Elements of Scientific Computing with Julia

March 5, 2015

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3. Julia is well equipped for parallel computing;
4. We can call C functions directly;
5. Power type system - support for arbitrary precision.

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```
# There are several basic types of numbers.
3 #=> 3 (Int64)
3.2 #=> 3.2 (Float64)
2 + 1im #=> 2 + 1im (Complex{Int64})
2//3 #=> 2//3 (Rational{Int64})

# All of the normal infix operators are available.
1 + 1 #=> 2
8 - 1 #=> 7
10 * 2 #=> 20
35 / 5 #=> 7.0
5 / 2 #=> 2.5 # dividing an Int by an Int always results
    in a Float
div(5, 2) #=> 2 # for a truncated result, use div
5 \ 35 #=> 7.0
2 ^ 2 #=> 4 # power, not bitwise xor
12 % 10 #=> 2
```

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```
# Boolean operators
!true #=> false
!false #=> true
1 == 1 #=> true
2 == 1 #=> false
1 != 1 #=> false
2 != 1 #=> true
1 < 10 #=> true
1 > 10 #=> false
2 <= 2 #=> true
2 >= 2 #=> true

# Comparisons can be chained
1 < 2 < 3 #=> true
2 < 3 < 2 #=> false
```

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```
# Strings are created with "
"This is a string."
# Character literals are written with '
'a'
# A string can be indexed like an array of characters
"This is a string"[1] #=> 'T' # Julia indexes from 1

# $ can be used for string interpolation:
"2 + 2 = $(2 + 2)" #=> "2 + 2 = 4"
# You can put any Julia expression inside the parenthesis.

# Another way to format strings is the printf macro.
@printf "%d is less than %f" 4.5 5.3 # 5 is less than
    5.300000

# Printing is easy
println("I'm Julia. Nice to meet you!")
```

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```
# Arrays store a sequence of values indexed by integers 1
    through n:
a = Int64[] #=> 0-element Int64 Array

# Note that arrays must be given a type, and all elements
    in the array must be of that type.

# 1-dimensional array literals can be written with
    comma-separated values.
b = [4, 5, 6] #=> 3-element Int64 Array: [4, 5, 6]
b[1] #=> 4
b[end] #=> 6

# 2-dimentional arrays use space-separated values and
    semicolon-separated rows.
matrix = [1 2; 3 4] #=> 2x2 Int64 Array: [1 2; 3 4]
```

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```
# Add stuff to the end of an array with push! and append!
push!(a,1)    #=> [1]
push!(a,2)    #=> [1,2]
push!(a,4)    #=> [1,2,4]
push!(a,3)    #=> [1,2,4,3]
append!(a,b) #=> [1,2,4,3,4,5,6]

# Remove from the end with pop
pop!(b)       #=> 6 and b is now [4,5]

# Let's put it back
push!(b,6)  # b is now [4,5,6] again.

a[1] #=> 1 # remember that Julia indexes from 1, not 0!
```

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```
# Function names that end in exclamations points indicate
    that they modify their argument.
arr = [5,4,6] #=> 3-element Int64 Array: [5,4,6]
sort(arr) #=> [4,5,6]; arr is still [5,4,6]
sort!(arr) #=> [4,5,6]; arr is now [4,5,6]

# You can initialize arrays from ranges
a = [1:5] #=> 5-element Int64 Array: [1,2,3,4,5]

# You can look at ranges with slice syntax.
a[1:3] #=> [1, 2, 3]
a[2:] #=> [2, 3, 4, 5]
a[2:end] #=> [2, 3, 4, 5]
```

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```
# Remove elements from an array by index with splice!
arr = [3,4,5]
splice!(arr,2) #=> 4 ; arr is now [3,5]

# Check for existence in an array with in
in(1, a) #=> true

# Examine the length with length
length(a) #=> 8
```

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```
# Tuples are immutable.
tup = (1, 2, 3) #=> (1,2,3) # an (Int64,Int64,Int64)
    tuple.
tup[1] #=> 1

# Many array functions also work on tuples
length(tup) #=> 3
tup[1:2] #=> (1,2)
in(2, tup) #=> true

# Tuples are created even if you leave out the parentheses
d, e, f = 4, 5, 6 #=> (4,5,6)

# Look how easy it is to swap two values
e, d = d, e #=> (5,4) # d is now 5 and e is now 4
```

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```
# Dictionaries store mappings
empty_dict = Dict() #=> Dict{Any,Any}()

# You can create a dictionary using a literal
filled_dict = ["one"=> 1, "two"=> 2, "three"=> 3]

# Look up values with []
filled_dict["one"] #=> 1

# Get all keys
keys(filled_dict)
# Get all values
values(filled_dict)

# Check for existence in a dictionary with in or haskey
in(("two", 3), filled_dict) #=> false
haskey(filled_dict, "one") #=> true
```

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```
# Here is an if statement. Indentation is not meaningful
    in Julia, but it is good for readability.

if some_var > 10
    println("some_var is totally bigger than 10.")
elseif some_var < 10  # This elseif clause is optional.
    println("some_var is smaller than 10.")
else                  # The else clause is optional too.
    println("some_var is indeed 10.")
end
#=> prints "some var is smaller than 10"
```

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```
# For loops iterate over iterables.
# Iterable types include Range, Array, Set, Dict, and
    String.
for animal=["dog", "cat", "mouse"]
    println("$animal is a mammal")
    # You can use $ to interpolate variables or
        expression into strings
end
# prints:
#    dog is a mammal
#    cat is a mammal
#    mouse is a mammal

# You can use 'in' instead of '='.
for animal in ["dog", "cat", "mouse"]
    println("$animal is a mammal")
end
```

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```
# While loops loop while a condition is true
x = 0
while x < 4
    println(x)
    x += 1 # Shorthand for x = x + 1
end
# prints:
#   0
#   1
#   2
#   3

# Handle exceptions with a try/catch block
try
   error("help")
catch e
   println("caught it $e")
```

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```
# The keyword 'function' creates new functions
#function name(arglist)
#  body...
#end
function add(x, y)
    println("x is $x and y is $y")

    # Functions return the value of their last statement
    x + y
end

add(5, 6) #=> 11 after printing out "x is 5 and y is 6"
```

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```
# You can define functions with optional positional
    arguments
function defaults(a,b,x=5,y=6)
    return "$a $b and $x $y"
end

defaults('h','g') #=> "h g and 5 6"
defaults('h','g','j') #=> "h g and j 6"
defaults('h','g','j','k') #=> "h g and j k"
try
    defaults('h') #=> ERROR: no method defaults(Char,)
    defaults() #=> ERROR: no methods defaults()
catch e
    println(e)
end
```

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```
# Julia supports functional programming - stuff like
    currying and higher order functions
function create_adder(x)
    function adder(y)
        x + y
    end
    adder
end

add_10 = create_adder(10)
add_10(3) #=> 13

# There are built-in higher order functions
map(add_10, [1,2,3]) #=> [11, 12, 13]
filter(x -> x > 5, [3, 4, 5, 6, 7]) #=> [6, 7]
```

Arbitrary Precision Arithmetic

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Write a Julia program to compute the mathematical constant e, the base of natural logarithms, from the definition:

$$e = \lim_{n \to \infty} (1 + 1/n)^n$$

Compute $(1 + 1/n)^n$ for $n = 10^k$, $k = 1, 2, ..., 20$ and determine the error in the successive approximations by comparing them with the value of the built in constant e.

Arbitrary Precision Arithmetic

If we enter the following *modified* code into IJulia:

```
for k = 1:2:20
    a = (1+BigFloat(1/10^k))^BigFloat(10^k)
    err = a - e
    @printf("For k = %d, we get the approximation: %1.12f
        and the error %1.12f \n",
    k, a, err)
end
```

Arbitrary Precision Arithmetic

We get the following output:

```
For k = 1,  we get the approximation: 2.593742460100 and
the error -0.12453936835904511060l357
For k = 3,  we get the approximation: 2.716923932236 and
the error -0.00135789622315272149114O
...
For k = 15, we get the approximation: 2.718281828459 and
the error -0.0000000000000011479157 38
For k = 17, we get the approximation: 2.718281828459 and
the error  0.000000000000000180881062
For k = 19, we get the approximation: 2.718281828459 and
the error -0.000000000000000253747066
```

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In this lecture we will look at quadrature methods for solving one dimensional definite integrals numerically.

Quadrature Methods

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We can chop up the area of an unfamiliar shape into slices, and approximate the area of each slice with the area of a familiar shape (such as a rectangle or a trapezoid).

If we add up the area of all these slices, we should get an approximation of the are under the given curve, and thus the approximate solution of the definite integral of the given function.

Rules, rules, rules!

For all of the rules below consider the definite integral $\int_a^b f(x)dx$, that is, the area under the curve f in the closed interval $[a, b]$. We divide $[a, b]$ into n subintervals of equal width $\Delta x = \frac{b-a}{n}$.

Midpoint Rule

This rule obtains the area under the curve by subdividing the area into rectangles of equal width Δx and height $f(x_i^*)$, where x_i^* is the **midpoint** of the subinterval $[x_{i-1}, x_i]$.

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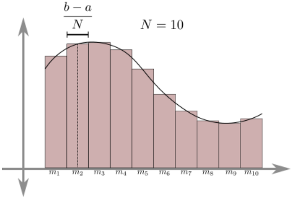
The area of each rectangle is then $\Delta x f(x_i^*)$, and therefore, we get that:

$$\int_a^b f(x)dx \approx \Delta x f(x_1^*) + \Delta x f(x_2^*) + \ldots + \Delta x f(x_n^*)$$



Trapezoidal Rule

This rule obtains the area under the curve by subdividing the area into trapezoids of equal trapezoidal height Δx, and base widths $f(x_{i-1})$ and $f(x_i)$ for each subinterval $[x_{i-1}, x_i]$.

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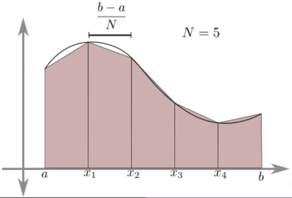
The area of each trapezoid is then $\dfrac{\Delta x}{2}(f(x_{i-1}) + f(x_i))$, and therefore, we get that: $\int\limits_a^b f(x)dx \approx$

$$\frac{\Delta x}{2}(f(x_0)+f(x_1))+\frac{\Delta x}{2}(f(x_1)+f(x_2))+\ldots+\frac{\Delta x}{2}(f(x_{n-1})+f(x_n))$$



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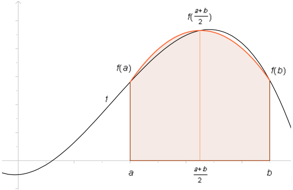
If subdivide the interval $[a, b]$ into $n = 2k$ sub-intervals, then we get that: $\int_a^b f(x)dx \approx$

$$\frac{\Delta x}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + ... + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)]$$



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However, if we are able to get the true value, then why are we bothering with the approximation?

Numerical Integration Error Bounds

Error bounds are quantities we can easily compute and are set as ceilings for our errors, that is, the error obtained by a certain mathematical model is guaranteed to be *less* than its error bound. As you might have already guessed, an error bound depends on the mathematical model used (there is no universal error bound).

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Below are the error bounds for the three methods of numerical integration we've discussed in this lecture.

Numerical Integration Error Bounds

Let f be the function we are numerically integrating. Suppose that $\max_{a \le x \le b} |f''(x)| = K$ and $\max_{a \le x \le b} |f^{(4)}(x)| = M$ for $a \le x \le b$, then:

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3. *The error bound for Simpson's Rule is*

$$\frac{M(b-a)^5}{180n^4}$$

The Error Function

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^2} dt$$

The error function (occurring in statistics to measure the behavior of a sample with respect to the population mean) given above is an example of a non-elementary function.

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However, this integral has no analytic solution...

Save us, Julia!

Let's use IJulia to implement the erf function using the midpoint rule. Our function will take two inputs: the upper bound x of the interval of integration, and the number of sub-intervals n.

Solution

```
# erf's integrand
function integrand(t)
    e^(-t^2)
end

# erf function using the midpoint rule
function middle_erf(x, n)

    delta_x = x / n
    result = 0
    # summing up the are of rectangles
    for i = 1:n
        x_mid = ((i-1)*delta_x + i*delta_x)/2
        result += delta_x*integrand(x_mid)
    end
```

Solution cont.

```
result *= 2 / sqrt(pi)

# since the SECOND derivative of e^(-t^2) is (4t^2 -
    2)*(e^(-t^2)),
# and since it obtains a maximum at t = sqrt(3/2) on
    the interval
# from 0 to x, when x >= sqrt(3/2), OR just at t = x,
    when
# x < sqrt(3/2), then our K in the error bound
    formula is:
if x >= sqrt(3/2)
  error_bound = (4/e^(3/2))*(x^3)/(24*n^2)
else
  error_bound = abs((4*x^2 -
      2)*(e^(-x^2)))*(x^3)/(24*n^2)
end
```

Solution cont.

```
    return ["result" => result, "error bound" =>
        error_bound]
end
```