Monte-Carlo (with randomness)

- direct MC: replace some physics by random process
- MC integration: use to calculate integrals
- "metropolis" MC: Markov chains

(slightly blurry boundaries).

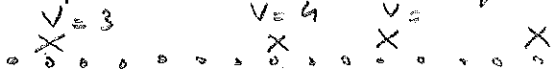
Direct MC: usually ad-hoc-ish

f.e random Lorentz gas
draw random collision parameter for next scatterer

f.e Langevin thermostat: heat bath → random noise + damping

end lecture 7

f.e simple traffic model: Nagel-Schreckenberg



road is 1d grid with cars + vel. some max sat velocity v_{max}

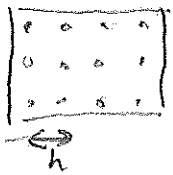
1) cars accelerate by 1: v_i++
2) if distance to car infront $(x_{i+1} - x_i) < v_i$: $v_i = x_{i+1} - x_i - 1$
3) with probability p v_i-- ← driver choice, or silliness of whatever
4) if $v_i < 0$: $v_i = 0$

⇒ widely studied, + additions, explains a lot of qualitative behaviour of traffic jams; real traffic $v_{max} \approx 5$

MC integration

$$\int dx\, f(x)$$

f smooth; hopefully from num. methods course



- usual integration methods based on regular grid
  to improve: points closer together (decrease h)
  (methods described in Thyssen's appendix using interpolation) $O(h^k)$ for some k.
- MC: instead of grid, random points

$\int dx\, f(x) = \text{area} \cdot \langle f(x) \rangle \approx \text{area} \cdot \frac{1}{N} \sum_{i=1}^{N} f(x_i)$

after N points error $= O(\frac{1}{\sqrt{N}})$

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in d dimensions:

grid: $N \propto (\frac{1}{h})^d$ ← high dimensional ⇒ many points

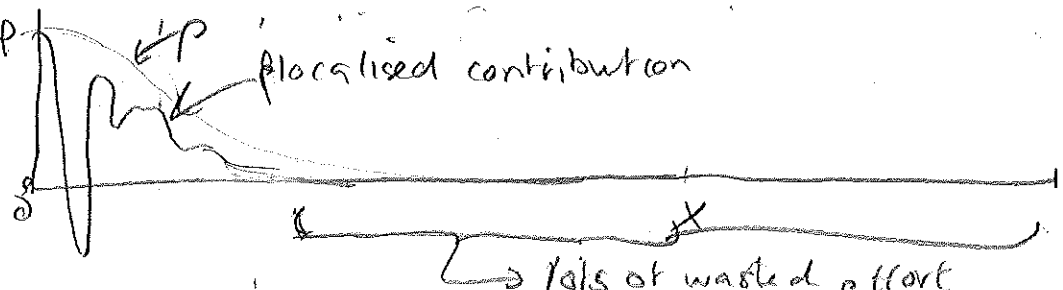
MC

error $O(\frac{1}{N})^{k/d}$ $\quad O((\frac{1}{N})^{1/2})$

⇒ if $k/d < 1/2$ MC is better

high d ⇒ MC more efficient compared to grid

example:



→ lots of wasted effort calculations, but almost no contribution

Suppose we know another function $\rho(x)$, which we can integrate, and which is some what similar and >0 if $f \neq 0$

$$\int dx\, f(x) = \int dx\, \rho(x) \frac{f(x)}{\rho(x)}$$

average this instead of f.

draw ρ-distributed points instead of homogeneous points concentrate where f is large

$$\int = \langle f/\rho \rangle_\rho$$

error in $\langle f \rangle$

$$\text{error}^2 = \left(\langle f^2 \rangle - \langle f \rangle^2\right) \frac{1}{N}$$

$$= \left[\frac{1}{N} \sum_i f(x_i)^2 - \left(\frac{1}{N} \sum_i f(x_i)\right)^2\right] \frac{1}{N}$$

big fluctuations in f

or: error in $\langle f/\rho \rangle_\rho$

$$\text{error}^2 = \left(\left\langle \left(\frac{f}{\rho}\right)^2 \right\rangle_\rho - \left\langle \frac{f}{\rho} \right\rangle_\rho^2 \right) \frac{1}{N}$$

not so big fluctuations in f/ρ

$$= \left[\frac{1}{N} \sum_i \left(\frac{f(x_i)}{\rho(x_i)}\right)^2 - \left(\frac{1}{N} \sum_i \frac{f(x_i)}{\rho(x_i)}\right)^2\right] \frac{1}{N}$$

Key is to pick good ρ

- analytically manageable
- easy to draw from

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drawing gaussian random variables

draw X_1, X_2 between 0, 1

$\phi = 2\pi X_1$

$R = [-\log(X_2)]^{1/2}$ R gets $\propto \exp(-x^2)$ type dist

$Y_1 = R \cos\phi$

$Y_2 = R \sin\phi$

$$p_R(R)\,dR = p_X(X_1)\,dX_1 \cdot \frac{dX}{dR}\,dR = \left[\frac{1}{(-\log(X_2))^{1/2}} \frac{1}{2} \frac{1}{X_2}\right]^{-1}$$

$$\propto R \exp(-R^2)$$

More MC

calculating some average:

$$\langle A \rangle = \frac{\sum_{\text{states}\,\alpha} A(\alpha) \exp(-\beta E(\alpha))}{\sum_{\alpha} \exp(-\beta E(\alpha)) = Z}$$

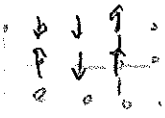
$$\int_{\text{phase space}} d\gamma\, A(\gamma) \exp(-\beta E(\gamma)) \Big/ \int d\gamma \exp(-\beta E(\gamma))$$

example: Ising model $\quad \mathcal{H} = -J \sum_{nn} s_i s_j - h \sum_i s_i$

(Hopefully Supriya has discussed this system just in 2d)

coupling in x direction ↑ field

every spin is just up or down
=> should be simple enough!



in 3d, 5x5x5 grid (not big)

$N = 125$ # states $2^{125} \approx 10^{37}$

calc Z or something

O(1 GHz) computer $= 10^9$ calcs/second.

$\Rightarrow O(10^{28}\,s) \approx O(10^{20})$ years, $\gg$ lifetime of universe.

considering all states is hopeless

MC says just some random subset instead a_i

$$\langle A \rangle = \frac{\frac{1}{B}\sum_{i=1}^{B} A(\alpha_i) \exp(-\beta E(\alpha_i))}{\frac{1}{B}\sum_{i=1}^{B} \exp(-\beta E(\alpha_i))} \quad \begin{matrix} \nearrow \langle A \exp(-\beta E) \rangle_{\text{set}} \\ \searrow \langle \exp(-\beta E) \rangle_{\text{set}} \end{matrix}$$

Now consider low T ... spins tend to align

↑ ↑ ↑ ↑ ↓ ↓ ↓ ↓ ↓

most random states do not look like this.

to get sensible convergence, we need these states to be sampled

O(1) out of 10^{37} .... B must be very large

same trick as with MC integration: importance sampling

solution: bias the random states $\quad p(\alpha)$: density

$$\langle A \rangle_{\exp(-\beta E)} = \frac{1}{B}\sum_{i=1}^{B} \xi(\alpha_i) \quad \text{with } \xi(\alpha) = \frac{A(\alpha)}{p(\alpha)} \exp(-\beta E)$$

same story about errors: $\left(\langle \xi^2 \rangle_p - \langle \xi \rangle_p^2\right)$

smaller than $\langle A^2 \rangle_1 - \langle A \rangle_1^2$

good choice would be $p(\alpha) \propto \exp(-\beta E(\alpha))$

IMPORTANCE SAMPLING

Markov-chain MC

all about obtaining samplings of $\exp(-\beta E)$

Markov chain { set of n states $\alpha_1 \dots \alpha_n$; transfer probs between states P_{ij}

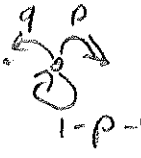
- no memory (depends only on previous state)
- used to model lots of processes; examples
  - N
  - simplistic attempt at modeling weather

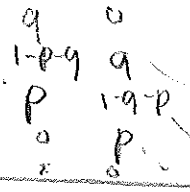
    precipitation / no precipitation (in a day)

	yes	no
yes	1-p	q
no	p	1-q

  - random walk on a line (large # states)

    state # wher walker is





  - NS model

end lecture 8

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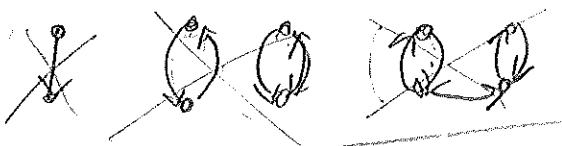
idea of metropolis type algorithms is to construct a Markov chain that moves the system to likely configurations (with the correct eq. dist)

- end up in the correct equilibrium
- accessibility: must be possible to reach all states (detailed)
- balance: there has to be an equilibrium in the Markov chain.

- accessibility:



on lecture 8

- balance or steady state

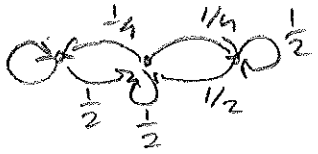
equilibrium: state α_i; population a_i

$P_{ij} a_j = a_i$ eigenvalue equation for $(a_1, \dots a_n)$ (eigenvalue 1)

example ①

$P = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} \\ \frac{2}{3} & \frac{2}{3} \end{pmatrix} \Rightarrow a_i = \frac{1}{3}(1,2)$

example ②



$\Rightarrow a = \left(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right)$