Numerische Methoden in der Festkörperphysik

Prof. Dr. Nils Blümer

http://komet337.physik.uni-mainz.de/Bluemer/lectures_SS2007
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Vorübergehend englischsprachige Notizen, übernommen von der Vorlesung "Computer Simulations in Statistical Physics": http://komet337.physik.uni-mainz.de/Bluemer/lectures_WS2006

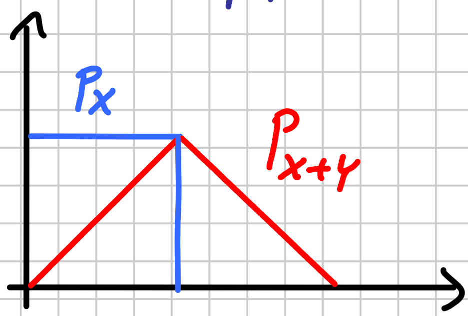
Full probability distribution of sum/average?

$$p_{X+Y}(z) = \int dX\, p_X(X) \int dY\, p_Y(Y)\, \delta(z-(X+Y))$$

$$= \int dX\, p_X(X)\, p_Y(z-X)$$

specifically for uniformly distributed X, Y:

$$p_{X+Y}(z) \begin{cases} z & \text{for } 0 \le z \le 1 \\ 2-z & \text{"} \quad 1 \le z \le 2 \\ 0 & \text{else} \end{cases}$$



Look at higher order cumulants $\rightsquigarrow$ normal distribution

$$\boxed{p_{\bar{X}}(x) \xrightarrow{N\to\infty} \frac{1}{\sigma_{\bar{X}}\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\bar{x}-\langle x\rangle}{\sigma_{\bar{X}}}\right)^2\right]; \quad \sigma_{\bar{X}} = \frac{\sigma}{\sqrt{N}}}$$

central limit theorem (uncorrelated case!)

Now: application to simulation / measurements

again: random variables X_i with same distribution,
non necessarily uncorrelated

Problem: probability distribution, mean, variance unknown. Best unbiased estimates?

easy: $\langle X\rangle \approx \bar{X} = \frac{1}{N}\sum_{i=1}^{N} X_i$

$\bar{X}$ is (best) unbiased estimator for $\langle X\rangle$ since

$$\langle \bar{X}\rangle = \frac{1}{N}\sum_{i=1}^{N} \underbrace{\langle X_i\rangle}_{=\langle X\rangle} = \langle X\rangle$$

(also unbiased: $\tilde{x} = \sum_{i=1}^{N} a_i X_i$ with $\sum_{i=1}^{N} a_i = 1$

also estimator: $\tilde{\tilde{x}} = \frac{1}{N-1}\sum_{i=1}^{N} X_i$ (since $\langle \tilde{\tilde{x}}\rangle = \frac{N}{N-1}\langle x\rangle \xrightarrow{N\to\infty} \langle x\rangle$))

difficult: best estimator for error of $\bar{X}$?

(i) unbiased estimator for σ_x?

$$\left\langle \sum_{i=1}^{N}(X_i-\bar{X})^2\right\rangle = N\langle (X_i-\bar{x})^2\rangle$$

$$= N\left\langle \left(X_i - \frac{1}{N}\sum_{j=1}^{N} X_j\right)^2\right\rangle$$

$$= N\left\langle \left[(X_i-\langle X\rangle) - \frac{1}{N}\sum_{j=1}^{N}(X_j-\langle X\rangle)\right]^2$$

$$= N\left\langle \left[\left(1-\frac{1}{N}\right)(X_i-\langle x\rangle) - \frac{1}{N}\sum_{\substack{j=1\\ j\neq i}}^{N}(X_j-\langle x\rangle)\right]^2\right\rangle$$

$$\overset{\text{no corr.}}{=} N\left[\left(1-\frac{1}{N}\right)^2\langle (X_i-\langle x\rangle)^2\rangle + \frac{1}{N^2}\sum_{\substack{j=1\\ j\neq i}}^{N}\langle (X_j-\langle x\rangle)^2\rangle\right]$$

$$= \frac{(N-1)^2}{N}\sigma^2 + \frac{N-1}{N}\sigma^2$$

$$= \sigma^2\frac{[(N-1)+1](N-1)}{N} = (N-1)\sigma^2$$

Thus, $\boxed{\sigma^2_{est} = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2}$ is an unbiased estimator for the variance σ^2 <u>if</u> the data is uncorrelated.

(Above estimator systematically underestimates σ^2 for autocorrelated data ($\frac{1}{N}$-effect). Better: $\sigma^2_{est,imp} = \frac{\sum_i (x_i - \bar{x})^2}{N - \tau}$.)

Step (ii) variance of mean value $\bar{x}$:

$$\langle (\bar{x} - \langle x \rangle)^2 \rangle = \langle \left(\frac{1}{N}\sum_{i=1}^{N} x_i - \langle x \rangle\right)^2 \rangle$$

$$= \langle \left[\frac{1}{N} \sum_{i=1}^{N} (x_i - \langle x \rangle)\right]^2 \rangle$$

$$= \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \langle (x_i - \langle x \rangle)(x_j - \langle x \rangle) \rangle$$

$\left(\text{gen. Def.: } C_{A,B} = \frac{\langle (A - \langle A \rangle)(B - \langle B \rangle) \rangle}{\sigma_A \; \sigma_B}\right)$

covariance

$$= \frac{\sigma^2}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} C_{i,j}$$

$$\overset{\text{translation inv.}}{\approx} \frac{\sigma^2}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} C_{i-j}$$

$k = i - j$

$j = i - k$

$$= \frac{\sigma^2}{N^2} \sum_{i=1}^{N} \sum_{k=i-N}^{i-1} C_k$$

$$\overset{C_k \approx 0 \text{ for } |k| > K \ll N}{\approx} \frac{\sigma^2}{N^2} \sum_{i=1}^{N} \sum_{k=-\infty}^{\infty} C_k = \frac{\sigma^2}{N} \tau$$

autocorrelation time $\tau = \sum_{k=-\infty}^{\infty} C_k \overset{C_k = C_{-k}}{=} 1 + 2 \sum_{k=1}^{\infty} C_k$

$$c_k \approx \frac{\frac{1}{N-k-1}\sum_{i=1}^{N-k}(x_i-\bar{x})(x_{i+k}-\bar{x})}{\frac{1}{N-1}\sum_{i=1}^{N}(x_i-\bar{x})^2}$$

autocorrelation function

Beispiel Datenanalyse: Vorgegeben sind 6 Zeitreihen (http://komet337.physik.uni-mainz.de/Bluemer/lectures_SS2007#Datenanalyse), diese sollen analysiert werden, z.B. mit dem Statistik-Tool stats_v1_4.

Mittelwert mit Fehler:

```
prompt> stats_v1_4 -a < data_set1_1000.dat
Average:  5.7610558, variance:  0.6616717, error: 0.025735851
Korrelation time:   1.105017, corrected error: 0.027053472, transient: -2.6028452e-05
prompt> stats_v1_4 -a < data_set1_10000.dat
Average:  5.7484945, variance: 0.64816593, error: 0.0080512779
Korrelation time:          1, corrected error: 0.0080512779, transient: 1.0067773e-06
```

Autokorrelationsfunktion:

```
prompt> stats_v1_4 -c < data_set1_10000.dat | head -11
# Autocorrelation function: (i,c(i))
   0   1.000000
   1  -0.006890
   2   0.004378
   3   0.001233
   4  -0.005135
   5  -0.010988
   6   0.013733
   7  -0.013954
   8   0.006322
   9   0.001616
  10  -0.005462
```