Computational Astrophysics I: Introduction and basic concepts

Helge Todt

Astrophysics
Institute of Physics and Astronomy
University of Potsdam

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Random numbers and Monte-Carlo methods

Motivation I

Many physical process can be described in two pictures:

- microscopic, individual, e.g., particle-particle interactions are considered realization usually with help of $\rightarrow$ Monte-Carlo (MC) methods
- macroscopic, only the *effective coaction* is described $\rightarrow$ usually analytical equations

Example: Thermodynamics

microscopic: motion of particles, e.g., $\overline{v^2} = \frac{1}{N}\sum_{i=1}^{N} v_i^2$
effective theory: thermodynamics (via statistical physics) averages particle quantities, e.g., $\frac{1}{2}m\overline{v^2} = \frac{3}{2}k_\mathrm{B}T$, so $\overline{v^2} \rightarrow\ T$

Monte-Carlo simulation

Computer algorithm based on a large number of repeated random experiments to obtain a representative sample of the possible configurations.

Motivation II

Example: Radiative transfer

- microscopic: interaction of photons with atoms/ions/molecules

  → `MOCASSIN` for Monte-Carlo simulation of photon propagation in gaseous nebulae
  → `MCRH` (Noebauer 2015) MC radiation hydrodynamics for stellar winds

  advantage: arbitrary geometries (e.g., torus) and density distributions (inhomogeneities) and processes; good for scattering (special non-LTE case)
  disadvantage: feedback on matter (often iteratively calculated) hard to implement because of MC noise

- macroscopic: radiative transfer equation (RTE) = effective theory, i.e. light (intensity I_ν) instead of single photons

  → `Cloudy` spectral synthesis code for astrophysical plasmas
  → `PoWR` for emergent spectra of stellar atmospheres

  advantage: feedback on matter (non-LTE) via iteration (boundary conditions, e.g., conservation of energy) → non-LTE population numbers
  disadvantage: hard to program (numerical stability); *consistent* only for some geometries, usually 1d, e.g., spherical symmetry

For MC methods we need *good* and *many* random numbers. Usual base are uniformly distributed random numbers (= same probability for every event).
Humans are not a good source for random numbers:

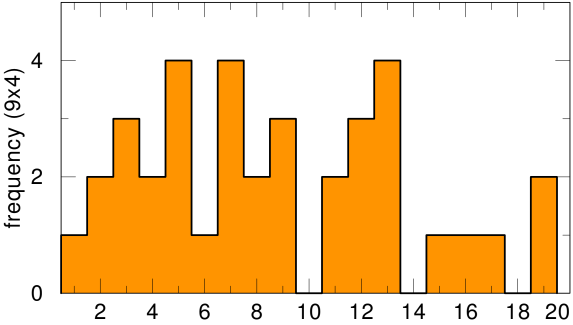


Figure: random numbers, created by colleagues → not uniformly distributed, too few

→ direct, severe consequence: don't make up your own passwords!

Random numbers II

Other sources: rolling dices, tossing coins $\rightarrow$ low rate

most programming languages have a builtin random function, which gives pseudo-random numbers, e.g., in C/C++ integers (!) from `[0,RAND_MAX]`

```
#include <cstdlib>
  ...
 int i = rand () ;
```

- output of next random number of a sequence
- restart by `srand(i) ;`

To get uniformly distributed random numbers $\in [0;1]$:

```
 r = rand()/double(RAND_MAX) ;
```

Random numbers III

Definition

A result (a state) is random if it was not predictable.

Quality tests for random numbers:

- *uniform distribution:* random numbers should be fair
- *sequential tests:* for $n$tuple repetitions (usually only for $n = 2$ und $n = 3$)
- *run tests:* for monotonically increasing/decreasing sequences, and duration of stay in a certain interval
- and more . . .

$\rightarrow$ there is no sufficient criterion for randomness tests

Non-uniform distributions

Non-uniform random numbers I

- random number generators give *uniform* (pseudo) random numbers $\in [0, \texttt{RAND\_MAX}]$ $\rightarrow r \in [0, 1]$ (from now on)
- we often need different distributions, e.g., normal (Gaussian) distributions or uniform distributions on an interval $x \in [a, b]$
- i.e., we need a transformation that maps r to x, so

Inverse transformation

$$x = P^{-1}(r) \tag{1}$$

Non-uniform random numbers II

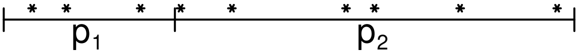
First, for the case of discrete numbers

- e.g., two events (1,2) with probabilities p_1 and p_2, such that

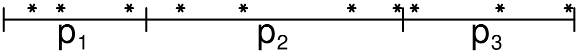
$$p_1 + p_2 = 1 \tag{2}$$

  How can we choose with help of r?

- obvious choice: for $r < p_1$ event 1, otherwise event 2



- for the case of 3 possible events with p_1, p_2, p_3: $r < p_1 \rightarrow$ event 1, $p_1 < r < p_1 + p_2 \rightarrow$ event 2, else event 3



- in general for n events, event i is selected if for r:

$$\sum_{j=0}^{i-1} p_j \leq r \leq \sum_{j=0}^{i} p_j \quad \text{where } p_0 \equiv 0 \tag{3}$$

Non-uniform random numbers III

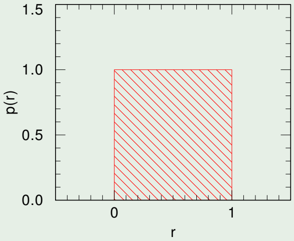
For continuous distributions:

- need the *probability density function* $p(x)$, where $p(x) \cdot dx$ is probability that x is in the interval $[x, x + dx]$
- moreover, $p(x)$ is normalized:

$$\int_{-\infty}^{+\infty} dx\, p(x) = 1 \tag{4}$$

Example: uniform distribution

$$p_\mathrm{u}(r) = \begin{cases} 1, & \text{if } 0 \leq r \leq 1 \\ 0, & \text{else} \end{cases} \tag{5}$$



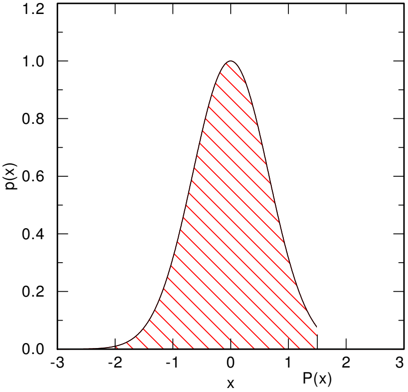
Non-uniform random numbers IV

- for the continuous case (continuum limit $i \to x$) in the Eqn. (3)

$$\sum_{j=0}^{i-1} p_j \leq r \leq \sum_{j=0}^{i} p_j \quad \text{where } p_0 \equiv 0$$

both sums are equal and become the integral:

$$P(x) = \int_{-\infty}^{x} p(x')\,dx' = r \qquad (6)$$



Non-uniform random numbers V

This corresponds to the cumulated distribution function

$$P(x) = \int_{-\infty}^{x} p(x')\,dx' \tag{7}$$

i.e. the probability to get a random number smaller or equal x. Geometrically: fraction of the area left of (smaller than) x. We state:

$$\begin{aligned} P(x) &= r \quad (8) \\ \Rightarrow x &= P^{-1}(r) \quad (9) \end{aligned}$$

i.e. exactly as r also $P(x)$ is uniformly distributed.
Therefore, the probability to find $P(x)$ in the interval $[P(x), P(x) + dP(x)]$ is $dP(x) = dr$ (Eq. 8).

Non-uniform random numbers VI

The relation between $dP(x)$ and dx is obtained by derivating Eq. (7) $\rightarrow$ Fundamental theorem of calculus:

$$\frac{dP(x)}{dx} = p(x) \tag{10}$$

for $0 \leq r \leq 1$ it is also:

$$dP(x) = p(x)\,dx = p_{\mathrm{u}}(r)\,dr \tag{11}$$

I.e., because of Eq. (8) $P(x) = r \rightarrow x$ is distributed according to $p(x)$

Non-uniform random numbers VII

To obtain such $p(x)$ distributed random numbers, one has to solve Eq. (9) $x = P^{-1}(r)$

Inverse transformation

1. Insert the required distribution $p(x)$ into:

$$r = P(x) = \int_{-\infty}^{x} p(x')\, dx' \tag{12}$$

2. solve for x, i.e. find

$$P^{-1}(r) = x \tag{13}$$

Not for all $p(x)$ are the corresponding conditions fulfilled (solvable integral and invertibility)

Example for inverse transformation

Let

$$p(x) = \begin{cases} a\, e^{-ax}, & \text{if } 0 \leq x \leq \infty \\ 0, & x < 0 \end{cases} \tag{14}$$

$$P(x) = \int_0^x a\, e^{-ax'} dx' = 1 - e^{-ax} = r \tag{15}$$

$$\Rightarrow x = -a^{-1} \ln(1-r) \tag{16}$$

and $(1-r)$ is exactly distributed as r, so:

$$x = P^{-1}(r) = -a^{-1} \ln r \tag{17}$$

The evaluation of ln on a computer is relatively time consuming
→ inverse transformation not always the best method

Probability distributions are fundamental in, e.g., statistical mechanics and non-relativistic quantum mechanics:

- Boltzmann distribution: $p_i \propto \exp\left(-\frac{E_i}{k_\mathrm{B} T}\right)$ for some state i

  usually: discrete states (statistical mechanics), hence

$$p_i = \frac{N_i}{N} = \frac{\exp\left(-\frac{E_i}{k_\mathrm{B} T}\right)}{\sum_{j=1}^{m} \exp\left(-\frac{E_j}{k_\mathrm{B} T}\right)} \tag{18}$$

  for N_i particles in state i and a total number of N particles with m states
  but might be also continuous, e.g., barometric formula for molecule of mass m, height h above ground

$$\rho(h) \propto \exp\left(-\frac{m\,g\,h}{k_\mathrm{B}\,T}\right) \tag{19}$$

  $\rightarrow$ computer generated samples via Markov Chain Monte Carlo (MCMC), in particular
  $\rightarrow$ Metropolis algorithm (see below)

- Maxwell-Boltzmann distribution: continuous distribution of particle velocity in one direction (e.g., radial sightline) with $v_{\mathrm{th}} = \sqrt{\frac{2k_{\mathrm{B}}T}{m}}$

$$p(v_x)\,dv_x = \left(\frac{m}{2\pi k_{\mathrm{B}}T}\right)^{1/2} \exp\left(-\frac{mv_x^2}{2k_{\mathrm{B}}T}\right)\,dv_x = \frac{1}{v_{\mathrm{th}}\sqrt{\pi}} \exp\left(-\frac{v_x^2}{v_{\mathrm{th}}^2}\right) \qquad (20)$$

Application: thermal Doppler broadening of spectral lines where $\Delta\nu_{\mathrm{th}} = \nu_0 \cdot v_{\mathrm{th}}/c$

Mean value $\langle v_x^2 \rangle = 2\int_0^\infty v_x^2\,p(v_x)dv_x = \frac{1}{2}v_{\mathrm{th}}^2 = \frac{k_{\mathrm{B}}T}{m} = v_{\mathrm{s}}^2$ → isothermal sound speed

→ example for a "moment" of a distribution

For 3D, absolute value, speed v: $d^3v = dv_x\,dv_y\,dv_z = v^2\,dv\,d\Omega$ integration → $4\pi v^2 dv$ and $v^2 = v_x^2 + v_y^2 + v_z^2$:

$$p(v)\,dv = 4\pi\left(\frac{m}{2\pi k_{\mathrm{B}}T}\right)^{3/2} v^2 \exp\left(-\frac{mv^2}{2k_{\mathrm{B}}T}\right)\,dv \qquad (21)$$

Hence, mean $\langle v^2 \rangle = \int_0^\infty v^2\,p(v)dv = \frac{3k_{\mathrm{B}}T}{m}$

→ compare definition of T as measure of mean kinetic energy

- in non-relativistic QM (1d):
  the squared modulus of the wave function $|\psi(x,t)|^2$ gives probability of particle in "volume" dx around x at time $t \rightarrow p(x,t)dx = |\psi(x,t)|^2 dx$

  Physical quantities (observables) have corresponding operators, e.g., momentum $p_{\text{op}} \rightarrow -\imath\hbar\partial/\partial x$; expectation or average value of observable A:

$$\langle A \rangle = \int \psi^*(x,t)\, A_{\text{op}}\, \psi(x,t) dx \tag{22}$$

  And ψ evolves according to Schrödinger equation

$$\imath\hbar \frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t) \tag{23}$$

  $\rightarrow$ because of similarity to diffusion equation (with imaginary time), solutions to Eq. (23) can be found by random walk (see below)

- the specific intensity $I_\nu(\vec{x}, t, \vec{n}, \nu) = \frac{dE}{d\vec{A}\cdot\vec{n}\, d\Omega\, d\nu\, dt}$ is a 7-dim distribution function on a 4-dim spacetime manifold $(\vec{x}, t)$, describing unpolarized radiation. Note: $I_\nu = n_\mathrm{phot} c h\nu \geq 0$ (where n_phot is photons / volume / solid angle / frequency interval)

  Moments of the specific intensity (radiation field) = integrals over all directions, in 1d (plane parallel, spherical symmetry) over $\mu = \cos\theta$, n-th moment: $\frac{1}{2}\int_{-1}^{+1} \mu^n\, I_\nu(\mu) d\mu$

n	symbol	integral	type
0.	J_ν	$= \frac{1}{2}\int_{-1}^{+1} I_\nu(\mu) d\mu$	mean intensity, energy density $E_\nu = \frac{4\pi}{c} J_\nu$, $J_\nu \geq 0$
1.	H_ν	$= \frac{1}{2}\int_{-1}^{+1} \mu\, I_\nu(\mu) d\mu$	(Eddington-) flux, can be neg. (e.g. "inward" flux)
2.	K_ν	$= \frac{1}{2}\int_{-1}^{+1} \mu^2\, I_\nu(\mu) d\mu$	radiation pressure $K_\nu = \frac{c}{4\pi} P_\nu$
3.	N_ν	$= \frac{1}{2}\int_{-1}^{+1} \mu^3\, I_\nu(\mu) d\mu$	flux-like, i.e., can be negative

$\rightarrow$ usually: MC simulations of radiation field require large number of runs for individual photons to recover macroscopic quantities I, J, etc. correctly

Non-uniform distributions II

Box-Muller method I

non-uniform distribution:

- with help of the *inversion* method we can get non-uniform random numbers from uniform random numbers $\rightarrow$ condition: $P(x)$ invertable
- for the Gaussian normal distribution:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right) \tag{24}$$

$P(x)$ is not analytical representable (error function)

- idea: 2d-transformation where:

$$p(x,y)\,dx\,dy = \frac{1}{2\pi\sigma^2} e^{-(x^2+y^2)/2\sigma^2}\,dx\,dy \tag{25}$$

- change to polar coordinates:

$$r = \sqrt{x^2+y^2} \quad \theta = \tan^{-1}\frac{y}{x} \tag{26}$$

Box-Muller method II

- let $\rho = r^2/2$ and set $\sigma = 1$:

$$p(x, y)dx\,dy = p(\rho, \theta)\,d\rho\,d\theta = \frac{1}{2\pi}\,e^{-\rho}\,d\rho\,d\theta \tag{27}$$

- now generate random numbers ρ according to exponential distribution, so $\rho = -\ln u$ (u standard uniform distributed) and θ uniform distributed on $[0, 2\pi)$, then

$$x = \sqrt{-2\ln u}\cos\theta \quad \text{und} \quad y = \sqrt{-2\ln u}\sin\theta \tag{28}$$

  are each according to Eq. (24) with $\sigma = 1$ and $\mu = 0$ distributed because of

$$re^{\imath z} = \sqrt{-\ln u}e^{\imath 2\pi\theta} = \sqrt{-2\ln u}\,[\cos(2\pi\theta) + \imath\sin(2\pi\theta)] \tag{29}$$

Alternative: Rejection method (see below)

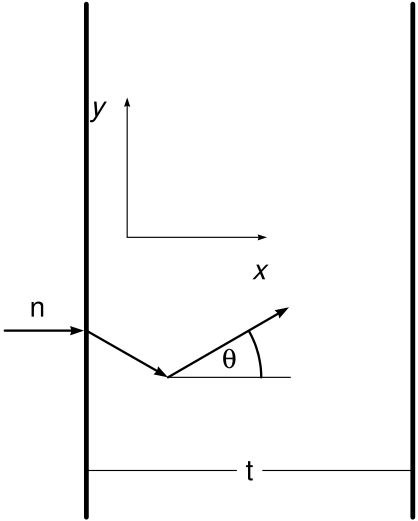
Example: Neutron transport

Neutron transport I

Application for non-uniform random numbers!

Transport of neutrons through matter – one of the first MC applications!

- consider a plate of thickness t
- plate is infinite in z and y direction, x-axis perpendicular to the plate
- at each point within the plate: probability p_c, that neutron gets absorbed (captured) and probability p_s that neutron is scattered
- after each scattering: find scattering angle θ in xy plane
- as motion in y, z direction irrelevant: azimuthal angle ϕ irrelevant



Determine scattering angle & scattering path length

1. Isotropic scattering:

$$p(\theta,\phi)\,d\theta\,d\phi = d\Omega/4\pi \tag{30}$$

$$\text{because of } d\Omega = \sin\theta\,d\theta\,d\phi \; : \tag{31}$$

$$p(\theta,\phi) = \frac{\sin\theta}{4\pi} \tag{32}$$

obtain $p(\theta)$ and $p(\phi)$ by integration over the complementary angle:

$$p(\theta) = \int_0^{2\pi} p(\theta,\phi)\,d\phi = 2\pi\,\frac{\sin\theta}{4\pi} = \frac{1}{2}\sin\theta \tag{33}$$

$$p(\phi) = \int_0^{\pi} p(\theta,\phi)\,d\theta = \frac{1}{4\pi}(-\cos\pi + \cos 0) = \frac{1}{2\pi} \tag{34}$$

I.e. $p(\theta,\phi) = p(\theta)p(\phi) \rightarrow$ independent variables

Neutron transport III

If random variable ϕ is wanted ($p(\phi) \equiv const.$):

$$\phi = 2\pi r \tag{35}$$

To get random θ according to Eq. (33) $\rightarrow$ inversion method:

$$r = P(\theta) = \int_0^\theta \frac{1}{2} \sin x \, dx = -\frac{1}{2}(\cos\theta - \cos 0) \tag{36}$$

$$\cos\theta = 1 - 2r \tag{37}$$

I.e. $\cos\theta$ is uniformly distributed on $[-1;1]$ and ϕ on $[0;2\pi]$. Solving for θ possible, but unnecessary, as only $\cos\theta$ required for x component of the path $\rightarrow$
2. scattering path length:

$$x = \ell \cos\theta \tag{38}$$

where ℓ from $p(\ell) \sim e^{-\ell/\lambda}$ (see example for inversion method):

$$\ell = -\lambda \ln r \tag{39}$$

$\lambda \rightarrow$ mean free path (e.g., $\lambda = (\sigma n)^{-1}$)

Algorithm, start at $x = 0$:

1. determine, if neutron is scattered or captured. If captured: increment number of absorbed neutrons, go to 5 step
2. scattering: “dice” $\cos\theta$ and ℓ, move to x position by $\ell\cos\theta$
3. if $x < 0$: increment number of reflected neutrons, if $x > t$: increment number of transmitted neutrones;
   go to 5
4. repeat step 1 - 3 until final result is achieved for all neutrons
5. repeat step 1 - 4 with more incident neutrons