nb-l04-float

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1 Recap

- Julia type system
- Multiple dispatch
- Performance issues
- Modules

1.1 Julia type system

- Julia is a strongly typed language
- Knowledge about the layout of a value in memory is encoded in its type
- Prerequisite for performance
- There are concrete types and abstract types
- See WikiBook for more

1.1.1 Concrete types

- Every value in Julia has a concrete type
- Concrete types correspond to computer representations of objects
- Inquire type info using `typeof()`
- One can initialize a variable with an explicitely given fixed type
  - Currently posible only in the body of funtions and for return values, not in the global context of Jupyter, REPL

1.1.2 Abstract types

- Abstract types label concepts which work for a several concrete types without regard to their memory layout etc.
- All variables with concrete types corresponding to a given abstract type (must) share a common interface
- A common interface consists of a set of methods working for all types exhibiting this interface
- The functionality of an abstract type is implicitely characterized by the methods working on it
- "duck typing": use the "duck test" — "If it walks like a duck and it quacks like a duck, then it must be a duck" — to determine if an object can be used for a particular purpose

1.1.3 The power of multiple dispatch

- Multiple dispatch is one of the defining features of Julia
- Combined with the the hierarchical type system it allows for powerful generic program design
- New datatypes (different kinds of numbers, differently stored arrays/matrices) work with existing code once they implement the same interface as existent ones.
- In some respects C++ comes close to it, but for the price of more and less obvious code

1.2 Just-in-time compilation and Performance

- Just-in-time compilation is another feature setting Julia apart
- Use the tools from the The LLVM Compiler Infrastructure Project to organize on-the-fly compilation of Julia code to machine code
- Tradeoff: startup time for code execution in interactive situations
- Multiple steps: Parse the code, analyze data types etc.
- Intermediate results can be inspected using a number of macros

1.3 Performance

Macros for performance testing: - @elapsed: wall clock time used - @allocated: number of allocations - @time: @elapsed and @allocated together - @benchmark: Benchmarking small pieces of code

1.3.1 Julia performace gotchas:

- Variables changing types
  - Type change assumed to be always possible in global context (outside of a function)
  - Type change due to inconsequential programming
- Memory allocations for intermediate results
- See # 7 Julia Gotchas to handle

1.4 Structuring your code: modules, files and packages

- Complex code is split up into several files
- Avoid name clashes for code from different places
- Organize the way to use third party code

1.4.1 Finding modules in the file system

- Put single file modules having the same name as the module into a directory which in on the `LOAD_PATH`
- Call "using" or "import" with the module
- You can modify your `LOAD_PATH` by adding e.g. the actual directory

1.4.2 Packages in the file system

- Packages are found via the same mechanism
- Part of the load path are the directory with downloaded packages and the directory with packages under development
- Each package is a directory named `Package` with a subdirectory `src`

- The file `Package/src/Package.jl` defines a module named `Package`
- More structures in a package:
  - Documentation build recipes
  - Test code
  - Dependency description
  - UUID (Universal unique identifier)
- Default packages (e.g. the package manager Pkg) are always available
- Use the package manager to checkout a new package via the registry

2 Julia Workflows

- REPL
- Atom/Juno

2.1 Developing code with the Julia REPL

- "using" a package involves compilation delay on startup of session
- Best way: never leave Julia session
- E.g. edit your code in the editor
- Write code, include, run,
  - repeat

2.1.1 Revise.jl

- Adds a command `includet` which triggers automatic recompile of the included file and those used therein upon change on the disk.
- Put this into your `~/.julia/config/startup.jl`:

[1]:
```
if isinteractive()
    try
        @eval using Revise
        Revise.async_steal_repl_backend()
    catch err
        @warn "Could not load Revise."
    end
end
```

Start Julia at the command prompt with `julia -i`

2.2 Atom/Juno

3 Calling code from other languages

- C
- python
- C++, R ...

3.1 ccall

- C language code has a well defined binary interface
  - `int` ↔ `Int32`
  - `float` ↔ `Float32`
  - `double` ↔ `Float64`
  - C arrays as pointers

- Create file cadd.c:

[2]:
```
open("cadd.c", "w") do io
    write(io, """double cadd(double x, double y) { return x+y; }""")
end
```

[2]:
```
47
```

- Create shared object (a.k.a. "dll") `cadd.so`
  - note the Julia command syntax using backtics

[3]:
```
run(`gcc --shared  cadd.c -o libcadd.so`)
```

[3]:
```
Process(`gcc --shared cadd.c -o
libcadd.so`, ProcessExited(0))
```

- Define wrapper function `cadd` using the Julia `ccall` method
  - `(:cadd, "libcadd")`: call cadd from `libcadd.so`
  - First `Float64`: return type
  - Tuple `(Float64,Float64,)`: parameter types
  - `x,y`: actual data passed
- At its first call it will load `libcadd.so` into Julia
- Direct call of compiled C function `cadd()`, no intermediate wrapper code

[4]:
```
cadd(x,y)=ccall((:cadd, "libcadd"), Float64, (Float64,Float64,),x,y)
```

[4]:
```
cadd (generic function with 1 method)
```

Call wrapper

[5]:
```
@show cadd(1.5,2.5);
```

```
cadd(1.5, 2.5) = 4.0
```

- Julia uses this method to access a number of higly optimized linear algebra and other libraries

3.2 PyCall

- Both Julia and Python are homoiconic language, featuring *reflection*
- They can parse the elemnts of their own data structures
- Possibility to automatically build proxies for python objects in Julia

- Define Python function

```
[6]: open("pyadd.py", "w") do io
         write(io, """
     def pyadd(x,y):
         return x+y
     """)
     end
```

```
[6]: 31
```

- Add PyCall package

```
[7]: using Pkg
     Pkg.add("PyCall")
```

```
  Updating registry at `~/.julia/registries/General`
  Updating git-repo
`https://github.com/JuliaRegistries/General.git`
 Resolving package versions…
  Updating `~/.julia/environments/v1.2/Project.toml`
  [438e738f] + PyCall v1.91.2
  Updating `~/.julia/environments/v1.2/Manifest.toml`
  [1914dd2f] + MacroTools v0.5.2
  [438e738f] + PyCall v1.91.2
```

- Use PyCall package

```
[8]: using PyCall
```

```
 Info: Recompiling stale cache file
/home/fuhrmann/.julia/compiled/v1.2/PyCall/GkzkC.ji for PyCall
[438e738f-606a-5dbb-bf0a-cddfbfd45ab0]
 @ Base loading.jl:1240
```

- Import python module:

```
[9]: pyadd=pyimport("pyadd")
```

```
[9]: PyObject <module 'pyadd' from
     '/home/fuhrmann/Wias/teach/scicomp/course/pyadd.py'>
```

- Call `pyadd` from imported module

```
[10]: @show pyadd.pyadd(3.5,6.5)
```

```
pyadd.pyadd(3.5, 6.5) = 10.0
```

```
[10]: 10.0
```

- Julia allows to call almost any python package
- E.g. matplotlib graphics

- There is also a pyjulia package allowing to call Julia from python

4 Number representation

Numbers of course are represented by bits

[11]:
```
@show bitstring(Int16(1))
@show bitstring(Float16(1))
@show bitstring(Int64(1))
@show bitstring(Float64(1))
```

```
bitstring(Int16(1)) = "0000000000000001"
bitstring(Float16(1)) = "0011110000000000"
bitstring(Int64(1)) =
"0000000000000000000000000000000000000000000000000000000000000001"
bitstring(Float64(1)) =
"0011111111110000000000000000000000000000000000000000000000000000"
```

[11]:
```
"0011111111110000000000000000000000000000000000000000000000000000"
```

4.1 Representation of real numbers

- Any real number $x \in \mathbb{R}$ can be expressed via representation formula:

$$x = \pm \sum_{i=0}^{\infty} d_i \beta^{-i} \beta^e$$

  - $\beta \in \mathbb{N}, \beta \geq 2$: *base*
  - $d_i \in \mathbb{N}, 0 \leq d_i < \beta$: *mantissa digits*
  - $e \in \mathbb{Z}$: *exponent*
- Infinite for periodic decimal numbers, irrational numbers

4.1.1 Scientific notation of floating point numbers: e.g.

- Let $x = 6.022 \cdot 10^{23}$
  - $\beta = 10$
  - $d = (6, 0, 2, 2, 0 \dots)$
  - $e = 23$
- Non-unique: e.g. $x_1 = 0.6022 \cdot 10^{24} = x$
  - $\beta = 10$
  - $d = (0, 6, 0, 2, 2, 0 \dots)$
  - $e = 24$

4.2 Computer representation of floating point numbers

- Computer representation uses $\beta = 2$, therefore $d_i \in \{0, 1\}$
- Truncation to fixed finite size:

$$x = \pm \sum_{i=0}^{t-1} d_i \beta^{-i} \beta^e$$

- t: mantissa length
- Normalization: assume $d_0 = 1 \Rightarrow$ save one bit for mantissa
  - normalization step after operations: adjust mantissa and exponent
- k: exponent size $-\beta^k + 1 = L \leq e \leq U = \beta^k - 1$
- Extra bit for sign
- $\Rightarrow$ storage size: $ (t-1) + k + 1$

4.2.1 IEEE 754 floating point types

- Standardized for many languages
- Hardware support usually for 64bit and 32bit

precision	Julia	C/C++	k	t	bits
quadruple	n/a	long double	16	111	128
double	Float64	double	11	53	64
single	Float32	float	8	23	32
half	Float16	n/a	5	10	16

- See also the Julia Documentation on floating point numbers

4.2.2 Storage layout for a normalized Float32 number ($d_0 = 1$)

- bit 0: sign, $0 \to +, \quad 1 \to -$
- bit $1 \dots 8$: $r = 8$ exponent bits
  - the value $e + 2^{r-1} - 1 = 127$ is stored $\Rightarrow$ no need for sign bit in exponent
- bit $9 \dots 31$: $t = 23$ mantissa bits $d_1 \dots d_{23}$
- $d_0 = 1$ not stored $\equiv$ "hidden bit"

[12]:
```
function floatbits(x::Float32)
    s=bitstring(x)
    return s[1]*" "*s[2:9]*" "*s[10:end]
end
function floatbits(x::Float64)
    s=bitstring(x)
    return s[1]*" "*s[2:12]*" "*s[13:end]
end
```

[12]:
```
floatbits (generic function with 2 methods)
```

- $e = 0$, stored $e = 127$:

[13]:
```
floatbits(Float32(1))
```

[13]:
```
"0 01111111 00000000000000000000000"
```

- $e = 1$, stored $e = 128$:

[14]:
```
floatbits(Float32(2))
```

[14]:
```
"0 10000000 00000000000000000000000"
```

- $e = -1$, stored $e = 126$:

[15]:
```
floatbits(Float32(1/2))
```

[15]:
```
"0 01111110 00000000000000000000000"
```

- Numbers which are exactly represented in decimal system may not be exactly represented in binary system! - Example: infinite periodic number in binary system:

[16]:
```
floatbits(Float32(0.1))
```

[16]:
```
"0 01111011 10011001100110011001101"
```

- positive zero:

[17]:
```
floatbits(zero(Float32))
```

[17]:
```
"0 00000000 00000000000000000000000"
```

- negative zero:

[18]:
```
floatbits(-zero(Float32))
```

[18]:
```
"1 00000000 00000000000000000000000"
```

4.2.3 Floating point limits

- Finite size of representation $\Rightarrow$ there are minimal and maximal possible numbers which can be represented
- symmetry wrt. 0 because of sign bit
- smallest positive denormalized number: $d_i = 0, i = 0 \ldots t-2, d_{t-1} = 1 \Rightarrow x_{min} = \beta^{1-t}\beta^L$

[19]:
```
@show nextfloat(zero(Float32));
@show floatbits(nextfloat(zero(Float32)));
```

```
nextfloat(zero(Float32)) = 1.0f-45
floatbits(nextfloat(zero(Float32))) = "0 00000000 00000000000000000000001"
```

[20]:
```
@show nextfloat(zero(Float64));
@show floatbits(nextfloat(zero(Float64)));
```

```
nextfloat(zero(Float64)) = 5.0e-324
floatbits(nextfloat(zero(Float64))) = "0 00000000000
0000000000000000000000000000000000000000000000000001"
```

- smallest positive normalized number: $d_0 = 1, d_i = 0, i = 1 \ldots t-1 \Rightarrow x_{min} = \beta^L$

[21]:
```
@show floatmin(Float32);
@show floatbits(floatmin(Float32));
```

```
floatmin(Float32) = 1.1754944f-38
floatbits(floatmin(Float32)) = "0 00000001 00000000000000000000000"
```

[22]:
```
@show floatmin(Float64);
@show floatbits(floatmin(Float64));
```

```
floatmin(Float64) = 2.2250738585072014e-308
floatbits(floatmin(Float64)) = "0 00000000001
0000000000000000000000000000000000000000000000000000"
```

- largest positive normalized number: $d_i = \beta - 1, 0 \dots t-1 \Rightarrow x_{max} = \beta(1-\beta^{1-t})\beta^U$

[23]:
```
@show floatmax(Float32)
@show floatbits(floatmax(Float32));
```

```
floatmax(Float32) = 3.4028235f38
floatbits(floatmax(Float32)) = "0 11111110 11111111111111111111111"
```

[24]:
```
@show floatmax(Float64)
@show floatbits(floatmax(Float64));
```

```
floatmax(Float64) = 1.7976931348623157e308
floatbits(floatmax(Float64)) = "0 11111111110
1111111111111111111111111111111111111111111111111111"
```

- largest representable number

[25]:
```
@show typemax(Float32)
@show floatbits(typemax(Float32))
@show prevfloat(typemax(Float32));
```

```
typemax(Float32) = Inf32
floatbits(typemax(Float32)) = "0 11111111 00000000000000000000000"
prevfloat(typemax(Float32)) = 3.4028235f38
```

[26]:
```
@show typemax(Float64)
@show floatbits(typemax(Float64))
@show prevfloat(typemax(Float64));
```

```
typemax(Float64) = Inf
floatbits(typemax(Float64)) = "0 11111111111
0000000000000000000000000000000000000000000000000000"
prevfloat(typemax(Float64)) = 1.7976931348623157e308
```

4.3 Machine precision

- There cannot be more than 2^{t+k} floating point numbers $\Rightarrow$ almost all real numbers have to be approximated
- Let x be an exact value and $\tilde{x}$ be its approximation. Then $|\frac{\tilde{x}-x}{x}| < \epsilon$ is the best accuracy estimate we can get, where
  - $\epsilon = \beta^{1-t}$ (truncation)
  - $\epsilon = \frac{1}{2}\beta^{1-t}$ (rounding)
- Also: ϵ is the smallest representable number such that $1 + \epsilon > 1$.
- Relative errors show up in particular when
  - subtracting two close numbers
  - adding smaller numbers to larger ones

4.4 How do operations work?

E.g. Addition - Adjust exponent of number to be added: - Until both exponents are equal, add one to exponent, shift mantissa to right bit by bit - Add both numbers - Normalize result

The smallest number one can add to 1 can have at most t bit shifts of normalized mantissa until mantissa becomes 0, so its value must be 2^{-t}.

4.4.1 Machine epsilon

- Smallest floating point number ϵ such that $1 + \epsilon > 1$ in floating point arithmetic
- In exact math it is true that from $1 + \varepsilon = 1$ it follows that $0 + \varepsilon = 0$ and vice versa. In floating point computations this is not true

[27]:
```
 =eps(Float32)
@show  , floatbits( )
@show one(Float32)+ /2
@show one(Float32)+ ,floatbits(one(Float32)+ )
@show nextfloat(one(Float32))-one(Float32);
```

```
( , floatbits( )) = (1.1920929f-7, "0 01101000 00000000000000000000000")
one(Float32) +   / 2 = 1.0f0
(one(Float32) +  , floatbits(one(Float32) +  )) = (1.0000001f0, "0 01111111
00000000000000000000001")
nextfloat(one(Float32)) - one(Float32) = 1.1920929f-7
```

[28]:
```
 =eps(Float64)
@show  , floatbits( )
@show one(Float64)+ /2
@show one(Float64)+ ,floatbits(one(Float64)+ )
@show nextfloat(one(Float64))-one(Float64);
```

```
( , floatbits( )) = (2.220446049250313e-16, "0 01111001011
0000000000000000000000000000000000000000000000000000")
one(Float64) +   / 2 = 1.0
(one(Float64) +  , floatbits(one(Float64) +  )) = (1.0000000000000002, "0
01111111111 0000000000000000000000000000000000000000000000000001")
nextfloat(one(Float64)) - one(Float64) = 2.220446049250313e-16
```

4.4.2 Associativity ?

- Normally: $(a+b)+c=a+(b+c)$
- But without optimization:

[29]:
```
@show (1.0 + 0.5*eps(Float64)) - 1.0
@show 1.0 + (0.5*eps(Float64) - 1.0);
```

```
(1.0 + 0.5 * eps(Float64)) - 1.0 = 0.0
1.0 + (0.5 * eps(Float64) - 1.0) = 1.1102230246251565e-16
```

- With optimization:

[30]:
```
 =eps(Float64)
@show (1.0 +  /2) - 1.0
@show 1.0 + ( /2 - 1.0);
```

```
(1.0 +   / 2) - 1.0 = 0.0
1.0 + (  / 2 - 1.0) = 1.1102230246251565e-16
```

4.4.3 Density of floating point numbers

[31]:
```
function fpdens(x::AbstractFloat;sample_size=1000)
    xleft=x
    xright=x
    for i=1:sample_size
        xleft=prevfloat(xleft)
        xright=nextfloat(xright)
    end
    return prevfloat(2.0*sample_size/(xright-xleft))
end
```

[31]:
```
fpdens (generic function with 1 method)
```

[32]:
```
x=10.0 .^collect(-10.0:0.1:10.0)
```

[32]:
```
201-element Array{Float64,1}:
 1.0e-10
 1.2589254117941662e-10
 1.584893192461111e-10
 1.9952623149688828e-10
 2.511886431509582e-10
 3.1622776601683795e-10
 3.9810717055349694e-10
 5.011872336272714e-10
 6.309573444801942e-10
```

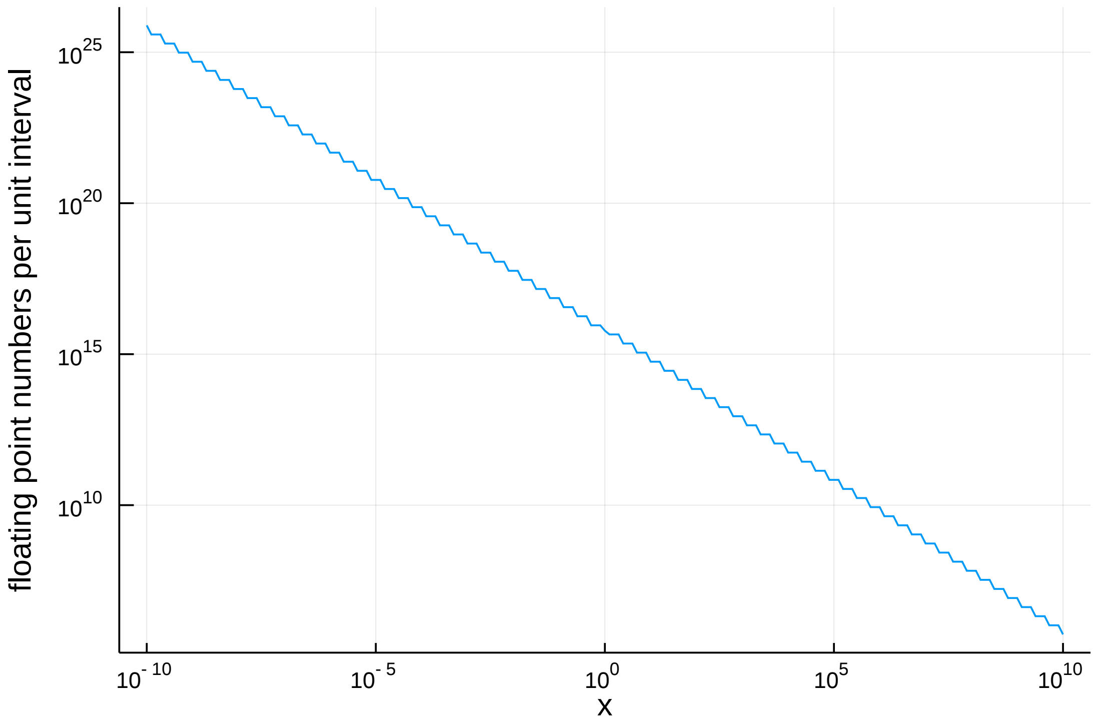
```
7.943282347242822e-10
1.0e-9
1.2589254117941663e-9
1.584893192461111e-9

7.943282347242821e8
1.0e9
1.258925411794166e9
1.5848931924611108e9
1.9952623149688828e9
2.511886431509582e9
3.1622776601683793e9
3.9810717055349693e9
5.011872336272715e9
6.309573444801943e9
7.943282347242822e9
1.0e10
```

[33]:
```
using Plots
using Plots
plot(x,fpdens.(x), xaxis=:log, yaxis=:log, label="",xlabel="x",␣
 ↪ylabel="floating point numbers per unit interval")
```

```
 Info: Recompiling stale cache file
/home/fuhrmann/.julia/compiled/v1.2/Plots/ld3vC.ji for Plots
[91a5bcdd-55d7-5caf-9e0b-520d859cae80]
 @ Base loading.jl:1240
```

[33]:



5 Matrix + Vector norms

5.1 Vector norms: let $x = (x_i) \in \mathbb{R}^n$

[34]:
```
using LinearAlgebra
x=[3.0,2.0,5.0]
```

[34]:
```
3-element Array{Float64,1}:
 3.0
 2.0
 5.0
```

- $||x||_1 = \sum_{i=1}^n |x_i|$: sum norm, l_1-norm

[35]:
```
@show norm(x,1);
```

```
norm(x, 1) = 10.0
```

- $||x||_2 = \sqrt{\sum_{i=1}^n x_i^2}$: Euclidean norm, l_2-norm

[36]:
```
@show norm(x,2);
@show norm(x);
```

```
norm(x, 2) = 6.164414002968976
norm(x) = 6.164414002968976
```

- $||x||_\infty = \max_{i=1}^n |x_i|$: maximum norm, l_∞-norm

[37]:
```
@show norm(x, Inf);
```

```
norm(x, Inf) = 5.0
```

Matrix $A = (a_{ij}) \in \mathbb{R}^n \times \mathbb{R}^n$ - Representation of linear operator $\mathcal{A} : \mathbb{R}^n \to \mathbb{R}^n$ defined by $\mathcal{A} : x \mapsto y = Ax$ with

$$y_i = \sum_{j=1}^n a_{ij} x_j$$

- Induced matrix norm:

$$\begin{aligned} ||A||_p &= \max_{x \in \mathbb{R}^n, x \neq 0} \frac{||Ax||_p}{||x||_p} \\ &= \max_{x \in \mathbb{R}^n, ||x||_p = 1} \frac{||Ax||_p}{||x||_p} \end{aligned}$$

5.2 Matrix norms induced from vector norms

[38]:
```
A=[3.0 2.0 5.0; 0.1  0.3  0.5 ; 0.6  2 3]
```

[38]:
```
3×3 Array{Float64,2}:
 3.0  2.0  5.0
 0.1  0.3  0.5
 0.6  2.0  3.0
```

- $||A||_1 = \max_{j=1}^n \sum_{i=1}^n |a_{ij}|$ maximum of column sums of absolute values of entries

[39]:
```
@show opnorm(A,1);
```

```
opnorm(A, 1) = 8.5
```

- $||A||_\infty = \max_{i=1}^n \sum_{j=1}^n |a_{ij}|$ maximum of row sums of absolute values of entries

[40]:
```
@show opnorm(A,Inf);
```

```
opnorm(A, Inf) = 10.0
```

- $||A||_2 = \sqrt{\lambda_{max}}$ with λ_{max}: largest eigenvalue of $A^T A$.

[41]:
```
@show opnorm(A,2);
```

```
opnorm(A, 2) = 7.083763693021976
```

6 Matrix condition number and error propagation

- Problem: solve $Ax = b$, where b is inexact
- Let Δb be the error in b and Δx be the resulting error in x such that

$$A(x + \Delta x) = b + \Delta b.$$

- Since $Ax = b$, we get $A\Delta x = \Delta b$
- Therefore

$$\left\{ \begin{array}{ll} \Delta x & = A^{-1}\Delta b \\ Ax & = b \end{array} \right\} \Rightarrow \left\{ \begin{array}{rl} ||A|| \cdot ||x|| & \geq ||b|| \\ ||\Delta x|| & \leq ||A^{-1}|| \cdot ||\Delta b|| \end{array} \right.$$

$$\Rightarrow \frac{||\Delta x||}{||x||} \leq \kappa(A) \frac{||\Delta b||}{||b||}$$

where $\kappa(A) = ||A|| \cdot ||A^{-1}||$ is the *condition number* of A.

6.0.1 Error propagation:

[42]:
```
A=[ 1.0 -1.0 ; 1.0e5 1.0e5];
Ainv=inv(A)
 =opnorm(A)*opnorm(Ainv)
@show Ainv
@show  ;
```

```
Ainv = [0.5 5.0e-6; -0.5 5.0e-6]
  = 100000.0
```

[43]:
```
x=[ 1.0, 1.0]
b=A*x
@show b
Δb=1*[eps(1.0), eps(1.0)]
Δx=Ainv*(b+Δb)-x
@show norm(Δx)/norm(x)
@show norm(Δb)/norm(b)
@show  *norm(Δb)/norm(b)
```

```
b = [0.0, 200000.0]
norm(Δx) / norm(x) = 7.850462293418875e-17
norm(Δb) / norm(b) = 1.5700924586837751e-21
(  * norm(Δb)) / norm(b) = 1.5700924586837752e-16
```

[43]:
```
1.5700924586837752e-16
```

This notebook was generated using Literate.jl.