Introduction

TMA4300: Computer Intensive Statistical Methods
(Spring 2019)

Sara Martino

[1]

[1] Slides are based on lecture notes kindly provided by Håkon Tjelmeland and Andrea Riebler.

General information

Lectures:

- Lectures: Sara Martino, room 1140
  `sara.martino@math.ntnu.no`
- Tuesday 10.12-12 ,
  Thursday 12.15-14:

Computer exercises:

- Exercises:Jorge Sicacha Parada, room 1144,
  `jorge.sicacha@ntnu.no`
- Tuesday 10.12-12 ,
  Thursday 12.15-14:
- Extra hour: Friday 10.15-12

See course webpage regularly for time plan!

Access to computer lab Nullrommet 380A

For those who do not have access to Nullrommet 380A: please send me (`sara.martino@math.ntnu.no`) as soon as possible your name, student number, NTNU username/e-mail address and study programme.

TMA4300: Course webpage

`https://wiki.math.ntnu.no/tma4300/2019v/start`

Please check this website regularly!

- Messages
- Course information
- Curriculum
- Lecture plan
- Exercise classes
- Statistical software
- Reference group
- Exam

Quality ensurance: Reference group

Three members preferably from different study programmes, such as Industrial Mathematics, Erasmus Programme, others.

Duties:

- Stay in dialogue with all students.
- Participate in three meetings distributed over the semester.
- Give feedback to lecturer and teaching assistant about lectures and exercises, and provide suggestions for improvement.
- Write a joint final report providing constructive feedback and evaluation of the course. This report will be published unedited in course evaluation.

A certificate will prove participation in the reference group.

Volunteers?

Course outline

Reference book:

- Givens, G.H., Hoeting, J.A., 2013, *Computational Statistics*, 2nd edition, John Wiley & Sons.

  The book is freely available as e-book within the NTNU network from the library.

- Gamerman, D. Lopes, H.F. 2006. *Markov chain Monte Carlo - Stochastic Simulation for Bayesian Inference*, 2nd edition

- Extra references might be used.

Course Structure

The course is divided in three topic blocks:

Part 1: Algorithms for stochastic simulation

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Part 3: Expectation-maximisation algorithms, bootstrap.

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- The exercises account for 30% of the final mark. The final exam counts for 70%. You must pass the final exam to pass the course (exercises + final exam).

Exercises

Each lecture block is followed by an exercise block

- The exercises MUST be done in groups of two persons.

Register your group until **18 January** by sending an email to (`jorge.sicacha@math.ntnu.no`). If you need help to find a team partner please send also an email to Jorge.

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- The exercises have to be done using the statistical package `R`.
- The exercises account for 30% of the final mark.
- In an oral presentation each group will once present their finding on a selected part of the exercises.

Exam

- The exam will be on 5th June 2019
- Examination aids: C (to be decided on)
- The exam counts for 70% of the final mark and must be passed in order to pass the course.

TMA4300: Learning outcome, Knowledge

- The student knows computational intensive methods for doing statistical inference.
- This includes direct and iterative Monte Carlo simulations, as well as the expectation-maximisation algorithm and the bootstrap.
- The student has basic knowledge in how hierarchical Bayesian models can be used to formulate and solve complex statistical problems.
- Finally, the student understands a number of classification techniques.

TMA4300: Learning outcome, Skills

- The student can apply computational methods, such as Monte Carlo simulations, the expectation-maximisation algorithm and the bootstrap, on simple applied problems.
- General competence. The student is able to give an oral presentation where he or she communicate his or her findings in a project.

Statistical software R

R is available for free download at The Comprehensive R Archive Network (Windows, Linux and Mac).

- Rstudio `http://www.rstudio.org` is an integrated development environment (system where you have your script, your run-window, overview of objects and a plotting window).
- A nice introduction to R is the book P. Dalgaard: Introductory statistics with R, 2nd edition, Springer which is also available freely to NTNU students as an ebook.

Intro to R

The word simulation . . .

. . . refers to the treatment of a real problem through reproduction in an environment controlled by the experimenter.

Gamerman & Lopes, Markov Chain Monte Carlo, 2nd Edition, Page 9

Motivation: Queueing problem

M/G/1 - queue:

- Customers arrive to a queueing system according to a Poisson process, i.e. interarrival times are exponentially distributed.
- One server
- Independent service times distributed according to $f(t)$.
- Queue system empty at time $t = 0$

$X(t)$ customers in queueing system at time t.

Motivation: Queueing problem (II)

What are we interested in:

- limiting distribution of $X(t)$, ie

$$\lim_{t \to \infty} P\{X(t) = i\}, i = 0, 1, \ldots$$

- Other quantities, for example

$$T = \min\{t > 0; X(t) > 7\}$$

Motivation: Queueing problem (III)

If service times are exponentially distributed, $X(t)$ is a Markov process and an explicit analytical formula for the limiting distribution is available.
For general f, analytical solutions might not be available.
$\Rightarrow$ Idea: Simulate the queueing process on a computer and return the quality of interest, e.g. $\min\{t > 0 : X(t) \geq 7\}$.

Show code `Queue.R`

Simulation, why do we need it?

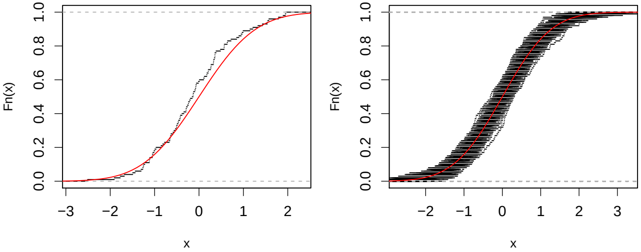
Necessity to produce chance on the computer:

- Evaluation of the behaviour of a complex system (Epidemics, weather forecast, networks, economic actions, etc)

Simulation, why do we need it?

Necessity to produce chance on the computer:

- Evaluation of the behaviour of a complex system (Epidemics, weather forecast, networks, economic actions, etc)
- Determine probabilistic properties of a novel statistical procedure or under an unknown distribution.



(Left: Estimation of CDF from a normal sample of 100 points,

Right: Variation of the estimation over 200 samples.)

Simulation, why do we need it?

- Approximation of an integral/area

$n = 1000$ ▷ (# of simulations)

$m = 0$ ▷ (# points in circle)

$i = 1$

while $i < n$ **do**

  $x = Rand(1), y = Rand(1)$

  if $x^2 + y^2 < 1$ **then**

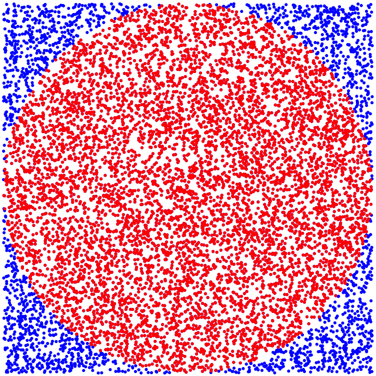
    $m \leftarrow m + 1$

  end if

  $i = i + 1$

end while

return $4 \cdot m/n$



$\hat{\pi} = 3.1353.$

Pseudo-random generator

Central building block of simulation: Always requires availability of uniform $\mathcal{U}(0,1)$ random variables.

```
[1] 0.6925103 0.2345950 0.7856542 0.3596010 0.2180535 0.2461511 0.7186286
[8] 0.7482534 0.6525447 0.5339895
```

Pseudo-random generator

A pseudo-random generator is a deterministic function f which takes a uniform random bit string as input and outputs a bit string which cannot be distinguished from a uniform random string.

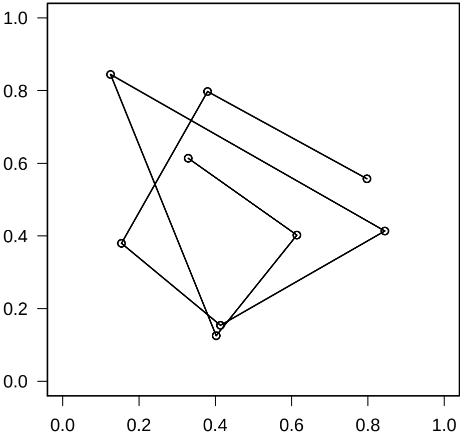
In more detail, this means that for starting value u_0 and any n, the sequence

$$\{u_0, f(u_0), f(f(u_0)), f(f(f(u_0))), \ldots, f^n(u_0)\}$$

behaves statistically like an $\mathcal{U}(0,1)$ sequence (when appropriately scaled).

Pseudo-random generator

Illustration of first 10 (u_t, u_{t+1}) steps



A standard uniform generator

The congruential random generator on $\{0, 1, \ldots, M-1\}$

$$f(x) = (a \cdot x + b) \mod M$$

has a period equal to M for proper choices (a, b) and becomes a generator on $[0, 1)$ when dividing by M.

Example

Take

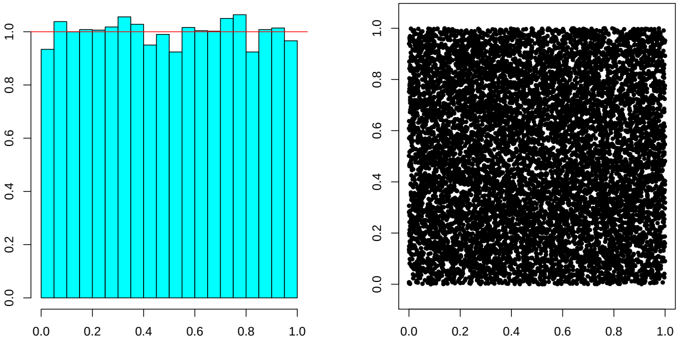
$$f(x) = (69069069 \cdot x + 12345) \mod (2^{32})$$

and produce

$\ldots, 69081414, 2406887111, 1109307232, 2802677792, 3651430880, 806776992, \ldots$

i.e.

$\ldots, 0.01608427, 0.56039708, 0.25828072, 0.65254927, 0.85016500, 0.18784241, \ldots$



Random number generator

From now on, we assume to have a random generator on the unit interval available.

Show code

Discrete and continuous random variables

Discrete

- Takes values in $\mathcal{N}$
- Probability mass func. $f(x)$

$$f(x) = \text{Prob}(X = x)$$

- Cum. distribution func. $F(x)$

$$F(x) = \sum_{u \leq x} f(u) = \text{Prob}(X \leq x)$$

Continuous

- Takes values in $\mathcal{R}$
- Probability density func. $f(x)$

$$\text{Prob}(a < X < b) = \int_a^b f(u)du$$

- Cum. distribution func. $F(x)$

$$\begin{aligned} F(x) &= \text{Prob}(X \leq x) \\ &= \int_{-\infty}^{x} f(u)du \end{aligned}$$

Normalising constant

A normalising constant c is a multiplicative term in $f(x)$, which does not depend on x. The remaining term is called core:

$$f(x) = c \underbrace{g(x)}_{\text{core}}$$

We often write $f(x) \propto g(x)$.

Examples of continuous distributions

- Uniform distribution $f(x) \propto 1$
- Exponential distribution $f(x) \propto e^{-\lambda x}$
- Normal distribution $f(x) \propto \exp\{-\frac{1}{\sigma^2}(x - \mu)^2\}$.
- ...

Generating from standard parametric families

We would like to find strategies to generate random variates from familiar distributions based on uniform random variates.

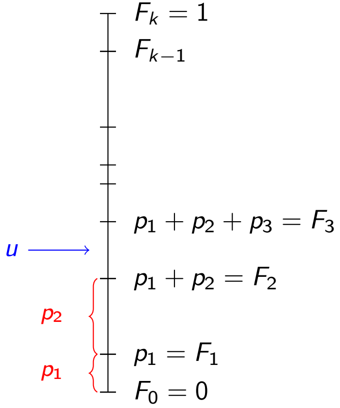
Discrete distributions

Let X be a stochastic variable with possible values $\{x_1, \ldots, x_k\}$ and $\mathrm{P}(X = x_i) = \mathrm{p}_i$. Of course $\sum_{i=1}^{k} p_i = 1$.

An algorithm for simulating a value for x is then:

$u \sim U[0, 1]$
for $i = 1, 2, \ldots, k$ **do**
  if $u \in (F_{i-1}, F_i]$ **then**
    $x \leftarrow x_i$
  end if
end for

Each interval $I_i = (F_{i-1}, F_i]$ corresponds to single value of x.



Proof & Note

Proof.

See Blackboard $\square$

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See Blackboard $\square$

Note: We may have $k = \infty$

- The algorithm is not necessarily very efficient. If k is large, many comparisons are needed.
- This generic algorithm works for any discrete distribution. For specific distributions there exist alternative algorithms.

Bernoulli distribution

Let $S = \{0, 1\}$, $\mathrm{P}(X = 0) = 1 - p$, $\mathrm{P}(X = 1) = p$.

Thus $X \sim \mathrm{Bin}(1, p)$.

The algorithm becomes now:

$u \sim U[0, 1]$

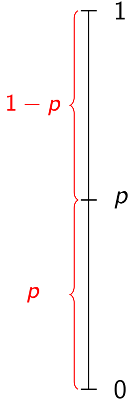
if $u \leq p$ **then**

$\quad x = 1$

else

$\quad x = 0$

end if



Binomial distribution

Let $X \sim \text{Bin}(n, p)$.

The generic algorithm from before can be used, but involves tedious calculations which may involve overflow difficulties if n is large.

An alternative is:

$x = 0$
for $i = 1, 2, \ldots, n$ **do**
  generate $u \sim U[0, 1]$
  if $u \leq p$ **then**
    $x \leftarrow x + 1$
  end if
end for
return x

Geometric and negative binomial distribution

The negative binomial distribution gives the probability of needing x trials to get r successes, where the probability for a success is given by p. We write $X \sim \mathrm{NB}(r, p)$.

The generic algorithm can still be used, but an alternative is:

$s = 0$ ▷ (# of successes)
$x = 0$ ▷ (# of tries)
while $s < r$ **do**
  $u \sim U[0, 1]$
  $x \leftarrow x + 1$
  if $u \leq p$ **then**
    $s \leftarrow s + 1$
  end if
end while
return x

Poisson distribution

Let $X \sim \text{Po}(\lambda)$, i.e. $f(x) = \frac{\lambda^x}{x!} e^{-\lambda}$, $x = 0, 1, 2, \ldots$.

An alternative to the generic algorithm is:

$x = 0$ ▷ (# of events)

$t = 0$ ▷ (time)

while $t < 1$ **do**

  $\Delta t \sim \text{Exp}(\lambda)$

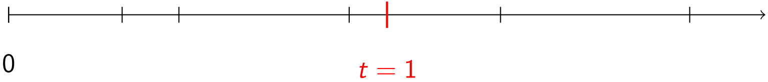
  $t \leftarrow t + \Delta t$

  $x \leftarrow x + 1$

end while

$x \leftarrow x - 1$

return x



It remains to decide how to generate $\Delta t \sim \text{Exp}(\lambda)$.

Sampling from continuous distribution functions

The inversion method (or probability integral transform approach) can be used to generate samples from an arbitrary continuous distribution with density $f(x)$ and CDF $F(x)$:

1. Generate random variable U from the standard uniform distribution in the interval $[0, 1]$.
2. Then is

   $$X = F^{-1}(U)$$

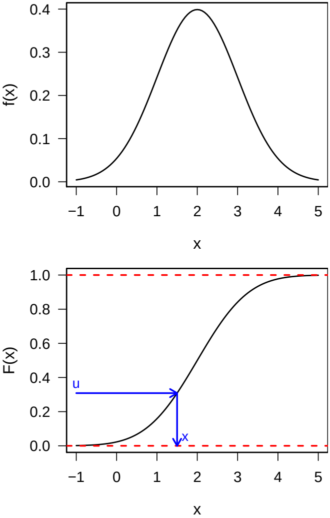
   a random variable from the target distribution.

Proof.

See blackboard □

Inverse cumulative distribution function (II)

Let X have density $f(x)$, $x \in \mathbb{R}$ and CDF $F(x) = \int_{-\infty}^{x} f(z)dz$:



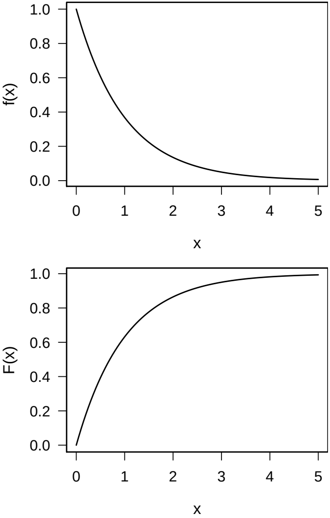
Simulation algorithm:

$u \sim U[0,1]$

$x = F^{-1}(u)$

return x

Example - Exponential Distribution



$$f(x) = \lambda \exp(-\lambda x) : \; x > 0$$

$$F(x) = 1 - \exp(-\lambda x)$$

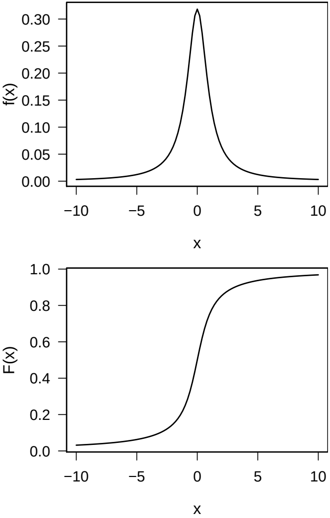
Simulation algorithm:

$u \sim U[0,1]$

$x = -\frac{1}{\lambda} \log(u)$

return x

Example - Standard Cauchy distribution



$$f(x) = \frac{1}{\pi} \cdot \frac{1}{1+x^2}$$
$$F(x) = \frac{1}{2} + \frac{\arctan(x)}{\pi}$$
$$F^{-1}(y) = \tan\left[\pi\left(y - \frac{1}{2}\right)\right]$$

Simulation algorithm:

$u \sim U[0,1]$

$x = \tan[\pi(U_i - \frac{1}{2})]$

return x

Inversion Sampling

Can we always use this algorithm??

- We have to be able to find $F^{-1}(u)$
- Not possible for many important distribution
  - Normal
  - Gamma
  - ...
- Need to know the normalizing constant