Monte Carlo Methods - Fall 2013/14

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Exercise Nr. 10

Discussion on January 22, after the lecture

28) Trotter product formula *(4 points)*

Consider the case of A, B being real or complex $N \times N$ matrices (a special case of linear operators, for which the Trotter product formula is also called Lie product formula). Show that this product formula

$$e^{A+B} = \lim_{P\to\infty} \left(e^{A/P} e^{B/P}\right)^P$$

is a corollary of the Baker-Campbell-Hausdorff formula

$$\log(e^X e^Y) = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}\left([X,[X,Y]] - [Y,[X,Y]]\right) + \dots .$$

What is the leading error induced by a finite P (this leading error regime is characterized as "Trotter scaling")?

29) Feynman Path Integral *(4 points)*

Consider a quantum mechanical system in the path integral formalism. Compute the typical interparticle mean-square displacement $\ell^2 = \left(\vec{r}_i^{(s+1)} - \vec{r}_i^{(s)}\right)^2$ for vanishing potential. A derived quantity is the "gyration radius" of a ring polymer with P monomers, $\langle R_g^2 \rangle = \ell^2 P/12$. Compare this to the thermal de Broglie wave length $\lambda_T = \frac{h}{\sqrt{2\pi m k_B T}}$ How do you interpret this finding in terms of the Heisenberg uncertainty principle? On which parameter does a good choice of the Trotter dimension P depend on?

30) Harmonic Oscillator *(12 points)*

Consider a single particle in a harmonic potential well with characteristic frequency of $\omega = \sqrt{k/m}$ Perform a path integral Monte Carlo simulation for $P = 1$, $P = 2$, and $P = 8$ at an inverse temperature of $\beta = 2.5$. Carry out multiple runs for 10000 MC steps and determine statistical error bars. Repeat the calculation for runs of 10^6 MC steps. Compare the results and comment.

Richard Philips Feynman

(May 11, 1918, - February 15, 1988) was an American physicist.

He grew up in Far Rockaway, Queens and when he was about 10, he started to buy old radios to use in his "personal laboratory," a collection of electric gadgets and components, and by the age of 12, he was already fixing radios in his neighborhood. [...] Feynman studied at the Massachusetts Institute of Technology and continued his studies at Princeton University, where he obtained his Ph.D. in physics in 1942 with a thesis supervised by John Wheeler. His thesis dealt with advanced waves, which can be described as the theory of electromagnetic waves that travel "backwards" in time. His first lecture at Princeton on the subject was interesting enough to draw an audience that included none less than Einstein, Pauli, and von Neumann. After completing his Ph.D., Feynman moved to Cornell University in 1945 as professor of theoretical physics. There, he met Hans Bethe and became involved in the Manhattan Project. While moving to the newly constructed secret laboratory at Los Alamos, Feynman flouted military discipline with a series of quirky practical jokes and tricks. He was particularly fond of pointing out the insufficiency of the security of the Los Alamos safes inside which the plans for the atomic bomb where entrusted. [...] While Feynman toiled at Los Alamos, his wife became very sick and subsequently died.

Soon after the war, Feynman was invited as a visiting professor to the University of Rio de Janeiro, Brazil. He subsequently accepted a professorship of theoretical physics at the California Institute of Technology in 1950, but loved Brazil so much that one of his "conditions" was to be able to visit Brazil again. As a result, he did not actually start lecturing at Caltech until 1951. While in Brazil, Feynman lectured about electromagnetism for ten months, at the same time preparing to parade in the carnival of a samba school in Copacabana, Rio de Janeiro.

Upon returning to Caltech the following year, Feynman returned his attention quantum electrodynamics and successfully developed the rules that all quantum field theories must obey. In the process, he discovered how to renormalize the theory of quantum electrodynamics and also invented a nice way of representing quantum interactions, now called Feynman diagrams. For all these contributions, especially to the renormalization of quantum electrodynamics, Feynman shared the 1965 Nobel Prize in physics with Shin-Ichiro Tomonaga and Julian Schwinger, each of whom also contributed to the renormalization of the theory. Feynman also contributed to the theory of nuclear interactions with Murray Gell-Mann.

Feynman was always concerned about the education of physics. [...] He also invigorated undergraduate physics education at Caltech, where his four years of lectures were edited and collected into the classic three-volume textbook The Feynman Lectures on Physics, which has become an inspiration for students of physics ever since. Feynman also published a number of popularizations of physics, including QED: The Strange Theory of Light and Matter.

After the explosion of NASA's Space Shuttle Challenger, Feynman was appointed to the council investigating the causes of the disaster. In his usual brusque and no-nonsense style, Feynman cut through the bureaucracy and identified the cause of disaster as the failure of an o-ring seal in the unusually cold launch-pad temperatures, even dunking a similar o-ring in a glass of ice water in front of other committee members to emphasize his conclusion.

In the early 1980s, Feynman developed an abdominal cancer. After a five-year fight, Feynman succumbed in 1988 at the age of 69. Feynman was the recipient of numerous awards during his lifetime, including the Albert Einstein Award (1954, Princeton) and Lawrence Award (1962). Feynman was also a member of the American Physical Society, the American Association for the Advancement of Science, the National Academy of Science, and was elected a foreign member of the Royal Society, London (Great Britain) in 1965.

`[http://scienceworld.wolfram.com/biography/Feynman.html]`