Monte Carlo methods

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1. Examples: Ising model etc.
2. Integration vs Sampling
3. Pseudo random number generators
4. Generation of random numbers with a given given distribution
5. Percolation, Random Walks
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10. **Potts model, Ising model, XY model, nonlinear $O(n)$ model**

We have an action with continous variables $S[q_i]$
Introduce Langevin time (similar to MC time)
q_i have an evolution as a function of τ using the **Langevin equation**, stochastic differential equation.

$$dq_i = -\frac{\partial S}{\partial q_i} d\tau + \sqrt{2} dw_i(\tau) \tag{1}$$

dw_i is an increment of a Wiener process: random walk in the continuum

$$\langle w_i(\tau) \rangle = 0, \quad \langle (w_i(\tau') - w_i(\tau))^2 \rangle = (\tau' - \tau) \tag{2}$$

Discretised with Ito calculus:

$$q_i(t + \Delta\tau) = q_i(\tau) + \left(-\frac{\partial S}{\partial q_i} \right) \Delta\tau + \eta_{i,\tau} \sqrt{2\Delta\tau} \tag{3}$$

with $\langle \eta_{i,\tau} \rangle = 0, \quad \langle \eta_{i,\tau} \eta_{j,\tau'} \rangle = \delta_{ij} \delta_{\tau,\tau'}$, Gaussian

$P(q_i, \tau)$ probability density of the variables
If we have

$$P(q_i, \tau) \rightarrow_{\tau \rightarrow \infty} e^{-S(q_i)} \tag{4}$$

than we can use this for simulating the thermal averages.

$$\int e^{-S(q)} F(q) d^n q = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T F(q(\tau)) d\tau \tag{5}$$

Averages collected along the trajectories.
$P(q_i, \tau) \rightarrow_{\tau \rightarrow \infty} e^{-S(q_i)}$ can be shown using the **Fokker-Planck eq.**

$$\frac{\partial P(q_i, \tau)}{\partial \tau} = \sum_i \frac{\partial}{\partial q_i} \left(\frac{\partial}{\partial q_i} + \frac{\partial S}{\partial q_i} \right) P(q_i, \tau) \tag{6}$$

(Stationarity of $e^{-S(q_i)}$ is easy to show, whether P converges to there is a bit harder to show)

We need $\partial_\tau P(q_i, \tau)$.

$$P(q_i', \tau + \Delta\tau) = \left\langle \int dq_i P(q_i, \tau) \prod_i \delta\left(q_i' - q_i + \delta\tau \frac{\partial S}{\partial q_i} - \eta_i \sqrt{2\Delta\tau}\right) \right\rangle_\eta \tag{7}$$

for a constant c we have $\int \delta(cx)dx = \int \delta(cx)d(cx)/c = 1/c$ This implies $\delta(cx) = (1/|c|)\delta(x)$ From that we have the rule:

$$\delta(f(x)) = \sum_{f(x_i)=0} \frac{\delta(x - x_i)}{|f'(x_i)|} \tag{8}$$

Now we can evaluate the formula above:

$$P(q_i', \tau + \Delta\tau) = \left\langle P(q_i' + \Delta\tau \frac{\partial S}{\partial q_i} - \eta_i \sqrt{2\Delta\tau}, \tau) \frac{1}{\prod_i \left| -1 + \Delta\tau \frac{\partial^2 S}{\partial q_i^2} \right|} \right\rangle_\eta \tag{9}$$

We have

$$\frac{1}{\prod_i \left| -1 + \Delta\tau \frac{\partial^2 S}{\partial q_i^2} \right|} = \frac{1}{\prod_i \left(1 - \Delta\tau \frac{\partial^2 S}{\partial q_i^2}\right)} \approx 1 + \sum_i \Delta\tau \frac{\partial^2 S}{\partial q_i^2} \tag{10}$$

Now we taylor expand

$$P(q_i', \tau + \Delta\tau) = \left\langle P(q_i' + \Delta\tau \frac{\partial S}{\partial q_i} - \eta_i \sqrt{2\Delta\tau}, \tau) \frac{1}{\prod_i \left| -1 + \Delta\tau \frac{\partial^2 S}{\partial q_i^2} \right|} \right\rangle_\eta \tag{11}$$

to order $\Delta\tau$ we have:

$$\begin{aligned} P(q_i', \tau + \Delta\tau) \quad = \quad & \left\langle P(q_i', \tau) + \sum_i \partial_i P(q_i', \tau) \Delta\tau \partial_i S - \sum_i \partial_i P(q_i', \tau) \eta_i \sqrt{2\Delta\tau} \right. \\ & \left. + \frac{1}{2} \sum_{i,j} \partial_i \partial_j P(q_i', \tau) \eta_i \eta_j 2\Delta\tau + \sum_i P(q_i', \tau) \Delta\tau \partial_i^2 S \right\rangle_\eta \end{aligned}$$

Now using $\langle \eta_i \rangle = 0, \quad \langle \eta_i \eta_j \rangle = \delta_{ij}$

$$P(\tau + \Delta\tau) = P + \Delta\tau \left(\sum_i \partial_i P \partial_i S + \sum_i \partial_i^2 P + \sum_i P \partial_i^2 S \right) \tag{12}$$

Which finally gives the Fokker-Planck equation:

$$\frac{\partial P(q_i, \tau)}{\partial \tau} = \sum_i \frac{\partial}{\partial q_i} \left(\frac{\partial}{\partial q_i} + \frac{\partial S}{\partial q_i} \right) P(q_i, \tau) \tag{13}$$

Here we show that using the Fokker-Planck eq. $\partial_\tau P = \sum_i \partial_i(\partial_i + \partial_i S)P$ $\implies$ P converges to e^{-S}.
Let's define $\Psi(q_i, \tau)$ such that

$$P(q_i, \tau) = \Psi(q_i, \tau)e^{-S(q_i)/2} \tag{14}$$

Writing this ansatz into Fokker Planck:

$$\begin{aligned}\dot{\Psi}e^{-S/2} &= \partial_i(\Psi' - \frac{1}{2}S'\Psi + S'\Psi)e^{-S/2} = \partial_i(\Psi' + \frac{1}{2}S'\Psi)e^{-S/2} = \\ &= \left(\Psi'' + \frac{1}{2}S''\Psi + \underbrace{\frac{1}{2}S'\Psi' - \frac{1}{2}S'\Psi'}_{=0} - \frac{1}{4}(S')^2\Psi\right)e^{-S/2}\end{aligned}$$

Now we note

$$\begin{aligned}-(-\partial_i + S'/2)(\partial_i + S'/2)\Psi &= -(-\partial_i + S'/2)(\Psi' + S'\Psi/2) \\ &= -(-\Psi'' - S''\Psi/2 \underbrace{-S'\Psi'/2 + S'\Psi'/2}_{=0} + S'S'\Psi/4)\end{aligned} \tag{15}$$

So we can write

$$\dot{\Psi} = -H_{FP}\Psi, \quad H_{FP} = Q^{+}Q \tag{16}$$

Where we defined the Fokker-Planck Hamiltonian H_{FP}, which we see is semi-positive definite
We have one stationary solution to $Q\Psi = 0$, which is $\Psi = e^{-S/2}$ (It's unique except for some special cases)
We can write

$$\Psi(\tau) = c_0 e^{-S/2} + \sum_i e^{-\lambda_i \tau}\Psi_i \tag{17}$$

with $\lambda_i > 0$ for all i.

$$\implies \Psi \to e^{-S/2}$$

$$P(\tau) = \Psi(\tau)e^{-S/2} \to e^{-S} \tag{18}$$

We are given the action $S(x) = ax^2 + bx^4$
Suppose we are interested in

$$\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} dx x^2 e^{-ax^2 - bx^4}}{\int_{-\infty}^{\infty} dx e^{-ax^2 - bx^4}} \tag{19}$$

Calculate the drift term:

$$K(x) = -\frac{\partial S}{\partial x} = -2ax - 4bx^3 \tag{20}$$

The discretised Langevin equation is thus:

$$x(\tau + \Delta\tau) = x(\tau) + \Delta\tau(-2ax - 4bx^3) + \sqrt{2\Delta\tau}\eta(\tau) \tag{21}$$

We choose some $\Delta\tau$, and an initial $x(\tau = 0)$
We solve the Langevin eq. numerically using an independent Gaussian random number at every timestep.

We thus have $x(\tau)$ for $\tau = n\Delta\tau$.
now we use

$$\lim_{T\to\infty} \frac{1}{T - T_0} \int_{T_0}^{T} f(x(\tau))d\tau = \int dx \Pi(x) f(x) \tag{22}$$

with $\Pi(x) \sim e^{-S(x)}$ the normalized equilibrium distribution. $T_0 > 0$ is used to get rid of the initial thermalization of the process, and thus get rid of the dependence on the initial conditions (similarly to Metropolis simulations).

We thus use

$$\langle f(x)\rangle \to \frac{1}{N} \sum_{\tau>\tau_0} f(x(\tau)) \tag{23}$$

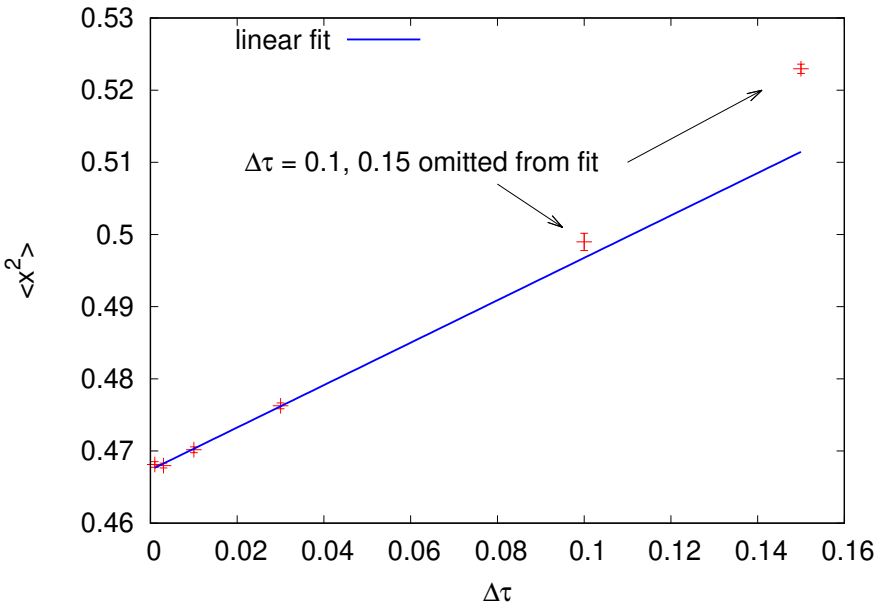
where N is the number of $x(\tau)$ steps we have with $\tau > \tau_0$.

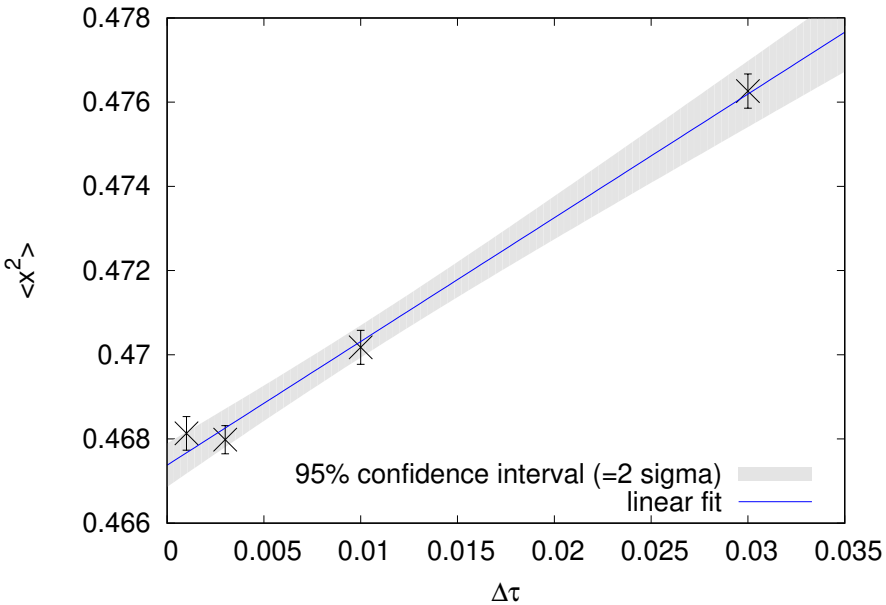
Numerically we use some $\Delta\tau > 0$, we have to carry out the extrapolation to $\Delta\tau = 0$. For the naive discretisation above the average observables are expected to have a linear dependence on $\Delta\tau$. (Higher order discretisations improve this)

$\to$ measure at 3 different $\Delta\tau$ values, fit linear to $\langle f(x)\rangle_{\Delta\tau}$ and extrapolate to $\Delta\tau = 0$ (i.e. read of the intercept)

We need $\langle x^2 \rangle_{\Delta\tau}$ at $\Delta\tau \to 0$

For the naive discretisation, a linear dependence is expected, so we fit:





Large $\Delta\tau$ values are omitted as linear behavior sets in at small $\Delta\tau$.

How do we calculate the confidence interval of the fit?

Let's look at fitting a linear to the data (Linear regression)

We have a dataset: $\{x_i, y_i, \delta_i\}$ where we have data point y_i with 1 σ error δ_i at coordinate x_i (Assuming no errors in x_i). We are looking for a and b such that $a + b * x$ best describes the dataset.
What is the error on a and b, what is their correlation?
Define the best fit by the minimal χ^2:

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - a - bx_i}{\delta_i} \right)^2 \tag{24}$$

Points with smaller errors are important, points with large errors are not.
Minimum:

$$0 = \frac{\partial \chi^2}{\partial a} = -2 \sum_{i=1}^{N} \frac{y_i - a - bx_i}{\delta_i^2} \tag{25}$$

$$0 = \frac{\partial \chi^2}{\partial b} = -2 \sum_{i=1}^{N} \frac{x_i(y_i - a - bx_i)}{\delta_i^2}$$

Using

$$S = \sum \frac{1}{\delta_i^2}, \quad S_x = \sum \frac{x_i}{\delta_i^2}, \quad S_{xx} = \sum \frac{x_i^2}{\delta_i^2}, \quad S_y = \sum \frac{y_i}{\delta_i^2}, \quad S_{xy} = \sum \frac{x_i y_i}{\delta_i^2},$$

and $\Delta = S S_{xx} - S_x^2$, we have:

$$\begin{array}{r} aS + bS_x = S_y, \\ aS_x + bS_{xx} = S_{xy} \end{array} \quad \Longrightarrow \quad \begin{array}{l} a = \frac{S_{xx} S_y - S_x S_{xy}}{\Delta} \\ b = \frac{S S_{xy} - S_x S_y}{\Delta} \end{array} \tag{26}$$

Using error propagation (assuming independent y_i variables):

$$\delta_a^2 = \sum_i \left(\frac{\partial a}{\partial y_i} \right)^2 \delta_i^2, \qquad \delta_b^2 = \sum_i \left(\frac{\partial b}{\partial y_i} \right)^2 \delta_i^2 \tag{27}$$

Covariance:

$$\mathrm{Cov}(a, b) = \langle ab \rangle - \langle a \rangle \langle b \rangle = \sum_i \frac{\partial a}{\partial y_i} \frac{\partial b}{\partial y_i} \delta_i^2 \tag{28}$$

$$\left(\frac{\partial a}{\partial y_i}\right)^2 = \left(\frac{S_{xx}\frac{1}{\delta_i^2} - S_x\frac{x_i}{\delta_i^2}}{\Delta}\right)^2 = \frac{S_{xx}^2 - 2S_{xx}S_x x_i + S_x^2 x_i^2}{\Delta\delta_i^4} \tag{29}$$

$$\delta_a^2 = \sum_i \left(\frac{\partial a}{\partial y_i}\right)^2 \delta_i^2 = \frac{S_{xx}^2 S - 2S_{xx}S_x^2 + S_x^2 S_{xx}}{\Delta^2} = \frac{S_{xx}(S_{xx}S - S_x^2)}{\Delta^2} = \frac{S_{xx}}{\Delta}$$

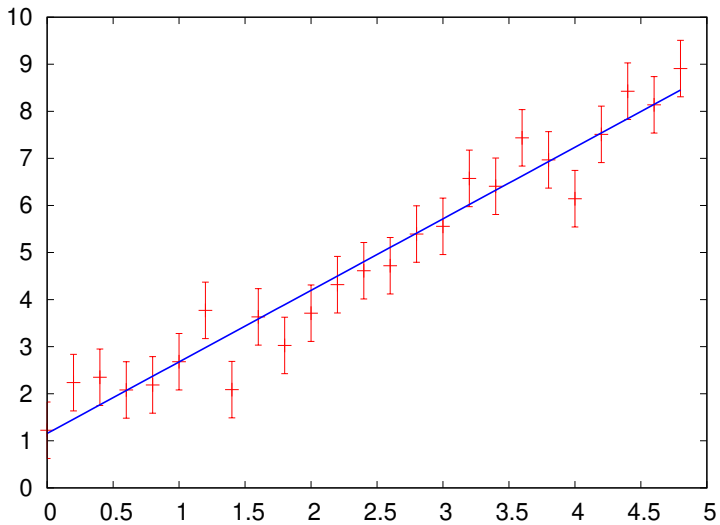
Similarly we can calculate:

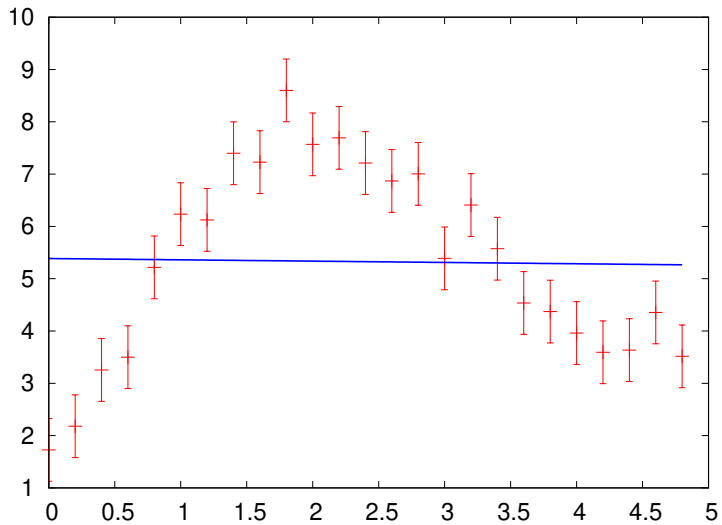
$$\delta_b^2 = \frac{S}{\Delta}, \quad \mathrm{Cov}(a,b) = -\frac{S_x}{\Delta} \tag{30}$$

Now we can get errors for any x:

$$\delta^2(a+bx) = \langle (a+bx)^2 \rangle - \langle a+bx \rangle^2 = \delta_a^2 + \delta_b^2 x^2 + 2x\mathrm{Cov}(a,b) \tag{31}$$

Which fit makes sense?





Besides looking at the plot (which is also important),
How can we decide whether the model (the function we fit) is probably OK or not?

We want to see if the data we get is described with the function $y = f(x)$. We use

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - f(x_i)}{\delta_i} \right)^2 \tag{32}$$

if the model is correct we get y_i from a Gaussian distribution

$$P(y_i) \sim e^{-\frac{y_i - f(x_i)^2}{2\delta_i^2}}, \quad x_i = \frac{y_i - f(x_i)}{\delta_i} \quad \Longrightarrow \quad P(x_i) \sim e^{-x_i^2/2} \tag{33}$$

So χ^2 is a sum of N Gaussian random variables with zero mean and $\sigma = 1$. Probability for haveing $\chi^2 > C^2$

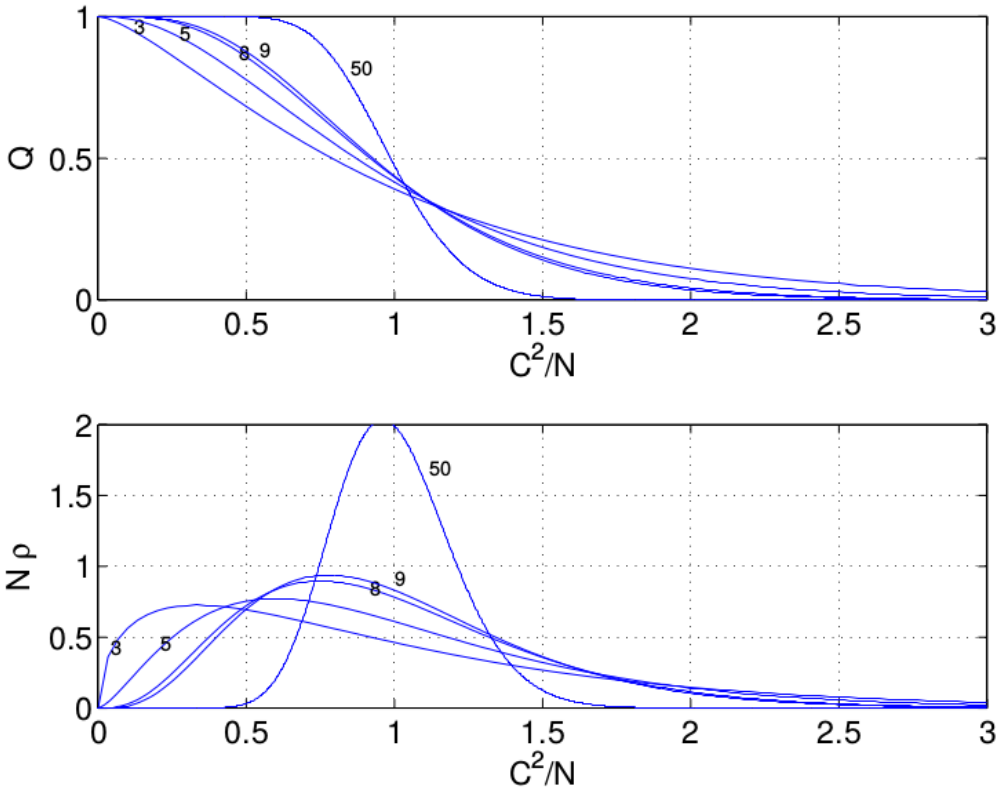
$$Q(C^2) = \frac{1}{(2\pi)^{N/2}} \int \prod dx_i e^{-\sum x_i^2/2} \Theta\left(\left(\sum x_i^2 \right) - C^2 \right) \tag{34}$$

Using polarcoordinates and then $\sum x_i^2/2 = t$, we have

$$1 - Q(C^2) = \frac{|S_{N-1}|}{(2\pi)^{N/2}} \int_0^{C^2/2} t^{N/2-1} e^{-t} = \Gamma_{inc}(C^2/2, N/2) \tag{35}$$

with the incomplete Gamma function.

Probability to find a χ^2/N value at least as large as a given C^2/N



small Q means :

- model is wrong
- errors are underestimated
- errors are not really Gaussian, but have long tail

Smoothed Step function – for large N gets steeper
Standard deviation of χ^2/N is $\sqrt{2/N}$

Usually we have some free parameters that we want to get from the data:

1. N data points x_i, y_i, δ_i
2. fit function: $f(x_i, a_j)$ with ν free parameters
3. $$\chi^2 = \sum_1^N \left(\frac{y_i - f(x_i, a_j)}{\delta_i^2} \right)^2 \tag{36}$$
4. Minimize χ^2 with respect to a_j. (calculate errors for a_j with e.g. Bootstrap, Jackknife, error propagation in simple cases)
5. χ^2 test: calculate χ^2/N_{dof} with $N_{dof} = (N - \nu)$
   if $\chi^2/N_{dof} \gg 1 \implies$: model is probably wrong (or other problems, as above)
   if $\chi^2/N_{dof} \ll 1 \implies$: This is called overfitting. Noise too large to say anything, or errors are overestimated.

Sometimes a linear fit cannot suffice, we want $f(x) = \sum a_k X_k(x)$ for e.g. a polynomial fit

$$\chi^2 = \sum \left(\frac{y_i - \sum a_k X_k(x_i)}{\sigma_i} \right)^2 \tag{37}$$

The minimum condition leads to $\sum \alpha_{kj} a_j = \beta_k$ with

$$\alpha_{kj} = \sum_{i=1}^{N} \frac{X_j(x_i) X_k(x_i)}{\sigma_i^2}, \quad \beta_k = \sum_{i=1}^{N} \frac{y_i X_k(x_i)}{\sigma_i^2}, \tag{38}$$

The errors and covariances are calculated from $C = \alpha^{-1}$

$$\delta^2(a_i) = C_{ii}, \quad \mathrm{Cov}(a_i, a_j) = C_{ij} \tag{39}$$

Typically LU decomposition, QR decomposition or similar is used to calculate the inverse.

Generally we have $f(x_i, a_j)$ nonlinear function.
We might be able to convert to a linear problem

$$y_i = \exp(-\lambda x_i) \quad \rightarrow \ln y_i = -\lambda x_i \tag{40}$$

Or even:

$$y_i = \frac{1}{e^{\beta x_i} + 1} \quad \rightarrow \ln\left(\frac{1}{y_i} - 1\right) = -\lambda x_i \tag{41}$$

Use error propagation to calculate errors.
Finally for the non-linear problems that remain, one uses a non-linear minimum search to get the fit parameters (e.g. gradient descent method)

The q-state Potts model is defined by the energy

$$H[S] = -\alpha \sum_x \sum_\nu \delta(S_x, S_{x+\hat{\nu}}) - h \sum_x \delta(S_n, 1), \tag{42}$$

with the spins $S_x \in \{1, 2, \ldots, q\}$, where x points to a lattice site on a d dimensional lattice and $x + \hat{\nu}$ is a neighbor in $+\nu$ direction.
$q = 2$ Potts model is is eqivalent to the Ising model: $\{1, 2\} \to \{-1, 1\}$, and the $H_{\text{Ising}} = H_{q=2\text{Potts}} + \text{Const}$

The symmetryes of the system play a central role in the type of phase transitions the system can have
At $h = 0$ Potts model is symmetric under permutation:

$$\begin{aligned} 1 &\to p(1) \\ 2 &\to p(2) \\ &\vdots \\ q &\to p(q) \end{aligned} \qquad \text{with } p(i) \text{ a permutation of the numbers } 1, 2, \ldots q$$

p is an element of the permutation group S_q

$$\delta(S_x, S_{x+\hat{\nu}}) = \delta(p(S_x), p(S_{x+\hat{\nu}})) \tag{43}$$

if $h \neq 0$, the symmetry is *explicity broken* by the magnetic field

Other symmetries:
The **Ising model** (for zero magnetic field is invariant under

$$S_i \to S_i, \quad S_i \to -S_i \tag{44}$$

as $S_1 S_2 = (-S_1)(-S_2)$.
Symmetry group: $Z_2 = \{-1, 1\}$, (which is equivalent to S_2)
Magnetic field again gives an explicit breaking

Nonlinear $O(n)$ spin model
Consider n component spin vectors (with real components) which satisfy $|S_i| = 1$
The action is given by:

$$S = -\beta \sum_x \sum_\nu S_x^T S_{x+\hat{\nu}} - h \sum_x S_1 \tag{45}$$

Transform all spins with $S_x \to MS_x$ with some $n \times n$ matrix M.

$$S_x^T S_{x+\hat{\nu}} \to S_x^T M^T M S_{x+\hat{\nu}} \tag{46}$$

This is a symmetry transformation if $M^T M = 1$, i.e. for orthogonal matrices.
The magnetic field term breaks the symmetry again.
XY-model $n = 2$ of the above is sometimes called the XY-model. ($n = 3$ is called Heisenberg model)
Writeing the spins in terms of an angle we have $S = (\cos(\phi), \sin(\phi))$

$$S = -\beta \sum_x \sum_\nu \cos(\phi_x - \phi_{x+\hat{\nu}}) - h \sum_x \cos(\phi_x) \tag{47}$$

The symmetry group is now the group of rotations in 2d, described with one angle.

We want to calculate the properties of these models couples to a heat bath with temperature T.
Partition function using $\beta = 1/(k_B T)$:

$$Z = \sum_{\{S\}} e^{-\beta H[S]}, \quad \langle O \rangle = \frac{1}{Z} \sum_{\{S\}} O(S) e^{-\beta H[S]} \tag{48}$$

Where we have to carry out the sum for all configurations
q-state Potts model has q^V, $V = L^d$ configurations
Continous models: sum $\rightarrow$ integration
We use the notation $J = \alpha\beta$, $M = h\beta$.

Observables:
Free energy: $F = -\frac{1}{\beta} \ln Z$
Internal energy:

$$E = U = \langle H \rangle = \frac{1}{Z} \sum_{\{S\}} H[S] e^{-\beta H[S]} = -\frac{1}{Z} \frac{\partial}{\partial \beta} \sum_{\{S\}} e^{-\beta H[S]} = -\frac{\partial}{\partial \beta} \ln Z = \frac{\partial}{\partial \beta}(\beta F)$$

Magnetization

Assuming the form $H[S] = \alpha A[S] + hM[S]$, with the magnetization $M[S]$ and A giving the rest of the terms.

$$\langle M \rangle = \frac{1}{Z} \sum_{\{S\}} M[S] e^{-\beta H[S]} = -\frac{1}{\beta} \frac{1}{Z} \frac{\partial}{\partial h} \sum_{\{S\}} e^{-\beta H[S]} = -\frac{1}{\beta} \frac{\partial}{\partial h} \ln Z = \frac{1}{\beta} \frac{\partial}{\partial h} (\beta F)$$

Specific heat is defined as $c_V = \partial_T E$. First we convert to β derivative:

$$\beta = \frac{1}{k_B T} \implies d\beta = -\frac{1}{k_B T^2} dT = -k_B \beta^2 dT \tag{49}$$

$$\begin{aligned} \frac{\partial}{\partial \beta} \langle H \rangle &= \frac{\partial}{\partial \beta} \left(\frac{1}{Z} \sum_{\{S\}} H[S] e^{-\beta H[S]} \right) = \\ &= \frac{1}{Z^2} \left(\sum_{\{S\}} H[S] e^{-\beta H[S]} \right)^2 - \frac{1}{Z} \sum_{\{S\}} H[S] H[S] e^{-\beta H[S]} = -\langle H^2 \rangle + \langle H \rangle^2 \end{aligned} \tag{50}$$

This is the energy fluctuation$*(-1)$

$$\frac{1}{k_B \beta^2} c_V = -\frac{\partial}{\partial \beta} \langle H \rangle = \langle H^2 \rangle - \langle H \rangle = -\frac{\partial}{\partial \beta} \left(-\frac{\partial}{\partial \beta} \ln Z \right) = -\frac{\partial^2}{\partial \beta^2} (\beta F) \tag{51}$$

Magnetic Susceptibility Defined as:

$$\chi = \langle (M - \langle M \rangle)^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2 \tag{52}$$

Can also be calculated starting from:

$$\begin{aligned} \frac{\partial}{\partial h}\left(\frac{1}{Z}\sum_{\{S\}} M[S] e^{-\beta H[S]}\right) &= -\frac{-\beta}{Z^2}\left(\sum_{\{S\}} M[S] e^{-\beta H[S]}\right)^2 + \frac{-\beta}{Z}\sum_{\{S\}} M[S]^2 e^{-\beta H[S]} \\ &= -\beta\left(\langle M^2 \rangle - \langle M \rangle^2\right) \end{aligned}$$

So we have

$$\chi = -\frac{1}{\beta}\frac{\partial}{\partial h}\langle M \rangle = \frac{1}{\beta^2}\frac{\partial^2}{\partial h^2}\ln Z = -\frac{1}{\beta^2}\frac{\partial^2}{\partial h^2}(\beta F) \tag{53}$$

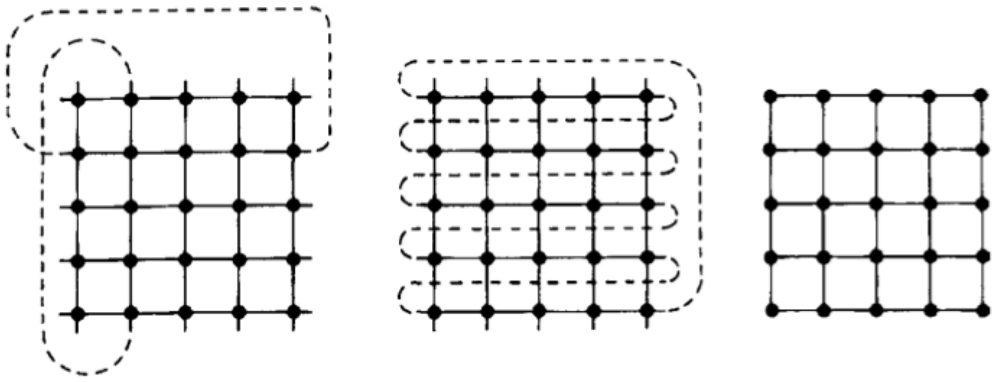
Generally: (one usually divides with the volume Ω for extensive quantities)

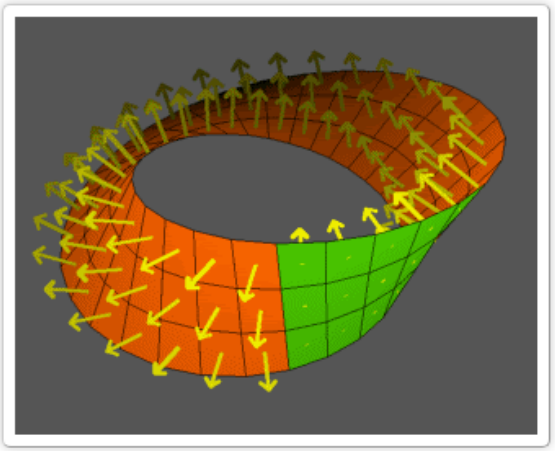
$$Z = \sum e^{-\beta(A[S] + jC[S])} \tag{54}$$

$$\text{average:} \qquad \langle C[S] \rangle / \Omega = -\frac{1}{\Omega\beta}\frac{\partial}{\partial j}\ln Z \tag{55}$$

$$\text{susceptibility:} \qquad \chi_C = \Omega\left(\left\langle (C/\Omega)^2 \right\rangle - \langle C/\Omega \rangle^2\right) = \frac{1}{\Omega\beta^2}\frac{\partial^2}{\partial j^2}\ln Z$$

On the computer we have a finite lattice. What happens at the edges?





- Periodic: makes the lattice a d dimensional torus. no boundary effect, but still finite size effects
- screw-periodic (aka. skew-periodic),free: easy to implement, some systematic effect always there, only gone at infinite volume limit
- antiperiodic: as periodic, but spin across the boundary gets a minus sign. This allows studying the interface between phases (can control the direction of the interface if combined with screw periodic)
- Möbius: Can be used to study topological effects

We calculate averages using Markov chains with local Metropolis update.

- Choose boundary conditions
- Choose initial configuration: Cold start: all spins $S_x = 1$
  Hot Start: Independent random Spins.
- Monte Carlo "hit": a proposed update for one of the spins. One hits all spins either sequentially or chooses a random lattice point for each hit
- "Sweep": All lattice points were hit. (Or do Ω hits)
- (if applicable) With some experimentation try to find proposals which lead to an acceptance rate of $0.5 - 0.8$
- Before measurements one needs typically $O(10^2) - O(10^5)$ sweeps to get rid of the effect of the initial conditions (e.g. compare hot and cold starts)
- Between two measurements one does $10 - 100$ sweeps to decrease autocorrelations on the data
- Analysis of the data: calculate averages, errors, correlations, do fits

We can also calculate averages using the Langevin equation, in case we are looking at a system with continous variables

- Choose boundary conditions
- Choose initial configuration: Cold start: all spins $S_x = 1$
  Hot Start: Independent random Spins.
- Langevin step: One update of the fields with the discretised Langevin eq. with stepsize $\Delta\tau$, increase Langevin time τ to $\tau + \Delta\tau$
- Before measurements one needs typically $O(10) - O(1000)$ Langeevin time for thermalization to get rid of the effect of the initial conditions (e.g. compare hot and cold starts)
- Between two measurements one waits $0.01 - 1$ Langevin time
- Analysis of the data: calculate averages, errors, correlations, do fits
- Carry out $\Delta\tau \to 0$ extrapolation

Representing fields on the lattice, one has to decide on the "layout".
From the coordinates $0 \leq n_i < L_i$ we calculate n the lattice index

$$n_1, n_2, \ldots, n_d \rightarrow n = n_1 + n_2 L_1 + n_3 L_1 L_2 + \ldots \tag{56}$$

which means $0 \leq n < \Omega$ with $\Omega = \prod_i L_i$, with a one to one relation $\{n_i\} \leftrightarrow n$
One can use more complex functions to improve performance on a given computer architecture

We need coordinates for neighbors:

$n_i^{(+\nu)} = n_i(x)$
$n_\nu^{(+\nu)} += 1$
`if` $n_\nu^{(+\nu)} == L_\nu$: $\quad n_\nu^{(+\nu)} = 0$
$n_i^{(+\nu)} \rightarrow n^{(+\nu)}$

We either store $n^{(\pm\nu)}$ in the memory ("neighbor map") or calculate on the fly when needed, depending on which is faster on a given architecture.