Introduction
Computer Arithmetics

732A90
Computational Statistics

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Computational Statistics — In brief

- Even simple data analysis (mean, variance) by hand is tedious
- Today: huge datasets, models capturing system complexity, interactions (between variables **and** observations)
- We will discuss:
  - Being careful with calculations—overflow
  - Generation of random variables including correlated ones
  - Numerically optimizing functions, esp. maximum likelihood
  - Computing confidence (credible) intervals for distributions when analytical ones are unobtainable

Lesson structure

- Lectures
- Computer Labs
- Seminars
- Examination: Reports, seminars, final exam
- Final exam: computer based
- Answer in English.
- Electronic reports as **.PDF**.
- Disclose **ALL** collaborations and sources.
- Provide source code (if used).
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Course materials, software

- Lecture slides
- 2016 lecture slides (732A38)
- Handouts, R code
- Various suggested www pages or articles
- **Googling**
- James E. Gentle "Computational Statistics", Springer, 2009
- Geof H. Givens, Jennifer A. Hoeting "Computational Statistics", Wiley, 2013

- R

Course contents

- Recap: R
- Recap: Basic Statistics
- Computer Arithmetics (JG pages 85–105)
- Optimization (JG pages 241–272, handouts)
- Random Number Generation (JG pages 305–312, 325–328, handouts)
- Monte Carlo Methods (JG pages 312–318, 328 417–429, handouts)
- Numerical Model Selection and Hypothesis Testing (JG pages 52–56, 424, 435–467, handouts)
- Expectation Maximization Algorithm and Stochastic Optimization (JG pages 275–284, 296–298, 480–483, handout)

Pages are recommended reading for each lecture, **NOT** exact lecture content. The lectures will build up on this material.

Examination

Computer labs (need to be passed)

Presentation or opposition and attendance at seminars (see 732A90_ComputationalStatisticsVT2019_CourseInformation.pdf).

Computer exam points
A: $[18, \infty)$, B: $[16, 18)$, C: $[14, 16)$, D: $[12, 14)$, E: $[10, 12)$, F: $[0, 10)$

Allowed aids for exam: printed books and own PDF document containing max 100 pages (see 732A90_ComputationalStatisticsVT2019_CourseInformation.pdf).

SHOULD YOU CARE?

For a detailed mathematical treatment see Ch. 4.2 in
D. E. Knuth (1998). The Art of Computer Programming, Volume 2, Addison–Wesley.

Computer Arithmetics: Examples

Computations can be affected by magnitudes of numbers.

```
x<-0.5^10000;y<-0.4^10000;x/(x+y)+y/(x+y)
x<-0.5^1000;y<-0.4^1000;x/(x+y)+y/(x+y)
x<-0.1^1000;y<-0.2^1000;x/(x+y)+y/(x+y)
```

```
t<-rnorm(5,10^18,1);t[3]-t[4];t[1]-t[2]
```

```
x<-10^800;sd<-10^400;y<-x/sd;y
```

And your are doing estimation under a nice, fancy model ...

Data presentation

- Computers store information in binary form
  0 1 0 1 1 0 0 1
- 1Byte=8bits (typical counting unit)
- 1Word=32 or 64bits (depending on architecture)
- 1KB=1024bytes
- 1MB=1024KB
- and so on

QUESTION: Why binary form?

Character encoding

- ASCII (American Standard Code for Information Interchange)
  - 1 byte per character, 7 bits coding, 1 parity check or 0
  - $2^7 = 128$ characters can be encoded
  - "Usual" English letters, Arabic numerals, punctuation, i.e. "standard" keyboard
  - 1–31 control characters, 0: NULL **WHY?**
  - Design influenced by contemporary (1960) hardware
  - Extended ASCII: all 8 bits, 256 characters

- Unicode
  - 8, 16 or 32 bits encoding
  - "of more than 128,000 characters covering 135 modern and historic scripts, as well as multiple symbol sets" (Wikipedia)

- `read.csv()`, `read.table()` have `fileEncoding` argument

Fixed–point system (integers)

- We use the base–10 (decimal) system, e.g.
  $1234 = 1 \cdot 10^3 + 2 \cdot 10^2 + 3 \cdot 10^1 + 4 \cdot 10^0$
- We could use base–m system for any m
- Computers: base–2 (binary) system
- Each integer represented as:
  $A = a_0 \cdot 2^0 + a_1 \cdot 2^1 + a_2 \cdot 2^2 + \dots$

EXERCISE: 5, 16, 17, 31, 32, 33, 255, 256 in binary
QUESTION: What is the range of a byte, word, double word?

- Negative numbers
  - **Leading bit:** first bit 0 if positive, 1 if negative
  - **Twos–complement:** sign bit 1, remaining bits to **opposite** value and then +1
    e.g. $5 = 00000101$, $-5 = 11111011$
    QUESTIONS $5 + (-5) =?$, try 12 and -12
  - Range: $[-2^{k-1}, 2^{k-1} - 1]$ on k bits **WHY?**

Arithmetic operations

R operations on binary

- Addition, multiplication: base–2 instead of base–10
- Subtraction: $A - B = A + (-B)$ (*twos–complement*)
- Division: tedious, rounded towards 0 `as.integer(17/3)`

- **Overflow:** adding two large numbers the sign bit can be treated as a high order bit and on some architectures results in a negative number

Floating–point system (rational, “real”)

- How can we represent fractions (rational numbers)?

- Sign
- Exponent (**signed**, read standards if interested)
- Mantissa or Significand
- on 64bits:

sign (1bit)	Exponent (11bits)	Mantissa (52 bits)

$$\pm 0.d_1 d_2 \ldots d_p \cdot b^e \qquad b = 2, \quad p = 52$$

- **Range:** $\approx [-10^{300}, 10^{300}] \approx [-b^{e_{max}}, b^{e_{max}}]$

Floating–point system

- Rationals rounded towards the nearest computer float

```
options(digits=22) #max possible
0.1
[1] 0.1000000000000000055511
```

- **EXAMPLE:** Assume base $b = 10$ and mantissa has 5 digits $p = 5$:
  $1.2345 = +0.12345 \cdot 10^1$
  $4.0000567 = +0.40000 \cdot 10^1$
- Problem remains whatever base (b) is chosen

- **EXERCISE:** Try to convert some numbers

Floating–point system

- Distribution of computer floats

- Dense from -1 to 1
- Density decreases
- same number of points for each exponent:

$$\ldots,\quad \cdot 10^{-3},\quad \cdot 10^{-2},\quad \cdot 10^{-1},\quad \cdot 10^{1},\quad \cdot 10^{2},\quad \cdot 10^{3},\quad \ldots$$

- What about integers?
  $5 = +0.50000 \cdot 10^1$

```
options(digits=22)
9007199254740992
9007199254740993
9007199254740994
```

Floating–point system, special “numbers”

- We do not discuss how the exponent is actually coded.
- Usually the maximum allowed number in the exponent is one unit less than possible.
- ±Inf: exponent is $\exp_{\max} + 1$, mantissa is 0
- NaN: exponent is $\exp_{\max} + 1$, mantissa is $\neq 0$
- 0 **WHY?**

Overflow: number larger than can be represented
Underflow: loss of significant digits

```
10^200*10^200  =  Inf
10^400/10^400  =  NaN
10^-200/10^200 =  0
10^-200*10^200 =
0*10^400 =
x<-10^300; while(1){x<-x+1}
```

Arithmetic operations

- Floats are rounded so usual mathematical laws do not hold — floating point arithmetic
- **Examples**

```
1/3+1/3 =  0.6666667
options(digits=22)
1/3+1/3 =  0.6666666666666666296592
10^(-200)/(10^(-200)+10^(-200)) =  0.5
10^(-200)/(10^(-200)+20^(-200)) = 1
```

- Software is designed to make operations as correct as possible
- **Do we need to work with such extreme numbers?**

Arithmetic operations

- $X + Y$, $X \cdot Y$ can display overflow, underflow
- $A \neq B$ but $X + A = B + X$
- $A + X = X$ but $A + Y \neq Y$
- $A + X = X$ but $X - X \neq A$
- **COMPARING FLOATS IS TRICKY!**

```
options(digits=22)
x<-sqrt(2)
x*x
[1] 2.000000000000000444089
(x*x)==2
[1] FALSE
isTRUE(all.equal(x*x,2))
[1] TRUE
```

Summation

Underflow problems can occur with any summation (`x<-x+1`)

```
options(digits=22)
x<-1:1000000; sum(1/x); sum(1/rev(x))
[1] 14.39272672286572252176
[1] 14.39272672286572429812
```

- **WHICH ONE IS CORRECT?**
- **WHICH ONE IS MORE ACCURATE?**

Potential solutions

Solution A:

1. Sort the numbers ascending **CAN BE EXPENSIVE**
2. Sum in this order

Solution B:

1. Sum numbers pairwise, from n obtain $n/2$ numbers **HOW TO CHOOSE PAIRS?**
2. Continue until 1 number left

More on summing

Example

- Computing exponent using Taylor series

$$e^x = 1 + x + x^2/2 + x^3/6 + \ldots = \sum_{i=0}^{\infty} \frac{x^i}{i!}$$

The exponential

```
options(digits=22)
fTaylor<-function(x,N){1+sum(sapply(1:N,
    function(i,x){x^i/prod(1:i)},x=x,simplify=
    TRUE))}
exp(20) #fine
[1] 485165195.4097902774811
fTaylor(20,100)
[1] 485165195.4097902774811
fTaylor(20,100)-exp(20)
[1] 0
exp(-20) #problem
[1] 2.061153622438557869942e-09
fTaylor(-20,100)
[1] -3.853877217352419393137e-10
fTaylor(-20,200)
[1] -3.853877217352419393137e-10
```

More on summing

Example

- Computing exponent using Taylor series

$$e^x = 1 + x + x^2/2 + x^3/6 + \ldots = \sum_{i=0}^{\infty} \frac{x^i}{i!}$$

- **WHY?**

- Varying sign of terms
- **CANCELLATION** adding two numbers of almost equal magnitude but of opposite sign
- Effects of cancellations accumulate
- **SOLUTION:** Different algorithm . . .

Can you explain why?

```
## Example due to Thomas Ericsson in his
   Numerical Analysis course at Chalmers
f1<-function(x){(x-1)^6}
f2<-function(x){1-6*x+15*x^2-20*x^3+15*x^4-6*x
   ^5+x^6}

x<-seq(from=0.995,to=1.005,by=0.0001)
y1<-f1(x);y2<-f2(x)

plot(x,y1,pch=19,cex=0.5,ylim=c(-5*10^(-15),20
   *10^(-15)),main="Two ways to calculate (x
   -1)^6",xlab="x",ylab="y")
points(x,y2,pch=18,cex=0.8)
```

Matrix Calculations

- Many problems (in Statistics, Numerical methods, e.t.c) can be reduced to solving

$$\mathbf{A}\vec{x} = \vec{b}$$

  A (design) matrix
  $\vec{x}$ vector of unknowns
  $\vec{b}$ vector of scalars (data)

- Algorithm should be **numerically stable**

  (small changes in **A** or $\vec{b}$ imply in small changes in $\vec{x}$)

Example: Linear regression models

Minimize

$$RSS(\beta_0, \beta_1, \ldots, \beta_m) = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{i1} - \ldots - \beta_m x_{im})^2$$

The system of equations

$$\frac{\partial RSS}{\beta_0} = \frac{\partial RSS}{\beta_1} = \ldots \frac{\partial RSS}{\beta_m} = 0$$

can be written as

$$\mathbf{X}^T \mathbf{X} \vec{\beta} = \mathbf{X} \vec{y}$$

where

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & \ldots & x_{1m} \\ 1 & x_{21} & \ldots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \ldots & x_{nm} \end{bmatrix}$$

Solving a linear system

- $\mathbf{A}\vec{x} = \vec{b}$ needs a stable numerical solution
- **Computer arithmetics**
-
  - Original system: $\mathbf{A}\vec{x} = \vec{b}$
  - Perturbed system: $\mathbf{A}\vec{x'} = \vec{b'}$, $\vec{x'} = \vec{x} + \delta\vec{x}$, $\vec{b'} = \vec{b} + \delta\vec{b}$
- Stable: small perturbation in $\vec{b}$, small perturbations in $\vec{x}$
- $\|\vec{b}\| = \|\mathbf{A}\vec{x}\| \leq \|\mathbf{A}\|\|\vec{x}\|$ implies $\|\vec{x}\|^{-1} \leq \|\mathbf{A}\|\|\vec{b}\|^{-1}$
  $\|\delta\vec{x}\| = \|\mathbf{A}^{-1}(\delta\vec{b})\| \leq \|\mathbf{A}^{-1}\|\|\delta\vec{b}\|$
  together

$$\frac{\|\delta\vec{x}\|}{\|\vec{x}\|} \leq \|\mathbf{A}^{-1}\|\|\mathbf{A}\|\frac{\|\delta\vec{b}\|}{\|\vec{b}\|}$$

Solving a linear system

Condition number of a matrix

$$\kappa(\mathbf{A}) = \|\mathbf{A}^{-1}\| \|\mathbf{A}\|$$

- Large $\kappa(\mathbf{A})$ is a bad sign, but does not imply ill–conditioning
- L_2 norm: $\kappa(\mathbf{A})$ is the ratio of the maximum and minimum eigenvalues of $\mathbf{A}$
- Under L_2 norm

$$\kappa(\mathbf{A}^T\mathbf{A}) \geq \kappa(\mathbf{A})^2 \geq \kappa(\mathbf{A})$$

(regression setting)

Solving a linear system

Dealing with ill–conditioning

- Rescale the variables (columns)
- Use a different algorithm for solving
  e.g. QR, Cholesky, SVD

Cholesky: $\mathbf{A}$ symmetric–positive–definite
$\mathbf{A}\vec{x} = \vec{b}$ is equivalent to $\mathbf{L}\mathbf{L}^T\vec{x} = \vec{b}$ **WHY?**

1. Solve $\mathbf{L}\vec{y} = \vec{b}$
2. Solve $\mathbf{L}^T\vec{x} = \vec{y}$

Summary

- Computations can behave “differently” at different numerical ranges.
- Floating point system.
- Computer arithmetics is not the same as “usual” arithmetic.
- Summing series, solving linear systems (inversion?)