Coefficients:
      Coef
             Std. Error
                                  Pr(>|t|)
                                             Lower 95%
                                                         Upper 95%
×1
     -0.5
              1.25565
                         -0.40
                                  0.7171
                                            -4.49605
                                                         3.49605
x2
      2.3
              0.378594
                         6.08
                                  0.0090
                                             1.09515
                                                         3.50485
```

```
julia > GLM.r2(result)
0.9248251748251748
```



### MLJ

### A Machine Learning Framework for Julia

```
julia > using MLJ
julia > models = MLJ. models()
julia > for m in models
            println (m[:name])
       end
ARDRegressor
AdaBoostClassifier
AdaBoostRegressor
AdaBoostStumpClassifier
KMedoids
KNNClassifier
NeuralNetworkRegressor
Random Forest Classifier
RandomForestImputer
RandomForestRegressor
SRRegressor
```





<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	у
1	1	0
1	0	1
0	1	1
0	0	0

Table:  $y = xor(x_1, x_2)$ 





```
using SymbolicRegression, MLJ

x = (
    x1 = Float64[1, 1, 0, 0],
    x2 = Float64[1, 0, 1, 0]
)

y = Float64[0, 1, 1, 0]
```



```
model = SRRegressor(
    niterations = 50,
    binary_operators = [+, -, *],
    unary_operators = [abs],
    should_simplify = true,
    save_to_file = false)
```





```
mach = machine(model, x, y)
fit!(mach)
report(mach)
@info predict(mach, x)
```





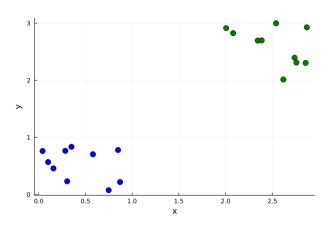
```
Hall of Fame:
------
Complexity Loss Score Equation
1 2.500e-01 3.604e+01 y = 0.5
4 0.000e+00 1.201e+01 y = abs(x1 - x2)
------
[ Info: [0.0, 1.0, 1.0, 0.0]
```





### Clustering Multivariate Data

### kmedoids

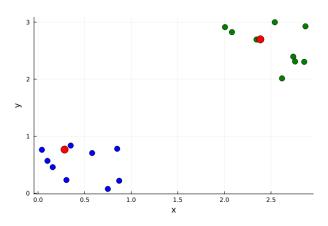






# Clustering Multivariate Data

### kmedoids





## Clustering Multivariate Data

Problem of Distance Matrices

```
using Clustering, Plots, Distances
# data = Code for loading data...
plt = scatter(data[:, 1], data[:, 2])
dist = pairwise(euclidean, eachrow(data))
result = kmedoids(dist, 2)
centers = data[result.medoids, :];
scatter!(centers[:, 1], centers[:, 2])
```



## A Distance Matrix

$$D = \begin{bmatrix} D_{11} & D_{12} & D_{13} & \dots & D_{1n} \\ D_{21} & D_{22} & D_{23} & \dots & D_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ D_{n1} & D_{n2} & D_{n3} & \dots & D_{nn} \end{bmatrix}_{n \times n}$$





## Clustering Multivariate Data

Problem of Distance Matrices

```
dist = pairwise(euclidean, eachrow(data))
```

- A distance matrix holds the distance data of *ith* and *jth* points, e.g.,  $D_{ij} = D_{ji}$  due to the symmetry.
- If data has n rows then the distance matrix is in dimension of  $n \times n$ .
- Each distance is measured in 64-bits float numbers (Float64).
- If *n* is large, your machine will probably throw an *Out of Memory* error!





```
struct OnDemandDistanceMatrix <: AbstractMatrix{Float64}
    rawdata::Matrix
end

function Base.getindex(odm::OnDemandDistanceMatrix, i::Int, j::Int)::Float64
    return euclidean(odm.rawdata[i, :], odm.rawdata[j, :])
end

function Base.size(odm::OnDemandDistanceMatrix)
    n, _ = size(odm.rawdata)
    return (n, n)
end</pre>
```





- On-demand distance matrix costs zero memory
- Caution: But it's really slow just because the requested distance is calculated on demand!
- But it makes it possible! <sup>(2)</sup>





# Big Matrices Memory Mapped IO

- We need an efficient way to cope with big distance matrices
- Memory-mapped IO is an OS level solution to this problem
- The content of a matrix is stored in files (on disk!)
- Access to data is really fast ⊕ (contrast to the previous one!)





# Big Matrices

### Memory-mapped IO

```
import Mmap

xio = open("/tmp/X.dat", "w+")
yio = open("/tmp/y.dat", "w+")

X = Mmap.mmap(xio, Matrix{Float64}, (n, 2))
y = Mmap.mmap(yio, Vector{Float64}, n)
```

- X and y are stored in files X.dat and y.dat
- But they are stored in files and mapped to memory (RAM).





# Big Matrices

## Memory-mapped IO

X and y are processed and accessed as normal matrices and vectors





#### The Normal Distribution

$$f(x; \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma}\right)^2}, \ -\infty < x < \infty \tag{5}$$

$$f(x; 0, 1) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}, -\infty < x < \infty$$
 (6)





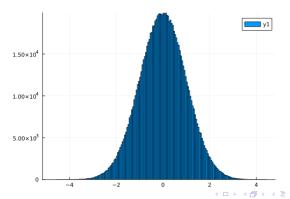
#### The Normal Distribution

```
julia > using Distributions
julia > quantile (Normal(), 0.05/2)
-1.9599639845400592
julia > quantile (Normal(), 0.10/2)
-1.6448536269514729
julia > quantile(Normal(), 0.01/2)
-2.5758293035489053
```



Monte Carlo Simulations - Drawing Random Numbers

```
julia > using Plots, Distributions
julia > x = rand(Normal(), 1000000);
julia> histogram(x)
```

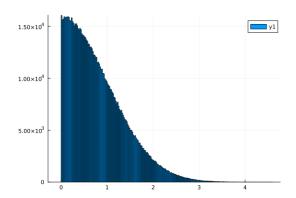




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Monte Carlo Simulations - Drawing Random Numbers

## julia > histogram(abs.(x))







## Numerical Integration

#### QuadGK

$$\int_{-1}^{1} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} dx = ? \tag{7}$$

```
using QuadGK
```

return 
$$1/sqrt(2pi) * exp(-0.5x^2)$$

end



## Simple Neural Network

$$H_{1} = f(w_{0} + x_{1}w_{11} + x_{2}w_{21})$$

$$W_{11}$$

$$W_{12}$$

$$W_{12}$$

$$W_{22}$$

$$W_{22}$$

$$W_{22}$$

$$W_{32}$$





#### Simple Neural Network

$$H_1 = f(w_{01} + x_1w_{11} + x_2w_{21})$$

$$H_2 = f(w_{02} + x_1w_{12} + x_2w_{22})$$

$$Y = f(w_{03} + w_{31}H_1 + w_{32}H_2)$$

What are the values of  $w_{ij}$ 's that minimize the total network error?





### Simple Neural Network

```
function sigmoid(x)
    return 1.0/(1.0 + exp(-x))
end

function cost(w)
    error = 0.0
    for i in 1:4
        H1 = sigmoid(w[1] + w[2]*x1[i] + w[3]*x2[i])
        H2 = sigmoid(w[4] + w[5]*x1[i] + w[6]*x2[i])
        yhat = sigmoid(w[7] + w[8] * H1 + w[9] * H2)
        error += (yhat - y[i])^2
    end
    return error
end
```





Simple Neural Network

```
using Metaheuristics
\times 1 = [1, 1, 0, 0]
x2 = [1, 0, 1, 0]
y = [0, 1, 1, 0]
bounds = vcat([-10000.0 \text{ for } i \text{ in } 1:9]),
                [10000.0 for i in 1:9]')
result = Metaheuristics.optimize(cost, bounds, MCCGA())
display (result)
```

# Feeding the trained network

```
function forward(w)
  yhat = zeros(length(y))
  for i in 1:4
      H1 = sigmoid(w[1] + w[2]*x1[i] + w[3]*x2[i])
      H2 = sigmoid(w[4] + w[5]*x1[i] + w[6]*x2[i])
      H3 = sigmoid(w[7] + w[8] * H1 + w[9] * H2)
      yhat[i] = H3
  end
  return yhat
end
```





## Mathematical Programming

max 
$$z=2x_1+3x_2$$
  
Subject to:  $x_1+2x_2\leq 100$   $2x_1+x_2\leq 150$   $x_1,x_2\geq 0$ 





**JuMP** 

```
using JuMP, HiGHS

m = Model(HiGHS.Optimizer)

@variable(m, x1 >= 0)
@variable(m, x2 >= 0)

@objective(m, Max, 2x1 + 3x2)

@constraint(m, x1 + 2x2 <= 100)
@constraint(m, 2x1 + x2 <= 150)
```





**JuMP** 

```
julia > optimize!(m)
Solving LP without presolve or with basis
Model status : Optimal
Objective value : 1.8333333333e+02
HiGHS run time
                              0.00
julia > value.([x1, x2])
2-element Vector{Float64}:
66.666666666667
16.6666666666657
```



# **SQL** Integration

#### **SQLite**

```
using SQLite

db = SQLite.DB("database.db")

sqlst = """
    select item, price from Prices
    where date = '2023.12.01'
    order by price

"""

resultsql = DBInterface.execute(db, sqlst)

for row in resultsql
    println(row[:item], ": ", row[:price])
end

close(db)
```



- Julia can operate with R and Python.
- R and Python objects can be transferred in both ways.
- We don't need to give up on them, let's talk to the strangers!





# Talking to Strangers

Calling into R

```
using RCall

x = [1, 2, 3, 4, 5]
y = [2, 5, 5, 8, 12]

@rput x y

R"result <- lm(y~x)"

jresult = @rget result</pre>
```





```
julia > jresult
  :coefficients \Rightarrow [-0.5, 2.3]
                  \Rightarrow [0.2, 0.9, -1.4, -0.7, 1.0]
  :residuals
  :rank
                   => 2
                  => [1.8, 4.1, 6.4, 8.7, 11.0]
  :fitted_values
                   => [0. 1]
  :assign
  :df_residual
                  => 3
  :xlevels
                   => OrderedDict(Symbol, Any)()
                   => y ~ x
  :terms
```



# Talking to Strangers

Calling into Python

```
using PyCall

np = pyimport("numpy")
linalg = pyimport("numpy.linalg")

x = np.matrix([1.0 1; 1 2; 1 3; 1 4; 1 5])
y = np.array([2.0, 5, 5, 8, 12])

result = linalg.lstsq(x, y)
```



# Talking to Strangers

Calling into Python

```
julia> include("pycaller.jl")
(
     [-0.500000000000023, 2.30000000000000],
     [4.299999999999],
     2,
     [7.69121313410482, 0.9193696350073228]
)
```







