$$I = \int_0^1 dx \underbrace{\left(x^{-\frac{1}{3}} + \frac{x}{10} \right)}_{f(x)} = \langle f \rangle = \frac{31}{20} = 1.55$$

$$\langle f^2 \rangle = \frac{937}{300} \approx 3.1233$$

$$\delta_{N_{meas}} = \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N_{meas}}} \approx \frac{0.849}{\sqrt{N_{meas}}}$$

Actual MC-integration:

N_{meas}	I	$\delta_{N_{meas}}$
100	1.4878	0.0751
10 000	1.5484	0.0080

↑ from simulations

Consider now $p(x) \equiv \frac{2}{3} x^{-\frac{1}{3}}$

Then $d\tilde{x} = \frac{2}{3} x^{-\frac{1}{3}} dx = d\left(x^{\frac{2}{3}}\right)$; $\tilde{x} = x^{\frac{2}{3}}$

$$g \equiv \frac{f(x)}{p(x)} = \frac{x^{-\frac{1}{3}} + \frac{x}{10}}{\frac{2}{3} x^{-\frac{1}{3}}} = \frac{3}{2} + \frac{3}{20} \tilde{x}^2$$

$$\langle g \rangle = \frac{31}{20} = 1.55$$

$$\langle g^2 \rangle = \frac{4809}{2000} \approx 2.4045$$

$$\delta_{N_{meas}} = \sqrt{\frac{\langle g^2 \rangle - \langle g \rangle^2}{N_{meas}}} \approx \frac{0.0447}{\sqrt{N_{meas}}}$$

$\Rightarrow$ error is $\frac{1}{19}$ of first attempt!

Actual MC-integration:

N_{meas}	I	$\delta_{N_{meas}}$
100	1.5792	0.0043
10 000	1.5503	0.0004

↑ from simulation

Exercise: Carry out the MC-integrations and check that you get the same results within errorbars!

Update algorithms

In our case the integral is of the form

$$\langle O \rangle = \frac{\left\{ \prod_{\vec{x}} \int ds(\vec{x}) \right\} O(\{s(\vec{y})\})\, e^{-S(\{s(\vec{z})\})}}{\left\{ \prod_{\vec{x}} \int ds(\vec{x}) \right\} e^{-S(\{s(\vec{z})\})}}$$

Thus, the integrand is exponentially localised. It will be extremely important to use importance sampling.

At the same time, the integration variable $\{s(\vec{x})\}$ is an $N_1 \cdot N_2 \cdots N_d$-dimensional vector, on which the action S depends in a non-trivial way. A change of integration variables can hardly be carried out analytically.

It is possible to implement importance sampling numerically, however, by employing various update algorithms. To find an effective one (i.e, one giving a small error with given computing resources) is an art as much as a science. But there are some basic principles to be satisfied.

Notation:

- $\left\{ \prod_{\vec{x}} \int ds(\vec{x}) \right\} \equiv \int \mathcal{D}s$
- $p(s) \equiv \dfrac{e^{-S(\{s(\vec{z})\})}}{\int \mathcal{D}s\, e^{-S(\{s(\vec{z})\})}}$

$$\Rightarrow \quad \langle O \rangle = \int \mathcal{D}s\, p(s)\, O(s)$$
$$\langle O^2 \rangle = \int \mathcal{D}s\, p(s)\, O^2(s)$$

Monte Carlo integration: $\quad \langle O \rangle \approx \dfrac{1}{N_{meas}} \sum_i O(s_i)$,

if $\quad \dfrac{\sum_i \delta(s - s_i)}{\sum_i} = \dfrac{\sum_i \delta(s - s_i)}{N_{meas}} = p(s)$,

or s_i are selected with probability $p(s_i)$.

How to generate configurations with probability $p(S_i)$?

The general principle is due to Metropolis et al, 1953.

- Generate a Markov chain of configurations,

  $$S_1 \to S_2 \to S_3 \to \cdots S_{N_{mcs}}.$$

- Let $W(S \to S')$ be the transition probability, i.e., probability distribution of S', given S.

- Transition probability must satisfy :

  (a) "ergodicity" : Starting from any configuration, all others can be reached.

  (b) "equilibration" : $p(S')$ is a fixed point of $W(S \to S')$, i.e.,

  $$\int \mathcal{D}S \; p(S) \, W(S \to S') = p(S').$$

Usually (b) is replaced with the stronger requirement of "detailed balance" :

$$p(S) \, W(S \to S') = p(S') \, W(S' \to S)$$

Since $\int \mathcal{D}S \; W(S' \to S) = 1$ (Something always happens !), (b) follows.

- These requirements are enough to guarantee that :

> Irrespective of initial S, the distribution of S_i in an infinite Markov chain is according to $p(S_i)$!

Proof: Introduce a norm $\| p' - p \| = \int \mathcal{D}S \; |p'(S) - p(S)|$, ...

(Usually some configurations are omitted from the beginning, to allow for "thermalisation".)

Thus such a Markov chain provides a method of Monte Carlo integration.

Common choices for $W(s \to s')$:

- "Metropolis"

$$W(s \to s') = C \times \begin{cases} \exp\left[S(s) - S(s')\right], & \text{if } S(s') > S(s) \\ 1, & \text{otherwise.} \end{cases}$$

≡ if new s' reduces S, accept always, otherwise with Boltzmann weight.

Does this satisfy detailed balance?

$$\frac{W(s \to s')}{W(s' \to s)} = \begin{cases} \exp\left[S(s) - S(s')\right], & \text{if } S(s') > S(s) \\ \dfrac{1}{\exp\left[S(s') - S(s)\right]}, & \text{if } S(s) > S(s') \end{cases} = \frac{\exp(-S(s'))}{\exp(-S(s))} \quad \checkmark$$

- "Heat bath"

$$W(s \to s') = C \cdot \exp\left[-S(s')\right] \quad \Rightarrow \text{detailed balance } \checkmark$$

$\Rightarrow$ independent of s!

- "Overrelaxation"

Some deterministic operation, e.g. a reflection

$$s \to s' = F(s)$$

such that $S(s') = S(s)$.

This is not ergodic, however, because S never changes. Often combine e.g.

5× overrelaxation + 1× heat bath.

- Glauber, cluster, ...

The best method depends on the problem and can often only be found with experimenting, or experience.

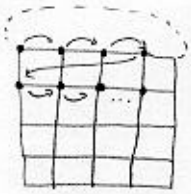
Example: updating the 2d Ising model (with zero external field, $\bar{h} = 0$).

p. 3: $S_{\bar{x}} \to \sigma_{\bar{x}} = \pm 1$

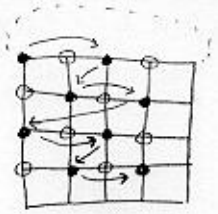
$$S = -\beta \sum_{\langle ij \rangle} \sigma_i \sigma_j = -\beta \sum_{\bar{x}} \sum_{i=1}^{d} \sigma_{\bar{x}} \sigma_{\bar{x}+\hat{\imath}} \quad ; \quad \beta_c = \frac{\ln(1+\sqrt{2})}{2}$$

- Assume periodic boundary conditions.
- Choose an order for going through the lattice.

"Typewriter":



"Checkerboard":

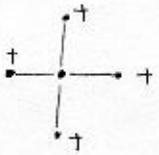


— and then white points.

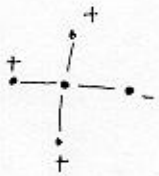
- Let us inspect a specific point $\bar{z}$. How does S depend on $\sigma_{\bar{z}}$?

$$S = \ldots - \beta \sigma_{\bar{z}} \left(\sigma_{\bar{z}+\hat{1}} + \sigma_{\bar{z}+\hat{2}} + \sigma_{\bar{z}-\hat{1}} + \sigma_{\bar{z}-\hat{2}} \right) \equiv \ldots + S_{\bar{z}}(\sigma_{\bar{z}})$$

- Possible configurations:



$$\Rightarrow \quad S_{\bar{z}}(+1) = -4\beta$$
$$S_{\bar{z}}(-1) = +4\beta$$



$$\Rightarrow \quad S_{\bar{z}}(+1) = -2\beta$$
$$S_{\bar{z}}(-1) = +2\beta$$

etc.

- Metropolis: Generate new $\sigma'_{\bar{z}}$. Compute $\delta S_{\bar{z}} = S_{\bar{z}}(\sigma'_{\bar{z}}) - S_{\bar{z}}(\sigma_{\bar{z}})$.
  If $\delta S_{\bar{z}} < 0$, accept new $\sigma'_{\bar{z}}$.
  If $\delta S_{\bar{z}} > 0$, generate random number $r \in (0,1)$.
  If $r < \exp(-\delta S_{\bar{z}})$, accept new $\sigma'_{\bar{z}}$.
  Otherwise keep old $\sigma_{\bar{z}}$, and move to next point.

- Heat bath: Compute $p(\sigma'_{\bar{z}}) = \dfrac{e^{-S_{\bar{z}}(\sigma'_{\bar{z}})}}{e^{-S_{\bar{z}}(+1)} + e^{-S_{\bar{z}}(-1)}}$ for $\sigma'_{\bar{z}} = \pm 1$.
  Generate random $r \in (0,1)$. If $r < p(+1)$, put $\sigma'_{\bar{z}} \equiv +1$, otherwise $\sigma'_{\bar{z}} \equiv -1$.
  Move to next lattice point.

- A single sweep: Go through all lattice points.