I Monte-Carlo-Simulationen des Ising-Modells

I.1 Statistische Eigenschaften von Zeitreihen

Motivation

Experimentelle Messungen und Simulationen liefern i.A. nicht ein exaktes Ergebnis, sondern eine Zeitreihe (d.h. eine geordnete Liste) von Ergebnissen (Skalaren, Vektoren etc.)

Frage/Problem: Wie lassen sich Zeitreihen (hier: Skalare) charakterisieren und interpretieren? Was sagen sie über das exakte Ergebnis aus?

Beispiel 1: Eine Simulations/Messreihe liefert die Zahlen 47.5, 47.7, 47.2, 46.8 – Charakterisierung?

- alle Werte ungefähr 47
- Mittelwert: 47.3
- Varianz der Einzelmessung: $0.153 = 0.39^2$ $\quad \frac{1}{3}(0.2^2+0.4^2+0.1^2+0.5^2)$
- Mittelwert mit Standardabweichung: 47.30 ± 0.20
- Trend/Transient: negativ (spätere Werte eher kleiner)
- Histogramm: nicht sinnvoll (zu wenige Werte)
- Autokorrelation: nicht erfassbar "

Ab hier vorübergehend englischsprachige Notizen, übernommen von der Vorlesung "Computer Simulations in Statistical Physics": http://komet337.physik.uni-mainz.de/Bluemer/lectures_WS2006

Fundamental question: how to get reliable results from simulations?

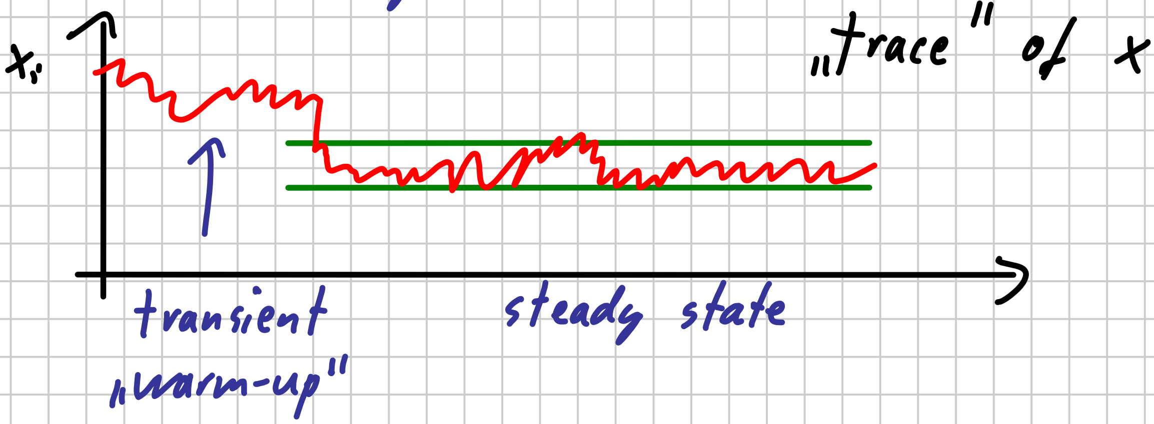
Result: estimate + error bars

- decide whether results are correct or incorrect
- essential for extrapolations (e.g. finite size)

Typical case in computer simulations:

simulations start with non-representative configurations and gradually approach steady state (e.g. thermal equilibrium)

$\rightsquigarrow$ both mean and variance of initial measurements can differ strongly from later ones and should be thrown away



Let us now assume that transient parts have been discarded. How to compute best estimate + error bars?

Mathematical excursion

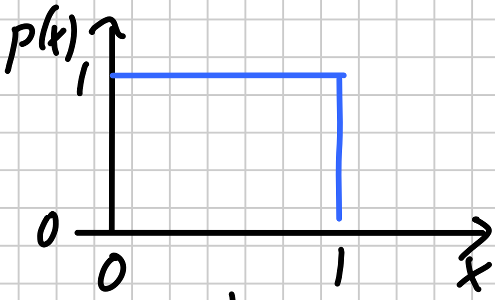
let X be a random variable with probability distribution p:

$$P(x \le X \le x+dx) = p(x)\,dx \qquad (p(x) \equiv p_X(x))$$

$\uparrow$ probability of the statement in brackets to be fulfilled

example: uniform distribution

$$p(x) = \begin{cases} 1 & \text{for } 0 \le x \le 1 \\ 0 & \text{else} \end{cases}$$



probability distribution is normalized: $\int_{-\infty}^{\infty} p(X)\,dX = 1$

mean (1^{st} moment): $\langle X \rangle = \int_{-\infty}^{\infty} X\, p(X)\, dX$ $\quad = \frac{1}{2}$

2^{nd} moment: $\langle X^2 \rangle = \int_{-\infty}^{\infty} X^2\, p(x)\, dx$ $\quad = \frac{1}{3}$

variance: $\sigma_X^2 = \langle (X - \langle X \rangle)^2 \rangle = \langle X^2 \rangle - \langle X \rangle^2$ $\quad = \frac{1}{12}$

$\sigma \equiv$ width of distribution $\quad \left(= \frac{1}{\sqrt{12}} \approx 0.29\right)$

for uniform dist.

The mean is always additive; the variance only for uncorrelated random variables:

$$\begin{aligned}
\langle X + Y \rangle &= \int dX \int dY\, p(X,Y)\, (X+Y) \\
&= \int dX\, X \int dY\, p(X,Y) + \int dY\, Y \int dX\, p(X,Y) \\
&= \langle X \rangle + \langle Y \rangle
\end{aligned}$$

$$\begin{aligned}
\sigma_{X+Y}^2 &= \langle [(X+Y) - \langle X+Y \rangle]^2 \rangle = \langle [(X - \langle X \rangle) + (Y - \langle Y \rangle)]^2 \rangle \\
&= \sigma_X^2 + \sigma_Y^2 + \underbrace{2 \langle (X - \langle X \rangle)(Y - \langle Y \rangle) \rangle}_{=0 \text{ for uncorrelated variables}}
\end{aligned}$$

Specifically for $\sigma_X = \sigma_Y \equiv \sigma$ in uncorrelated case:

$$\sigma\left[\frac{X+Y}{2}\right] = \frac{\sigma}{\sqrt{2}}$$

(and in fully correlated case $X=Y$: $\sigma\left[\frac{X+Y}{2}\right] = \sigma$)

and for arithmetic average of N uncorrelated random numbers with equal variance σ:

$$\sigma_{\bar{X}} = \sigma\left[\frac{1}{N}\sum_{i=1}^{N} X_i\right] = \frac{\sigma}{\sqrt{N}}$$

This is one formulation of the central limit theorem