Computer Arithmetic

Computer Arithmetic in Hardware

- Computer hardware supports two kinds of numbers:
  - fixed precision integers
  - floating point numbers
- Computer integers have a limited range
- Floating point numbers are a finite subset of the (extended) real line.

Overflow

- Calculations with native computer integers can overflow.
- Low level languages usually do not detect this.
- Calculations with floating point numbers can also overflow to $\pm\infty$.

Underflow

- Floating point operations can also underflow (be rounded to zero).

A Simple Example

A simple C program, available in

```
http://www.stat.uiowa.edu/~luke/classes/STAT7400/
                    examples/fact
```

that calculates *n*! using integer and double precision floating point produces

```
luke@itasca2 notes% ./fact 10
ifac = 3628800, dfac = 3628800.000000
luke@itasca2 notes% ./fact 15
ifac = 2004310016, dfac = 1307674368000.000000
luke@itasca2 notes% ./fact 20
ifac = -2102132736, dfac = 2432902008176640000.000000
luke@itasca2 notes% ./fact 30
ifac = 1409286144, dfac = 265252859812191032188804700045312.000000
luke@itasca2 notes% ./fact 40
ifac = 0, dfac = 815915283247897683795548521301193790359984930816.000000
luke@itasca2 fact% ./fact 200
ifac = 0, dfac = inf
```

- Most current computers include $\pm\infty$ among the finite set of representable real numbers.
- How this is used may vary:
  - On our x86_64 Linux workstations:

    ```
    > exp(1000)
    [1] Inf
    ```

  - On a PA-RISC machine running HP-UX:

    ```
    > exp(1000)
    [1] 1.797693e+308
    ```

    This is the largest finite floating point value.

Arithmetic in R

Higher level languages may at least detect integer overflow. In R,

```
> typeof(1:100)
[1] "integer"
> p<-as.integer(1)   # or p <- 1L
> for (i in 1:100) p <- p * i
Warning message:
NAs produced by integer overflow in: p * i
> p
[1] NA
```

Floating point calculations behave much like the C version:

```
> p <- 1
> for (i in 1:100) p <- p * i
> p
[1] 9.332622e+157
> p <- 1
> for (i in 1:200) p <- p * i
> p
[1] Inf
```

The `prod` function converts its argument to double precision floating point before computing its result:

```
> prod(1:100)
[1] 9.332622e+157
> prod(1:200)
[1] Inf
```

Bignum and Arbitrary Precision Arithmetic

Other high-level languages may provide

- arbitrarily large integers(often called *bignums*)
- rationals (ratios of arbitrarily large integers)

Some also provide arbitrary precision floating point arithmetic.

In Mathematica:

```
In[3]:= Factorial[100]

Out[3]= 933262154439441526816992388562667004907159682643816214685929638952175\
>    99993229915608941463976156518286253697920827223758251185210916864000000\
>    0000000000000000
```

In R we can use the `gmp` package available from CRAN:

```
> prod(as.bigz(1:100))
[1]    "933262154439441526816992388562667004907159682643816214685929638952175
     99993229915608941463976156518286253697920827223758251185210916864000000
     0000000000000000"
```

- The output of these examples is slightly edited to make comparison easier.
- These calculations are *much* slower than floating point calculations.
- C now supports `long double` variables, which are often (but not always!) slower than `double` but usually provide more accuracy.
- Some FORTRAN compilers also support *quadruple precision* variables.

Rounding Errors

A simple, doubly stochastic 2×2 Markov transition matrix:

```
> p <- matrix(c(1/3, 2/3, 2/3,1/3),nrow=2)
> p
          [,1]      [,2]
[1,] 0.3333333 0.6666667
[2,] 0.6666667 0.3333333
```

Theory says:

$$P^n \to \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}$$

Let's try it:

```
> q <- p
> for (i in 1:10) q <- q %*% q
> q
     [,1] [,2]
[1,]  0.5  0.5
[2,]  0.5  0.5
```

The values aren't exactly equal to 0.5 though:

```
> q - 0.5
              [,1]          [,2]
[1,] -1.776357e-15 -1.776357e-15
[2,] -1.776357e-15 -1.776357e-15
```

We can continue:

```
> for (i in 1:10) q <- q %*% q
> q
     [,1] [,2]
[1,]  0.5  0.5
[2,]  0.5  0.5
> for (i in 1:10) q <- q %*% q
> for (i in 1:10) q <- q %*% q
> q
          [,1]      [,2]
[1,] 0.4999733 0.4999733
[2,] 0.4999733 0.4999733
```

Rounding error has built up.

Continuing further:

```
> for (i in 1:10) q <- q %*% q
> q
          [,1]      [,2]
[1,] 0.4733905 0.4733905
[2,] 0.4733905 0.4733905
> for (i in 1:10) q <- q %*% q
> q
             [,1]         [,2]
[1,] 2.390445e-25 2.390445e-25
[2,] 2.390445e-25 2.390445e-25
> for (i in 1:10) q <- q %*% q
> for (i in 1:10) q <- q %*% q
> for (i in 1:10) q <- q %*% q
> q
     [,1] [,2]
[1,]    0    0
[2,]    0    0
```

As another example, the log-likelihood for right-censored data includes terms of the form $\log(1-F(x))$. For the normal distribution, this can be computed as

```
log(1 - pnorm(x))
```

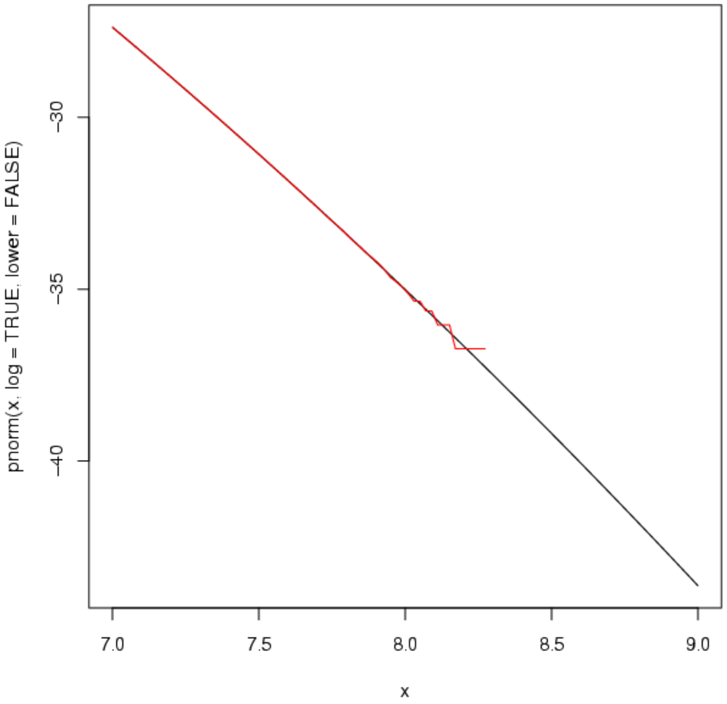
An alternative is

```
pnorm(x, log = TRUE, lower = FALSE)
```

The expressions

```
x <- seq(7,9,len=100)
plot(x, pnorm(x, log = TRUE,lower = FALSE), type = "l")
lines(x, log(1 - pnorm(x)), col = "red")
```

produce the plot



Some notes:

- The problem is called *catastrophic cancellation*.
- Floating point arithmetic is not associative or distributive.
- The range considered here is quite extreme, but can be important in some cases.
- The expression `log(1 - pnorm(x))` produces invalid results ($-\infty$) for `x` above roughly 8.3.
- Most R cdf functions allow `lower.tail` and `log.p` arguments (shortened to `log` and `lower` here)
- The functions `expm1` and `log1p` can also be useful.

  $$\begin{aligned} \texttt{expm1(x)} &= e^x - 1 \\ \texttt{log1p(x)} &= \log(1+x) \end{aligned}$$

  These functions also exist in the standard C math library.

Another illustration is provided by the behavior of the expression

$$e^{-2x^2} - e^{-8x^2}$$

near the origin:

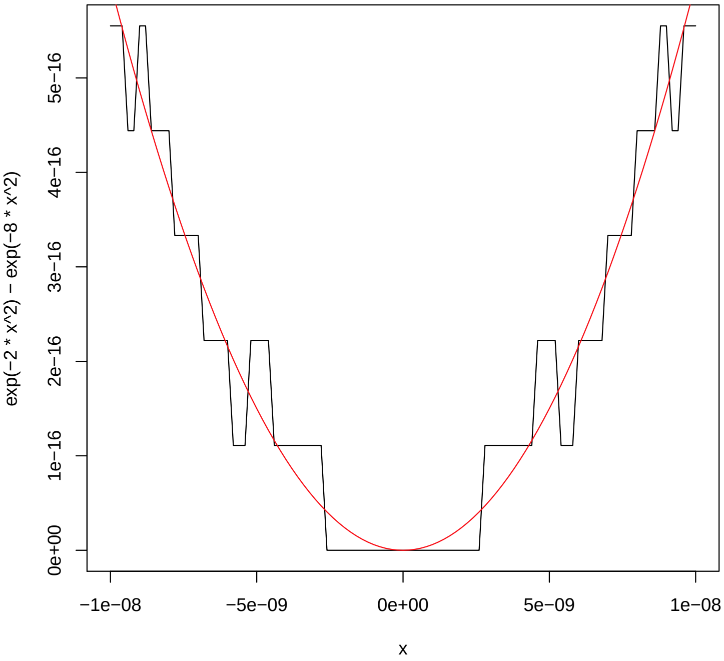
```
x <- seq(-1e-8, 1e-8, len = 101)
plot(x, exp(-2 * x ^ 2) - exp(-8 * x ^ 2), type = "l")
```

Rewriting the expression as

$$e^{-2x^2}\left(1 - e^{-6x^2}\right) = -e^{-2x^2}\mathrm{expm1}(-6x^2)$$

produces a more stable result:

```
lines(x, -exp(-2 * x ^ 2) * expm1(-6 * x ^ 2), col = "red")
```



Example: Sample Standard Deviations

```
> x <- 100000000000000 + rep(c(1,2), 5)
> x
 [1] 1e+14 1e+14 1e+14 1e+14 1e+14 1e+14 1e+14 1e+14 1e+14 1e+14
> print(x, digits = 16)
 [1] 100000000000001 100000000000002 100000000000001 100000000000002
 [5] 100000000000001 100000000000002 100000000000001 100000000000002
 [9] 100000000000001 100000000000002
> n <- length(x)
> s <- sqrt((sum(x^2) - n * mean(x)^2) / (n - 1))
> s
[1] 0
> s == 0
[1] TRUE
> y <- rep(c(1,2), 5)
> y
 [1] 1 2 1 2 1 2 1 2 1 2
> sqrt((sum(y^2) - n * mean(y)^2) / (n - 1))
[1] 0.5270463
> sd(x)
[1] 0.5270463
> sd(y)
[1] 0.5270463
```

- The “computing formula” $\sum x_i^2 - n\overline{x}^2$ is not numerically stable.
- A two-pass algorithm that first computes the mean and then computes $\sum (x_i - \overline{x})^2$ works much better.
- There are also reasonably stable one-pass algorithms.

Example: Truncated Normal Distribution

- Sometimes it is useful to simulate from a standard normal distribution conditioned to be at least a, or truncated from below at a.
- The CDF is

  $$F(x|a) = \frac{\Phi(x) - \Phi(a)}{1 - \Phi(a)}$$

  for $x \geq a$.
- The inverse CDF is

  $$F^{-1}(u|a) = \Phi^{-1}(\Phi(a) + u(1 - \Phi(a)))$$

- This can be computed using

  ```
  Finv0 <- function(u, a) {
      p <- pnorm(a)
      qnorm(p + u * (1 - p))
  }
  ```

- Some plots:

  ```
  u <- (1:100) / 101
  plot(u, Finv0(u, 0), type = "l")
  plot(u, Finv0(u, 2), type = "l")
  plot(u, Finv0(u, 4), type = "l")
  plot(u, Finv0(u, 8), type = "l")
  ```

- An improved version:

  ```
  Finv1 <- function(u, a) {
      q <- pnorm(a, lower.tail = FALSE)
      qnorm(q * (1 - u), lower.tail = FALSE)
  }

  lines(u, Finv1(u, 8), col = "red")
  ```

- This could be further improved if the tails need to be more accurate.

Interger Arithmetic

- Integer data types can be signed or unsigned; they have a finite range.
- Almost all computers now use *binary place-value* for unsigned integers and *two's complement* for signed integers.
- Ranges are

$$\begin{array}{ll} \text{unsigned:} & 0,1,\ldots,2^n-1 \\ \text{signed:} & -2^{n-1},\ldots,2^{n-1}-1. \end{array}$$

  For C `int` and Fortran `integer` the value $n = 32$ is almost universal.
- If the result of `+`, `*`, or `-` is representable, then the operation is exact; otherwise it *overflows*.
- The result of `/` is typically truncated; some combinations can overflow.
- Typically overflow is silent.
- Integer division by zero signals an error; on Linux a SIGFPE (floating point error signal!) is sent.
- statistical calculations rarely need to use integers directly except
  - as dimension sizes and indices for arrays
  - as sizes in storage allocation requests
  - as frequencies for categorical data
- Storing scaled floating point values as small integers (e.g. single bytes) can save space.
- As data sets get larger, being able to represent integers larger than $2^{31}-1$ is becoming important.
- Double precision floating point numbers can represent integers up to 2^{53} exactly.

- Detecting integer overflow portably is hard; one possible strategy: use double precision floating point for calculation and check whether the result fits.
  - This works if integers are 32-bit and double precision is 64-bit IEEE
  - These assumptions are almost universally true but should be tested at compile time.

  Other strategies may be faster, in particular for addition, but are harder to implement.
- You can find out how R detects integer overflow by looking in the file

  ```
  src/main/arithmetic.c
  ```

  The R sources are available at

  ```
  https://svn.r-project.org/R/
  ```

Floating Point Arithmetic

- Floating point numbers are represented by a sign s, a *significand* or *mantissa sig*, and an *exponent exp*; the value of the number is

  $$(-1)^s \times sig \times 2^{exp}$$

  The significand and the exponent are represented as binary integers.

- Bases other than 2 were used in the past, but virtually all computers now follow the IEEE standard number 754 (IEEE 754 for short; the corresponding ISO standard is ISO/IEC/IEEE 60559:2011).

- IEEE 754 specifies the number of bits to use:

	sign	significand	exponent	total
single precision	1	23	8	32
double precision	1	52	11	64
extended precision	1	64	15	80

- A number is *normalized* if $1 \leq sig < 2$. Since this means it looks like

  $$1.something \times 2^{exp}$$

  we can use all bits of the mantissa for the *something* and get an extra bit of precision from the implicit leading one.

- Numbers smaller in magnitude than $1.0 \times 2^{exp_{min}}$ can be represented with reduced precision as

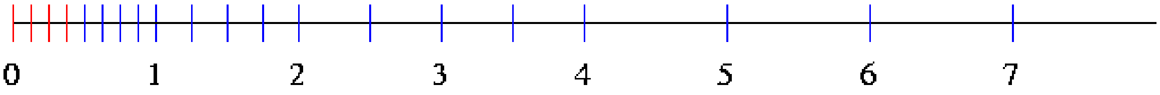
  $$0.something \times 2^{exp_{min}}$$

  These are *denormalized* numbers.

- Denormalized numbers allow for *gradual underflow*. IEEE 745 includes them; many older approaches did not.

- Some GPUs set denormalized numbers to zero.

For a significand with three bits, $exp_{min} = -1$, and $exp_{max} = 2$ the available nonnegative floating point numbers look like this:



Normalized numbers are blue, denormalized numbers are red.

- Zero is not a normalized number (but all representations include it).
- Without denormalized numbers, the gap between zero and the first positive number is larger than the gap between the first and second positive numbers.

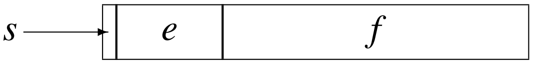
There are actually two zeros in this framework: $+0$ and -0. One way to see this in R:

```
> zp <- 0          ## this is read as +0
> zn <- -1 * 0     ## or zn <- -0; this produces -0
> zn == zp
[1] TRUE
> 1 / zp
[1] Inf
> 1 / zn
[1] -Inf
```

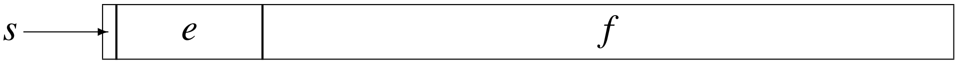
This can identify the direction from which underflow occurred.

- The IEEE 754 representation of floating point numbers looks like

Single precision, exponent bias $b = 127$



Double precision, exponent bias $b = 1023$



- The exponent is represented by a nonnegative integer e from which a *bias b* is subtracted.
- The fractional part is a nonnegative integer f.
- The representation includes several special values: $\pm\infty$, NaN (*Not a Number*) values:

	e	f	Value
Normalized	$1 \leq e \leq 2b$	*any*	$\pm 1.f \times 2^{e-b}$
Denormalized	0	$\neq 0$	$\pm 0.f \times 2^{-b+1}$
Zero	0	0	± 0
Infinity	$2b+1$	0	$\pm\infty$
NaN	$2b+1$	$\neq 0$	NaN

- 1.0/0.0 will produce $+\infty$; 0.0/0.0 will produce NaN.
- On some systems a flag needs to be set so 0.0/0.0 does not produce an error.
- Library functions like exp, log will behave predictably on most systems, but there are still some where they do not.
- Comparisons like `x <= y` or `x == y` should produce `FALSE` if one of the operands is NaN; most Windows C compilers violate this.
- Range of exactly representable integers in double precision:

$$\pm(2^{53}-1) \approx \pm 9.0072 \times 10^{15}$$

- Smallest positive (denormalized) double precision number:

$$2^{-b+1} \times 2^{-52} = 2^{-1074} \approx 4.940656 \times 10^{-324}$$

Machine Characteristics

Machine Characteristics in R

The variable `.Machine` contains values for the characteristics of the current machine:

```
> .Machine
$double.eps
[1] 2.220446e-16
$double.neg.eps
[1] 1.110223e-16
$double.xmin
[1] 2.225074e-308
$double.xmax
[1] 1.797693e+308
$double.base
[1] 2
$double.digits
[1] 53
$double.rounding
[1] 5
$double.guard
[1] 0
$double.ulp.digits
[1] -52
$double.neg.ulp.digits
[1] -53
$double.exponent
[1] 11
$double.min.exp
[1] -1022
$double.max.exp
[1] 1024
$integer.max
[1] 2147483647
$sizeof.long
[1] 8
$sizeof.longlong
[1] 8
$sizeof.longdouble
[1] 16
$sizeof.pointer
[1] 8
```

The help page gives details.

Machine Epsilon and Machine Unit

Let m be the smallest and M the largest positive finite normalized floating point numbers.

Let $\mathrm{fl}(x)$ be the closest floating point number to x.

Machine Unit

The *machine unit* is the smallest number $\mathbf{u}$ such that

$$|\mathrm{fl}(x) - x| \leq \mathbf{u}\,|x|$$

for all $x \in [m,M]$; this implies that for every $x \in [m,M]$

$$\mathrm{fl}(x) = x(1+u)$$

for some u with $|u| \leq \mathbf{u}$. For double precision IEEE arithmetic,

$$\mathbf{u} = \frac{1}{2}2^{1-53} = 2^{-53} \approx 1.110223 \times 10^{-16}$$

Machine Epsilon

The *machine epsilon* ε_m is the smallest number x such that

$$\mathrm{fl}(1+x) \neq 1$$

For double precision IEEE arithmetic,

$$\varepsilon_m = 2^{-52} = 2.220446 \times 10^{-16} = 2\mathbf{u}$$

$\mathbf{u}$ and ε_m are very close; they are sometimes used interchangeably.

Computing Machine Constants

A standard set of routines for computing machine information is provided by

> Cody, W. J. (1988) MACHAR: A subroutine to dynamically determine machine parameters. Transactions on Mathematical Software, 14, 4, 303-311.

Simple code for computing machine epsilon is in

```
http://www.stat.uiowa.edu/~luke/classes/STAT7400/
                examples/macheps
```

The R code looks like

```
eps <- 2
neweps <- eps / 2
while (1 + neweps != 1) {
    eps <- neweps
    neweps <- neweps / 2.0
}
eps
```

and produces

```
> eps
[1] 2.220446e-16
> .Machine$double.eps
[1] 2.220446e-16
> eps == .Machine$double.eps
[1] TRUE
```

Analogous C code compiled with

```
cc -Wall -pedantic -o eps eps.c
```

produces

```
luke@itasca2 macheps% ./eps
epsilon = 2.22045e-16
```

The *same* C code compiled with optimization (and an older gcc compiler) on a i386 system

```
cc -Wall -pedantic -o epsO2 eps.c -O2
```

produces

```
luke@itasca2 macheps% ./epsO2
epsilon = 1.0842e-19
```

Why does this happen?

Here is a hint:

```
> log2(.Machine$double.eps)
[1] -52
> log2(1.0842e-19)
[1] -63
```

Some Notes

- Use equality tests `x == y` for floating point numbers with caution
- Multiplies can overflow—use logs (log likelihoods)
- Cases where care is needed:
  - survival likelihoods
  - mixture likelihoods.
- Double precision helps a lot

Floating Point Equality

- R FAQ 7.31: Why doesn't R think these numbers are equal?

  ```
  > b <- 1 - 0.8
  > b
  [1] 0.2
  > b == 0.2
  [1] FALSE
  > b - 0.2
  [1] -5.551115e-17
  ```

- Answer from FAQ:

  > The only numbers that can be represented exactly in R's numeric type are integers and fractions whose denominator is a power of 2. Other numbers have to be rounded to (typically) 53 binary digits accuracy. As a result, two floating point numbers will not reliably be equal unless they have been computed by the same algorithm, and not always even then. For example
  >
  > ```
  >    > a <- sqrt(2)
  >    > a * a == 2
  >    [1] FALSE
  >    > a * a - 2
  >    [1] 4.440892e-16
  > ```
  >
  > The function `all.equal()` compares two objects using a numeric tolerance of `.Machine$double.eps ^ 0.5`. If you want much greater accuracy than this you will need to consider error propagation carefully.

- The function `all.equal()` returns either `TRUE` or a string describing the failure. To use it in code you would use something like

  ```
  if (identical(all.equal(x, y), TRUE)) ...
  else ...
  ```

  but using an explicit tolerance test is probably clearer.

- Bottom line: be **VERY CAREFUL** about using equality comparisons with floating point numbers.