Computersimulations

W. von der Linden and E. Schachinger

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Appendix A

A.1 The Correlation Coefficient

Two random variables X and Y are measured and they an be combined to a random vector (X, Y). If we have

$$P((X, Y) \in G|\mathcal{B}) = \int\limits_G dxdy\, p(x, y)$$

with

$$\int\limits_{\mathbb{R}^2} dxdy\, p(x, y) = 1,$$

then, $P((X, Y) \in G|\mathcal{B})$ is the probability for the random vector (X, Y) to be within the set G and $p(x, y)$ is the corresponding PDF of the random vector.

The correlation coefficient r is defined as:

$$r = \frac{\text{cov}(X, Y)}{\text{std}(X)\,\text{std}(Y)}, \qquad -1 \leq r \leq 1, \quad r^2 \leq 1.$$

We also define that the random variables X and Y are stronger correlated to each other with increasing values of r^2.

Such a definition becomes plausible if we make use of the fact the two random variables are independent of each other if the PDF $p(x, y)$ can be factorized:

$$p(x, y) = p(x)p(y).$$

The covariance of two independent (uncorrelated) random variables is zero and, thus, $r = 0$ in this case. Therefore, a value $r \neq 0$ necessarily indicates correlated random variables.

A typical motivation for the definition of the correlation coefficient is found from the following minimalization problem:

$$\left\langle (y - a - bx)^2 \right\rangle \overset{!}{=} \text{Min}, \qquad a, b \in \mathbb{R}.$$

We search the linear function $f(x) = a + bx$ which optimally represents y. This is precisely GAUSS' method of minimizing the square of errors, with the solution

$$y = \langle X \rangle + r\frac{\text{std}(X)}{\text{std}(Y)}(x - \langle X \rangle),$$

wich is known as *linear regression*. We find

$$\left\langle (y - a - bx)^2 \right\rangle = \text{var}(Y)(1 - r^2),$$

with the best result for $r^2 = 1$ and the worst for $r^2 = 0$.

Appendix B

B.1 Virial Theorem

We assume an n-particle system to be confined and autonomous. It is described by the equations of motion:

$$\begin{aligned} m_1\ddot{\mathbf{r}}_1 &= \mathbf{F}_{21} + \mathbf{F}_{31} + \cdots + \mathbf{F}_{n1} + \mathbf{K}_1 \\ \vdots &= \vdots \\ m_n\ddot{\mathbf{r}}_n &= \mathbf{F}_{1n} + \mathbf{F}_{2n} + \cdots + \mathbf{F}_{n-1,n} + \mathbf{K}_n. \end{aligned}$$

Thus,

$$m_i\ddot{\mathbf{r}}_i = \sum_{k\neq i}^{n} \mathbf{F}_{ki} + \mathbf{K}_1, \quad \mathbf{F}_{ki} = -\mathbf{F}_{ik}, \tag{B.1}$$

with $\mathbf{F}_{ik}$ the force exerted by particle i on particle k (internal force). $\mathbf{K}_i$ is the external force acting on particle i. The internal forces are described by a potential but they are not necessarily central forces. General solutions of Eqs. (B.1) for $n > 2$ can, if at all, only be found for very specific configurations. Nevertheless, it is possible to find some qualitative results and in order to find those we assume the solutions $\mathbf{r}_i(t)$ to be known. We define the mapping

$$V(t) = \sum_{i=1}^{n} \mathbf{r}_i(t)\mathbf{p}_i(t) \tag{B.2}$$

from phase space to real numbers $V(t)$, the *virial*. We assume, furthermore, that the solutions of Eqs. (B.1)never allow a particle to escape to infinity (thus, n is constant) are to acquire infinite momentum. In this case, $V(t)$ stays finite for all times.

We define the time average

$$\langle f \rangle := \lim_{t\to\infty} \frac{1}{2t} \int_{-t}^{t} dt'\, f(t'),$$

and find for the time average of the time derivative of the virial:

$$\langle \dot{V} \rangle = \lim_{t\to\infty} \int_{-t}^{t} dt \, \frac{dV(t)}{dt} = \lim_{t\to\infty} \frac{V(t) - V(-t)}{2t} = 0, \tag{B.3}$$

because $V(t)$ was assumed to be finite. The time derivative of the virial is given by:

$$\begin{aligned} \dot{V}(t) &= \sum_{i=1}^{n} \left[\dot{\mathbf{r}}_i(t)\mathbf{p}_i(t) + \mathbf{r}_i(t)\dot{\mathbf{p}}_i(t) \right] \\ &= \sum_{i=1}^{n} \left[m_i \dot{\mathbf{r}}_i^2(t) + \mathbf{r}_i(t) \underbrace{m_i \ddot{\mathbf{r}}_i(t)}_{\to(\text{B.1})} \right]. \end{aligned}$$

If we keep in mind that

$$\mathbf{F} = -\nabla U \left[\mathbf{r}_1(t), \ldots, \mathbf{r}_n(t) \right]$$

and use Eqs. (B.1), as indicated, we find the following expression for $\dot{V}(t)$

$$\dot{V}(t) = \sum_{i=1}^{n} m_i \dot{\mathbf{r}}_i^2(t) - \sum_{i=1}^{n} \mathbf{r}_i(t) \nabla_i U \left[\mathbf{r}_1(t), \ldots, \mathbf{r}_n(t) \right].$$

Thus, Eq. (B.3) results in

$$\langle \dot{V} \rangle = 2\langle T \rangle - \left\langle \sum_{i=1}^{n} \mathbf{r}_i \nabla_i U \right\rangle = 0, \tag{B.4}$$

with $\langle T \rangle$ the time average of the kinetic energy. Eq. (B.4) establishes the *Virial Theorem*.

If the potential U is assumed to be a homogeneous function of rank k in it's arguments $\mathbf{r}_i$ then we can make use of EULER's theorem which results in

$$\sum_{i=1}^{n} \nabla_i U = kU,$$

and the virial theorem gives:

$$2\langle T \rangle - k\langle U \rangle = 0.$$

Appendix C

C.1 Kolmogorov's Zero-One Law

Kolmogorov's Zero-One Law specifies that a certain type of event, called a *tail event* will either certainly happen or certainly not happen, that is, the probability of such an event occurring is zero or one.

Tail events are defined in terms of infinite sequences of random variables. Suppose X_1, X_2, X_3, … is an infinite sequence of independent random variables (not necessarily identically distributed). Then, a tail event is an event whose occurrence or failure is determined by the values of these random variables but which is probabilistically independent of each finite subsequences of these random variables.

For example, the event that the series

$$\sum_{k=1}^{\infty} X_k$$

converges is a tail event. The event that the sum to which it converges is more than 1 is not a tail event, since, for instance, it is not independent of the value of X_1. In an infinite sequence of coin-tosses that a sequence of 100 consecutive heads eventually occurs, is a tail event.

In a book published 1909, Émile Borel stated that a monkey which hits typewriter keys randomly forever (the 'dactylographic monkey') will eventually type every book in France's National Library. This is a special case of the Zero-One Law: Since there is a positive, though tiny, chance that the monkey 'gets it right' the first time it tries, the probability of the tail event that it 'gets it right' given an infinite amount of time cannot be zero. Therefore, that probability must be one by the Zero-One Law.