Scientific Computing and (Big) Data Analysis with Julia

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2024.02.23

Julia Programming Language

julialang.org

Julia Programming Language
High Performance Computing & Dynamic
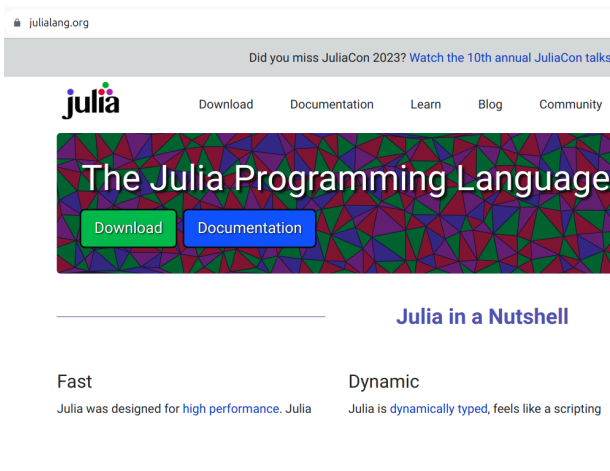
- Julia was designed for high performance. Julia programs automatically compile to efficient native code via LLVM, and support multiple platforms (Windows, MacOS, Linux, etc.).
- Julia is dynamically typed, feels like a scripting language, and has good support for interactive use, but can also optionally be separately compiled[1].

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[1]https://julialang.org/

Julia Programming Language
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[2].

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[2]https://julialang.org/

Julia Programming Language
Compilation to Binary

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

```
julia> @code_native 2 - 5
        .text
        .file   "-"
        .globl  "julia_-_199"                    # -- Begin function julia_-_199
        .p2align        4, 0x90
        .type   "julia_-_199",@function
"julia_-_199":                                   # @julia_-_199
; r @ int.jl:86 within `-`
# %bb.0:                                          # %top
        push    rbp
        mov     rax, rdi
        mov     rbp, rsp
        sub     rax, rsi
        pop     rbp
        ret
.Lfunc_end0:
        .size   "julia_-_199", .Lfunc_end0-"julia_-_199"
; L
                                                 # -- End function
        .section        ".note.GNU-stack","",@progbits
```

Julia Programming Language
First things first!

helloworld.jl file

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

```
julia> include("helloworld.jl")
Hello, world!
```
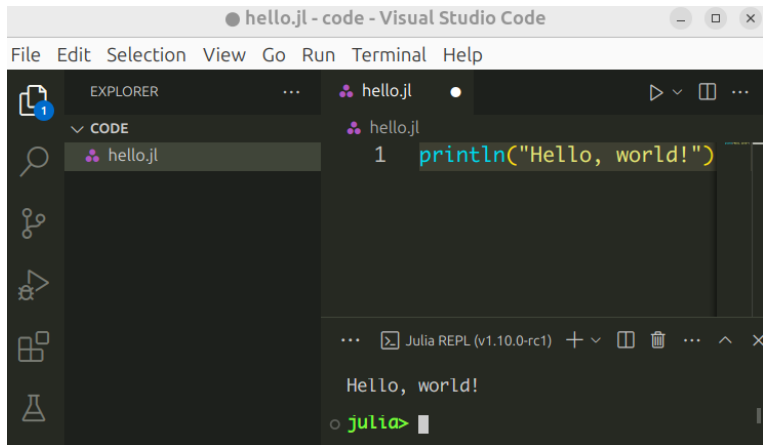
Julia Programming Language
Welcome!

Julia Programming Language
The editor: Visual Studio Code

Julia Programming Language
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
```

Julia Programming Language
Vectors

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
Matrices

```
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
```

Julia Programming Language
Matrices

```
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)
```

Julia Programming Language
Installing packages

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

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

Julia Programming Language
Importing Data

```
using CSV, DataFrames

mydata = CSV.read("data.csv",
                  delim = ";",
                  DataFrame)

show(mydata)
```

Julia Programming Language
Importing Data

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

X	Y
1	2
2	4
3	5
4	−1
5	2

Julia Programming Language
if/elseif/else

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

Julia Programming Language
Pattern Matching

```
using Rematch

function numberofrealroots(delta)
    @match delta begin
        x where x > 0  => 2
        x where x == 0 => 1
        _              => 0
    end
end
```

Julia Programming Language
Sum Types a.k.a. tagged unions (just like enum in Rust)

```
using  SumTypes

@sum_type Expression begin
    ConstantI64(::Int64)
    Add(::Expression, ::Expression)
end

function eval(e::Expression)
    result = @cases e begin
        ConstantI64(i) => i
        Add(e1, e2)    => eval(e1) + eval(e2)
        _              => error("Cannot understand :")
    end
    return result
end

eval(Add(ConstantI64(6), ConstantI64(5)))
```

Julia Programming Language
Loops

For loops are single threaded by design

```
results = zeros(10)

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

Julia Programming Language
Threads

Using multiple threads[3]

```julia
using Base.Threads

results = zeros(10)

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

---

[3]# julia -t 10

Julia Programming Language
Distributed Programming

```
julia> using Distributed
julia> addprocs(5);
julia> pmap(abs, [1, 2, -5, 10, 100, -6])
6-element Vector{Int64}:
    1
    2
    5
   10
  100
    6
```

Julia Programming Language
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.

Julia Programming Language
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.

Julia Programming Language
Multiple Dispatch

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

```
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.

Julia Programming Language
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.

Linear Regression
The formulation

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

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

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

Linear Regression
Sample Data

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

Linear Regression
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]
```

Linear Regression
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]
```

Linear Regression
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)
```

Linear Regression
The GLM package - Results

```
julia> include("reg-glm.jl")

Coefficients:
          Coef.    Std. Error    t       Pr(>|t|)   Lower 95%   Upper 95%

x1       -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
...
RandomForestClassifier
RandomForestImputer
RandomForestRegressor
...
SRRegressor
```

XOR
eXclusive OR

x_1	x_2	y
1	1	0
1	0	1
0	1	1
0	0	0

Table: $y = \text{xor}(x_1, x_2)$

Symbolic Regression

```
using SymbolicRegression, MLJ

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

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

Symbolic Regression

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

Symbolic Regression

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

Symbolic Regression

```
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]
```
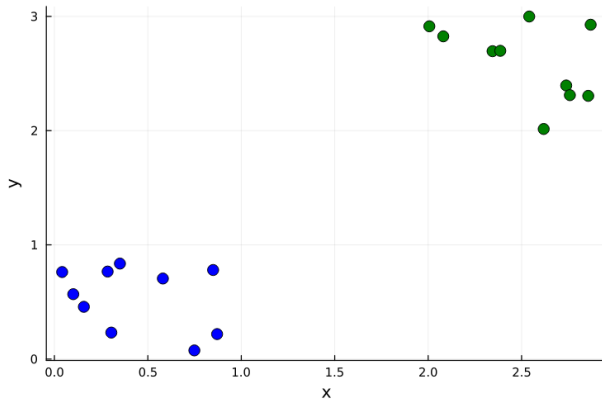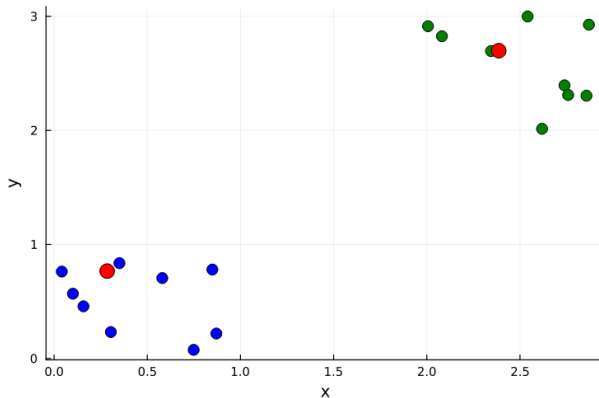
one more cup of coffee?

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

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

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!

Big Distance Matrices
On-demand Distance Matrix

```julia
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
```

Big Distance Matrices
On-demand Distance Matrix

```
# Example
data = Float64[
            1 2;
            0 5;
            1 2]

d = OnDemandDistanceMatrix(data)

println(d[1, 3])
```

Big Distance Matrices
On-demand Distance Matrix

```
data = Float64[
        1 2;
        0 5;
        1 2]

d = OnDemandDistanceMatrix(data)

# d is a usual distance matrix now!
kmedoids(d, 2)
```

Big Distance Matrices
On-demand Distance Matrix

- 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! ☺

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

```
X[1, :] = [1, 3]
y[5] = 9.7
betahats = inv(X'X)X'y
```

Distributions
The Normal Distribution

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

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

Distributions
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
```
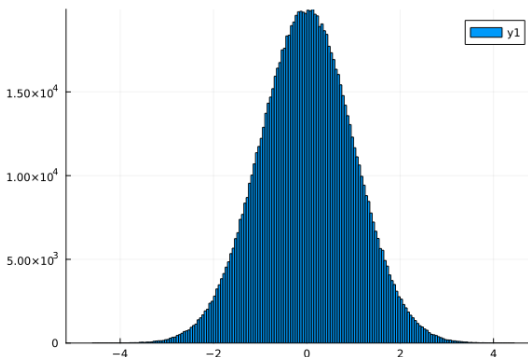
Distributions
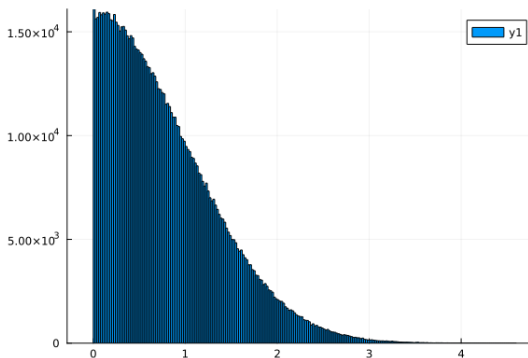
Monte Carlo Simulations - Drawing Random Numbers

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

Distributions
Monte Carlo Simulations - Drawing Random Numbers

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

Hypothesis Tests
Jarque-Bera Test for Normality

```julia
julia> using HypothesisTests
julia> x = randn(30);
julia> JarqueBeraTest(x)
```

The null hypothesis is a joint hypothesis of the skewness being 0 and the kurtosis being 3.

$$H_0 : \text{Data comes from a Normal distribution}$$

$$H_a : \text{🐱}$$

Hypothesis Tests
Jarque-Bera Test for Normality

```
Jarque−Bera normality test
─────────────────────────────
Population details:
    parameter of interest:      skewness and kurtosis
    value under h_0:            "0 and 3"
    point estimate:             "−0.065 and 1.873"
Test summary:
    outcome with 95% confidence: fail to reject h_0
    one−sided p−value:          0.4474
Details:
    number of observations:     30
    JB statistic:               1.60881
```

Numerical Integration
QuadGK

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

```
using QuadGK

function f(x)
    return 1/sqrt(2pi) * exp(-0.5x^2)
end

quadgk(f, -1.0, 1.0)
```
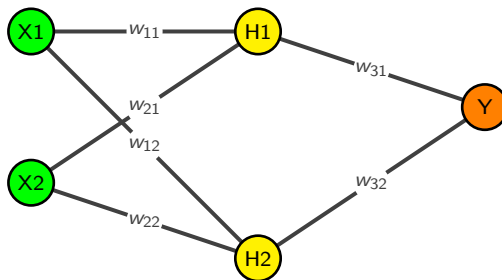
Optimizations
Simple Neural Network

$$H_1 = f(w_0 + x_1 w_{11} + x_2 w_{21})$$

Optimizations
Simple Neural Network

$$H_1 = f(w_{01} + x_1 w_{11} + x_2 w_{21})$$

$$H_2 = f(w_{02} + x_1 w_{12} + x_2 w_{22})$$

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

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

Optimizations
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
```

Optimizations
Simple Neural Network

```
using Metaheuristics

x1 = [1, 1, 0, 0]
x2 = [1, 0, 1, 0]
y  = [0, 1, 1, 0]

bounds = vcat([-10000.0 for i 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
```

Neural Networks with Flux.jl - The model

```
using Flux

model = Chain(
    Dense(2, 3, Flux.sigmoid),
    Dense(3, 1, Flux.sigmoid)
)

loss_fn(x, y) = Flux.mse(model(x), y)

opt = Flux.ADAM(0.1)
```

Neural Networks with Flux.jl - Training

```
for _ in 1:B
    train!(loss_fn, params(model), [(X, y)], opt)
end

# The Output:
println(model(X))
```

Optimizations
Mathematical Programming

$$\max z = 2x_1 + 3x_2$$

Subject to:

$$x_1 + 2x_2 \leq 100$$
$$2x_1 + x_2 \leq 150$$
$$x_1, x_2 \geq 0$$

Optimizations
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)
```

Optimizations
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}:
 66.66666666666667
 16.666666666666657
```

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

```julia
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
```

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

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")
(
    [-0.5000000000000023, 2.3000000000000003],
    [4.299999999999995],
     2,
    [7.69121313410482, 0.9193696350073228]
)
```

Talking to Strangers
Calling C Functions

C Function for integrating single variable function

```
typedef double (*F)(double);

double integrate(F f, double a, double b, double eps){

    double start = a;
    double mysum = 0.0;

    while(start <= b){
        mysum += f(start) * eps;
        start += eps;
    }

    return mysum;
}
```

Talking to Strangers
The Makefile

Generating dynamic link library in Linux

```
integration.so: integration.c
    cc -shared -o integration.so integration.c

clean: integration.so
    rm -f integration.so
```

Talking to Strangers
Integrating Julia function using C library

```julia
function normal(x::Cdouble)::Cdouble
    return (1 / sqrt(2*pi)) * exp(-0.5 * x * x)
end

normal_c = @cfunction(normal, Cdouble, (Cdouble,))

function integrate(f, a, b, eps)
    ccall((:integrate, "./integration.so"), Cdouble,
          (Ptr{Cdouble}, Cdouble, Cdouble, Cdouble), f, a, b, eps)::Cdouble
end

result = integrate(normal_c, -1.0, 1.0, 0.00001);

println(result)
```

Thank you!
Any questions? ☕