The Monte Carlo Method in Quantum Field Theory

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HUGS June 2006

Outline

- Path integrals in quantum mechanics
- Monte Carlo integration and Markov chains
- Monte Carlo evaluation of path integral in quantum mechanics
- Free Klein-Gordon scalar field theory in $2+1$ dimensions
- Interacting ϕ^4 scalar field theory in $2+1$ dimensions
- Applications in quantum chromodynamics
- Topics for future study

Part I

Path integrals in quantum mechanics

Transition amplitudes in quantum mechanics

- key quantity in quantum mechanics: transition amplitude

$$Z(b,a) \equiv \langle x_b(t_b) \mid x_a(t_a) \rangle$$

  - $Z(b,a)$ is probability amplitude for particle to go from point x_a at time t_a to point x_b at time t_b
- in this talk, will work in Heisenberg picture
  - state vectors $|\Psi\rangle$ are stationary
  - operators and their eigenvectors evolve with time

$$\begin{aligned} x(t) &= e^{iHt/\hbar}\, x(0)\, e^{-iHt/\hbar} \\ |x(t)\rangle &= e^{iHt/\hbar}\, |x(0)\rangle \end{aligned}$$

- often will shift Hamiltonian so ground state energy is zero

$$\begin{aligned} H\,|\phi_n(t)\rangle &= E_n\,|\phi_n(t)\rangle, \qquad E_0 = 0 \\ |\phi_0(t)\rangle &= |\phi_0(0)\rangle \equiv |0\rangle \end{aligned}$$

Spectral representation of transition amplitude

- insert complete (discrete) set of Heisenberg-picture eigenstates $|\phi_n(t)\rangle$ of Hamiltonian H into transition amplitude

$$Z(b,a) \equiv \langle x_b(t_b) \mid x_a(t_a)\rangle = \sum_n \langle x_b(t_b)\ |\phi_n(t_a)\rangle\langle\phi_n(t_a)|\ x_a(t_a)\rangle$$

- now use $|\phi_n(t)\rangle = e^{iHt/\hbar}|\phi_n(0)\rangle \stackrel{n}{=} e^{iE_nt/\hbar}|\phi_n(0)\rangle$ to obtain

$$Z(b,a) = \sum_n e^{iE_n(t_a-t_b)/\hbar}\langle x_b(t_b)\ |\phi_n(t_b)\rangle\langle\phi_n(t_a)|\ x_a(t_a)\rangle$$

- finally, $\langle x(t)|\phi_n(t)\rangle \stackrel{n}{\equiv} \varphi_n(x)$ is the wavefunction in coordinate space, so

$$Z(b,a) = \sum_n \varphi_n^*(x_b)\varphi_n(x_a)\ e^{-iE_n(t_b-t_a)/\hbar}$$

- transition amplitude contains information about all energy levels and all wavefunctions $\longrightarrow$ spectral representation

Vacuum saturation

- take $t_a = -T$ and $t_b = T$ in the limit $T \to (1 - i\epsilon)\infty$

$$\begin{aligned} \langle x_b(T)|x_a(-T)\rangle &= \langle x_b(0)|e^{-iHT/\hbar}\, e^{iH(-T)/\hbar}|x_a(0)\rangle \\ &= \sum_{n=0}^{\infty}\langle x_b(0)|\phi_n(0)\rangle\langle\phi_n(0)|x_a(0)\rangle\, e^{-2iE_nT/\hbar} \\ &\to \langle x_b(0)|0\rangle\langle 0|x_a(0)\rangle \end{aligned}$$

  - insert complete set of energy eigenstates, use $E_{n+1} \geq E_n, \quad E_0 = 0$, assume nondegenerate vacuum
- possibility of probing ground state (vacuum) properties

Vacuum expectation values

- now apply limit $T \to (1-i\epsilon)\infty$ to more complicated amplitude

$$\begin{aligned}
& \langle x_b(T)|x(t_2)x(t_1)|x_a(-T)\rangle \\
= \;& \langle x_b(0)|e^{-iHT/\hbar}\, x(t_2)x(t_1)\, e^{-iHT/\hbar}|x_a(0)\rangle \\
= \;& \sum_{n,m}\langle x_b(0)|\phi_n(0)\rangle\langle\phi_n(0)|x(t_2)x(t_1)|\phi_m(0)\rangle\langle\phi_m(0)|x_a(0)\rangle \\
& \qquad \times e^{-i(E_n+E_m)T/\hbar} \\
\to \;& \langle x_b(0)|0\rangle\langle 0|x(t_2)x(t_1)|0\rangle\langle 0|x_a(0)\rangle
\end{aligned}$$

- hence, vacuum expectation values from

$$\langle 0|x(t_2)x(t_1)|0\rangle = \lim_{T\to(1-i\epsilon)\infty} \frac{\langle x_b(T)|x(t_2)x(t_1)|x_a(-T)\rangle}{\langle x_b(T)|x_a(-T)\rangle}$$

- result generalizes to higher products of position operator

Observables from correlation functions

- all observables can be extracted from the correlation functions (vacuum expectation values)
- example: energies of the stationary states

$$\begin{aligned}\langle 0|x(t)x(0)|0\rangle &= \langle 0|e^{iHt/\hbar}x(0)e^{-iHt/\hbar}x(0)|0\rangle \\ &= \sum_n \langle 0|x(0)e^{-iHt/\hbar}|\phi_n(0)\rangle\langle\phi_n(0)|x(0)|0\rangle \\ &= \sum_n |\langle 0|x(0)|\phi_n(0)\rangle|^2 e^{-iE_nt/\hbar}\end{aligned}$$

- similarly for more complicated correlation functions

$$\begin{aligned}\langle 0|x^2(t)x^2(0)|0\rangle &= \langle 0|e^{iHt/\hbar}x^2(0)e^{-iHt/\hbar}x^2(0)|0\rangle \\ &= \sum_n |\langle 0|x^2(0)|\phi_n(0)\rangle|^2 e^{-iE_nt/\hbar}\end{aligned}$$

- but difficult to extract energies E_n from above oscillatory functions $\rightarrow$ much easier if we had decaying exponentials

The imaginary time formalism

- can get decaying exponentials if we rotate from the real to the imaginary axis in time (Wick rotation) $t \to -i\tau$

$$\begin{aligned} \langle 0|x(t)x(0)|0\rangle &= \sum_n |\langle 0|x(0)|\phi_n(0)\rangle|^2 e^{-E_n\tau/\hbar} \\ &\overset{\tau\to\infty}{\longrightarrow} |\langle 0|x(0)|0\rangle|^2 + |\langle 0|x(0)|\phi_1(0)\rangle|^2 e^{-E_1\tau/\hbar} \end{aligned}$$

- later, will see this imaginary time formalism provides another important advantage for Monte Carlo applications

Quantum mechanics and path integrals

- in the 1940s, Feynman developed an alternative formulation of quantum mechanics (his Ph.D. thesis)
  - Richard Feynman, Rev Mod Phys **20**, 367 (1948)

- quantum mechanical law of motion:
  - probability amplitude from *sum over histories*

$$Z(b,a) \sim \sum_{\substack{\text{all paths } x(t) \\ \text{from } a \text{ to } b}} \exp\left(iS[x(t)]/\hbar\right)$$

- all paths contribute to probability amplitude, but with different *phases* determined by the *action* $S[x(t)]$
- classical limit: when small changes in path yield changes in action large compared to $\hbar$, phases cancel out and path of least action $\delta S = 0$ dominates sum over histories

Defining the path integral

- action = time integral of Lagrangian (kinetic minus potential energy)

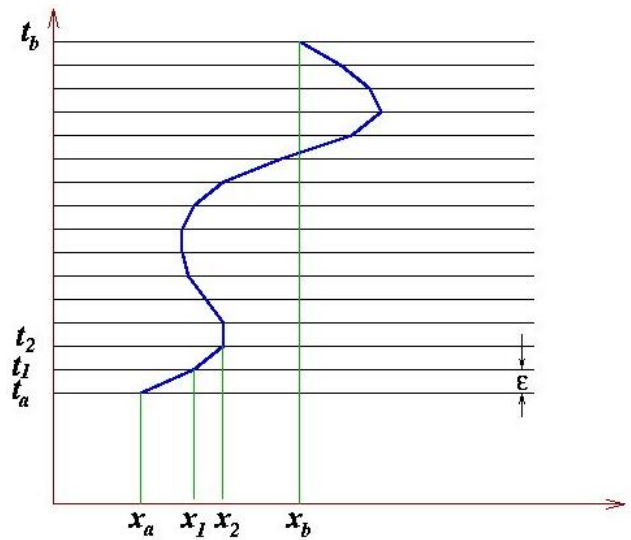
$$S = \int dt\, L(x, \dot{x}) = \int dt\, \Big(K - U \Big)$$

- divide time into steps of width ε where $N\varepsilon = t_b - t_a$
- path integral is defined as

$$Z(b,a) = \lim_{\varepsilon \to 0} \frac{1}{A} \int_{-\infty}^{\infty} \frac{dx_1}{A} \frac{dx_2}{A} \cdots \frac{dx_{N-1}}{A}\, e^{iS[x(t)]/\hbar}$$

where A is a normalization factor depending on ε chosen so path integral well-defined

- in nonrelativistic theory, paths cannot double-back in time



Schrödinger equation

- probability amplitude $\psi(x_b, t_b)$ at time t_b given amplitude $\psi(x_a, t_a)$ at earlier time t_a given by
$$\psi(x_b, t_b) = \int Z(b,a)\, \psi(x_a, t_a)\, dx_a$$
- take $t_a = t$ and $t_b = t + \varepsilon$ one time slice away
$$\psi(x_b, t+\varepsilon) = \frac{1}{A} \int_{-\infty}^{\infty} \exp\left[\frac{i\varepsilon}{\hbar} L\left(\frac{x_b + x_a}{2}, \frac{x_b - x_a}{\varepsilon}\right)\right] \psi(x_a, t)\, dx_a$$
  - in L, take $\dot{x} = (x_b - x_a)/\varepsilon$ and mid-point prescription $x \to (x_b + x_a)/2$
- particle in potential: $L = \frac{1}{2} m\dot{x}^2 - V(x,t)$, write $x_b = x,\ x_a = x + \eta$
$$\psi(x, t+\varepsilon) = \frac{1}{A} \int_{-\infty}^{\infty} e^{im\eta^2/(2\hbar\varepsilon)} e^{-i\varepsilon V(x+\eta/2, t)/\hbar} \psi(x+\eta, t)\, d\eta$$

Schrödinger equation (continued)

$$\psi(x,t+\varepsilon) = \frac{1}{A}\int_{-\infty}^{\infty} e^{im\eta^2/(2\hbar\varepsilon)} e^{-i\varepsilon V(x+\eta/2,t)/\hbar}\psi(x+\eta,t)\,d\eta$$

- rapid oscillation of $e^{im\eta^2/(2\hbar\varepsilon)}$ except when $\eta \sim O(\sqrt{\varepsilon}) \rightarrow$ integral dominated by contributions from η having values of this order
- expand to $O(\varepsilon)$ and $O(\eta^2)$, except $e^{im\eta^2/(2\hbar\varepsilon)}$ (ψ refers to $\psi(x,t)$)

$$\begin{aligned}\psi + \varepsilon\frac{\partial\psi}{\partial t} &= \frac{1}{A}\int_{-\infty}^{\infty} e^{im\eta^2/(2\hbar\varepsilon)}\left[1-\frac{i\varepsilon}{\hbar}V(x,t)\right]\left[\psi+\eta\frac{\partial\psi}{\partial x}+\frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}\right]d\eta \\ &= \frac{1}{A}\int_{-\infty}^{\infty} e^{im\eta^2/(2\hbar\varepsilon)}\left[\psi-\frac{i\varepsilon}{\hbar}V(x,t)\psi+\eta\frac{\partial\psi}{\partial x}+\frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}\right]d\eta\end{aligned}$$

Schrödinger equation (continued)

$$\psi + \varepsilon \frac{\partial \psi}{\partial t} = \frac{1}{A} \int_{-\infty}^{\infty} e^{im\eta^2/(2\hbar\varepsilon)} \left[\psi - \frac{i\varepsilon}{\hbar} V(x,t)\psi + \eta \frac{\partial \psi}{\partial x} + \frac{\eta^2}{2} \frac{\partial^2 \psi}{\partial x^2} \right] d\eta$$

- matching leading terms on both sides determines A (analytic continuation to evaluate integral)

$$1 = \frac{1}{A} \int_{-\infty}^{\infty} e^{im\eta^2/(2\hbar\varepsilon)} d\eta = \frac{1}{A} \left(\frac{2\pi i \hbar \varepsilon}{m} \right)^{1/2} \quad \Rightarrow \quad A = \left(\frac{2\pi i \hbar \varepsilon}{m} \right)^{1/2}$$

- two more integrals:

$$\frac{1}{A} \int_{-\infty}^{\infty} e^{im\eta^2/(2\hbar\varepsilon)} \, \eta \, d\eta = 0, \qquad \frac{1}{A} \int_{-\infty}^{\infty} e^{im\eta^2/(2\hbar\varepsilon)} \, \eta^2 d\eta = \frac{i\hbar\varepsilon}{m}$$

- $O(\varepsilon)$ part of equation at top yields

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x,t)\psi$$

- the Schrödinger equation!

Free particle in one dimension

- Lagrangian of free particle in one dimension $L = \frac{1}{2}m\dot{x}^2$
- amplitude for particle to travel from x_a at time t_a to location x_b at later time t_b is
$$\langle x_b(t_b)|x_a(t_a)\rangle = \int_a^b \mathcal{D}x(t)\exp(iS[b,a]/\hbar)$$
summing over all allowed paths with $x(t_a) = x_a$ and $x(t_b) = x_b$.
- classical path $x_{\rm cl}(t)$ from $\delta S = 0$ and boundary conditions:
$$\ddot{x}_{\rm cl}(t) = 0, \qquad x_{\rm cl}(t) = x_a + (x_b - x_a)\frac{(t-t_a)}{(t_b-t_a)}$$
- classical action is
$$S_{\rm cl}[b,a] = \int_{t_a}^{t_b} dt\ \tfrac{1}{2}m\dot{x}_{\rm cl}^2 = \frac{m(x_b-x_a)^2}{2(t_b-t_a)}$$
- write $x(t) = x_{\rm cl}(t) + \chi(t)$ where $\chi(t_a) = \chi(t_b) = 0$ then
$$S[b,a] = S_{\rm cl}[b,a] + \int_{t_a}^{t_b} dt\ \tfrac{1}{2}m\dot{\chi}^2$$
where $S_{\rm cl}[b,a]$ is classical action; no terms linear in $\chi(t)$ since $S_{\rm cl}$ is extremum

Path integral for free particle

- amplitude becomes

$$\begin{aligned} Z(b,a) &= F(T)\exp(iS_{\rm cl}/\hbar) \\ F(T) &= \int_0^0 \mathcal{D}\chi\ \exp\left\{\frac{im}{2\hbar}\int_0^T dt\ \dot{\chi}^2\right\} \end{aligned}$$

- partition time into discrete steps of length ε, use midpoint prescription, and note that $\chi_0 = \chi_N = 0$

$$\int_0^0 \mathcal{D}\chi = \frac{1}{A}\int_{-\infty}^{\infty}\left(\prod_{l=1}^{N-1}\frac{d\chi_l}{A}\right) \qquad A = \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{1/2}$$

$$\int_0^T dt\ \dot{\chi}^2 = \frac{1}{\varepsilon}\sum_{j=0}^{N-1}(\chi_{j+1}-\chi_j)^2$$

$$F(T) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2}\int_{-\infty}^{\infty}\left(\prod_{l=1}^{N-1}d\chi_l\right)\exp\left\{\frac{im}{2\hbar\varepsilon}\chi_j M_{jk}\chi_k\right\}$$

Gaussian integration

- a multivariate Gaussian integral remains

$$F(T) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2} \int_{-\infty}^{\infty} \left(\prod_{l=1}^{N-1} d\chi_l\right) \exp\left\{\frac{im}{2\hbar\varepsilon}\chi_j M_{jk}\chi_k\right\}$$

  where M is a symmetric $(N-1)\times(N-1)$ matrix

$$M = \begin{bmatrix} 2 & -1 & 0 & 0 & \cdots \\ -1 & 2 & -1 & 0 & \cdots \\ 0 & -1 & 2 & -1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

- Gaussian integrals of symmetric matrix A easily evaluated

$$\int_{-\infty}^{\infty} \left(\prod_{i=1}^{n} d\chi_i\right) \exp\left(-\chi_j A_{jk}\chi_k\right) = \left(\frac{\pi^n}{\det A}\right)^{1/2}$$

- result:

$$F(T) = \left(\frac{m}{2\pi i\hbar\varepsilon \det M}\right)^{1/2}$$

Determinant evaluation

- now need to compute $\det(M)$
- consider $n \times n$ matrix B_n of form

$$B_n = \begin{pmatrix} 2b & -b & 0 & 0 & \cdots \\ -b & 2b & -b & 0 & \cdots \\ 0 & -b & 2b & -b & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}_{n,n}$$

- notice that

$$\begin{aligned} \det B_n &= 2b \det B_{n-1} + b \det \left(\begin{array}{c|ccc} -b & -b & 0 & \cdots \\ \hline 0 & & & \\ \vdots & & B_{n-2} & \end{array}\right) \\ &= 2b \det B_{n-1} - b^2 \det B_{n-2} \end{aligned}$$

- define $I_n = \det B_n$ then have recursion relation

$$I_{n+1} = 2bI_n - b^2 I_{n-1}, \qquad I_{-1} = 0, \quad I_0 = 1, \qquad n = 0, 1, 2, \ldots$$

Transition amplitude for free particle

- rewrite $I_{n+1} = 2bI_n - b^2 I_{n-1}, \qquad I_{-1} = 0, \quad I_0 = 1$ as

$$\begin{pmatrix} I_{n+1} \\ I_n \end{pmatrix} = \begin{pmatrix} 2b & -b^2 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} I_n \\ I_{n-1} \end{pmatrix} = \begin{pmatrix} 2b & -b^2 \\ 1 & 0 \end{pmatrix}^n \begin{pmatrix} I_1 \\ I_0 \end{pmatrix}$$

- straightforward to show that

$$\begin{pmatrix} 2b & -b^2 \\ 1 & 0 \end{pmatrix}^n = \begin{pmatrix} (n+1)b^n & -nb^{n+1} \\ nb^{n-1} & -(n-1)b^n \end{pmatrix}$$

- so that

$$\begin{pmatrix} I_{n+1} \\ I_n \end{pmatrix} = \begin{pmatrix} (n+1)b^n & -nb^{n+1} \\ nb^{n-1} & -(n-1)b^n \end{pmatrix} \begin{pmatrix} 2b \\ 1 \end{pmatrix}$$

- and thus, $I_n = \det B_n = (n+1)b^n$
- here, $b = 1$ and $n = N - 1$ so $\det M = N$ and using $N\varepsilon = t_b - t_a$ obtain

$$F(t_b, t_a) = \left(\frac{m}{2\pi i\hbar(t_b - t_a)} \right)^{1/2}$$

- Final result:

$$\langle x_b(t_b) | x_a(t_a) \rangle = \left(\frac{m}{2\pi i\hbar(t_b - t_a)} \right)^{1/2} \exp\left\{ \frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)} \right\}$$

Infinite square well

- one of the first systems usually studied when learning quantum mechanics is the infinite square well
- particle moving in one dimension under influence of potential

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{for } x \leq 0 \text{ and } x \geq L \end{cases}$$

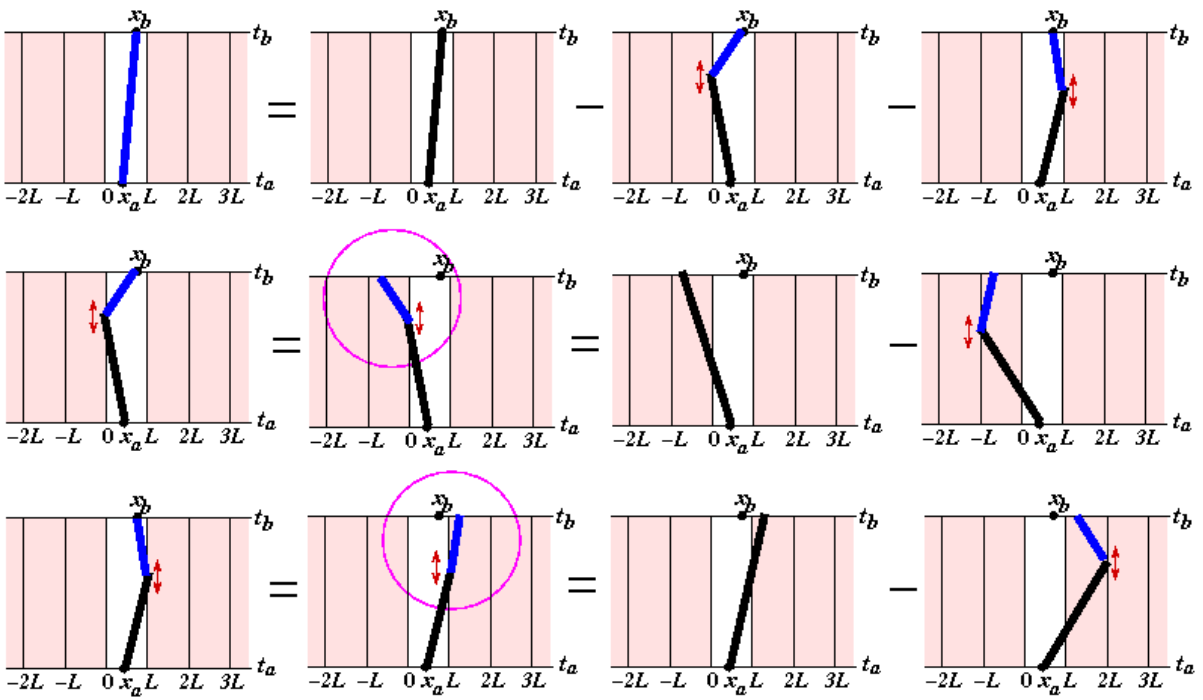
- path integral for transition amplitude given by

$$Z(b,a) = \lim_{\varepsilon \to 0} \frac{1}{A} \int_0^L \frac{dx_1}{A} \cdots \int_0^L \frac{dx_{N-1}}{A} \exp\left\{ \frac{im}{2\varepsilon\hbar} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2 \right\}$$

- paths limited to $0 < x < L$
- gaussian integrals over bounded domains produce error functions $\rightarrow$ direct evaluation difficult in closed form
- extend regions of integration to $-\infty < x < \infty$, but subtract off forbidden paths
  - M. Goodman, Am. Jour. Phys. **49**, 9 (1981)

Path cancellations

- **black** lines: all unbounded paths between end points
- blue lines: paths between end points that do not cross an nL boundary
- no doubling back in time
- magenta circle indicates action preserving reflection

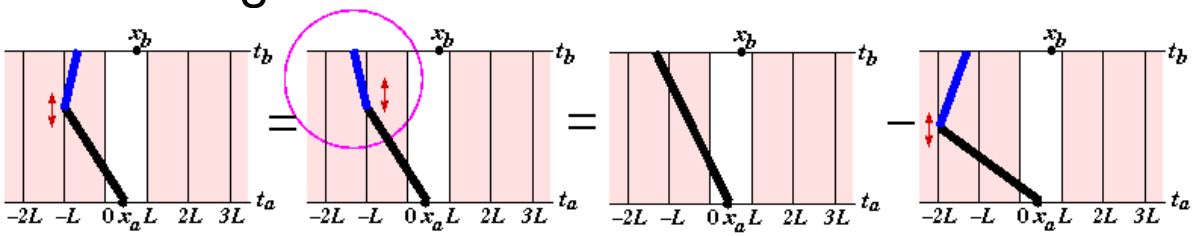


end point $-x_b$

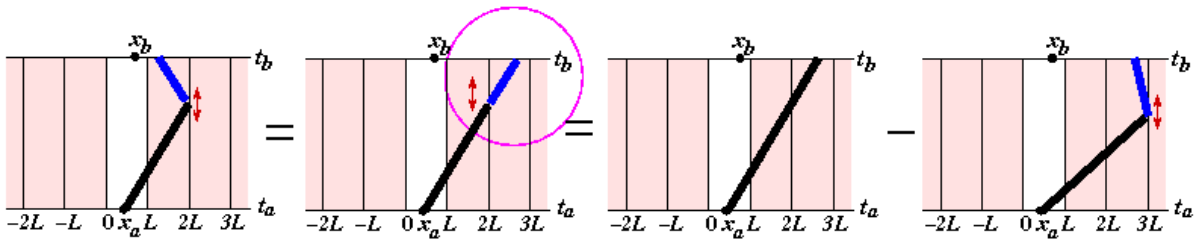
end point $2L - x_b$

Path cancellations (continued)

- continuing



end point $-2L + x_b$



end point $2L + x_b$

- and so on forever $\longrightarrow$ final result is

$$\langle x_b, t_b | x_a, t_a \rangle_{\text{well}} = \langle x_b, t_b | x_a, t_a \rangle_{\text{free}} - \langle -x_b, t_b | x_a, t_a \rangle_{\text{free}} - \langle 2L - x_b, t_b | x_a, t_a \rangle_{\text{free}} + \langle -2L + x_b, t_b | x_a, t_a \rangle_{\text{free}} + \langle 2L + x_b, t_b | x_a, t_a \rangle_{\text{free}} + \cdots$$

$$= \sum_{n=-\infty}^{\infty} \left\{ \langle 2nL + x_b, t_b | x_a, t_a \rangle_{\text{free}} - \langle 2nL - x_b, t_b | x_a, t_a \rangle_{\text{free}} \right\}$$

Transition amplitude for infinite square well

- substitute amplitude for free particle

$$\langle x_b(t_b)|x_a(t_a)\rangle = \left(\frac{m}{2\pi i\hbar(t_b-t_a)}\right)^{1/2}$$

$$\times \sum_{n=-\infty}^{\infty}\left(\exp\left\{\frac{im(2nL+x_b-x_a)^2}{2\hbar(t_b-t_a)}\right\} - \exp\left\{\frac{im(2nL-x_b-x_a)^2}{2\hbar(t_b-t_a)}\right\}\right)$$

- apply Poisson summation and integrate the gaussian

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{j=-\infty}^{\infty}\int_{-\infty}^{\infty} ds\, f(s)e^{2\pi ijs}$$

$$\int_{-\infty}^{\infty} ds \exp\left(-i\alpha s^2 \pm i\beta s\right) = \sqrt{\frac{\pi}{i\alpha}}\exp\left(\frac{i\beta^2}{4\alpha}\right)$$

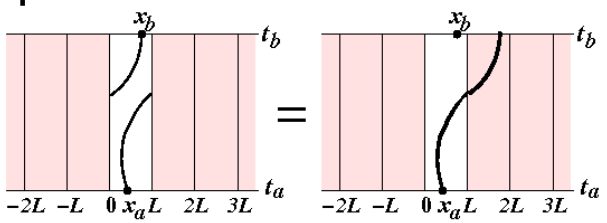
- spectral representation of transition amplitude

$$\langle x_b(t_b)|x_a(t_a)\rangle = \sum_{n=1}^{\infty}\varphi_n(x_b)\varphi_n^*(x_a)e^{-iE_n(t_b-t_a)/\hbar}$$

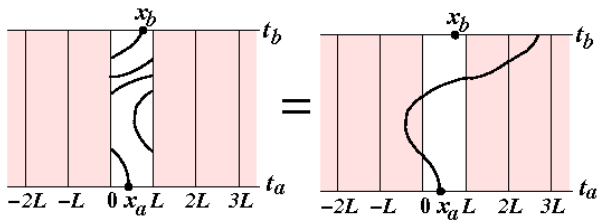
$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad \varphi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

Free particle in 1D periodic box

- consider particle moving in one-dimension with periodic boundary conditions at $x = 0$ and $x = L$
- enforcing boundary conditions on paths difficult
- use trick similar to that used in infinite square well
- express set of allowed paths in terms of equivalent set of unrestricted paths



end point $x_b + L$



end point $x_b + 2L$

- result:

$$\langle x_b, t_b | x_a, t_a \rangle_{\text{periodic}} = \sum_{n=-\infty}^{\infty} \langle x_b + nL, t_b | x_a, t_a \rangle_{\text{free}}$$

Transition amplitude for periodic boundary

- substitute amplitude for free particle

$$\langle x_b(t_b)|x_a(t_a)\rangle = \left(\frac{m}{2\pi i\hbar(t_b-t_a)}\right)^{1/2} \sum_{n=-\infty}^{\infty} \exp\left\{\frac{im(nL+x_b-x_a)^2}{2\hbar(t_b-t_a)}\right\}$$

- apply Poisson summation and integrate the gaussian

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{j=-\infty}^{\infty} \int_{-\infty}^{\infty} ds\, f(s) e^{2\pi ijs}$$

$$\int_{-\infty}^{\infty} ds \exp\left(-i\alpha s^2 \pm i\beta s\right) = \sqrt{\frac{\pi}{i\alpha}} \exp\left(\frac{i\beta^2}{4\alpha}\right)$$

- spectral representation of transition amplitude

$$\langle x_b(t_b)|x_a(t_a)\rangle = \sum_{n=-\infty}^{\infty} \varphi_n(x_b)\varphi_n^*(x_a) e^{-iE_n(t_b-t_a)/\hbar}$$

$$E_n = \frac{p_n^2}{2m} \qquad p_n = \frac{2\pi n\hbar}{L} \qquad \varphi_n(x) = \frac{1}{\sqrt{L}} e^{ip_n x/\hbar}$$

- quantization of momenta

The simple harmonic oscillator

- kinetic and potential energy of a simple harmonic oscillator of mass m and frequency ω

$$K = \tfrac{1}{2}m\dot{x}^2 \qquad U = \tfrac{1}{2}m\omega^2 x^2$$

- action is given by

$$S[x(t)] = \int_{t_a}^{t_b} dt \ \left(\tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2 x^2\right)$$

- classical equations of motion

$$\delta S = 0 \quad \Rightarrow \quad \ddot{x}_{\rm cl} + \omega^2 x_{\rm cl} = 0$$

- value of action for the classical path

$$S_{\rm cl} = \frac{m\omega}{2\sin(\omega T)}\left[(x_a^2 + x_b^2)\cos(\omega T) - 2x_a x_b\right]$$

- to calculate, write path as deviation from classical path

$$x(t) = x_{\rm cl}(t) + \chi(t) \qquad \chi(t_a) = \chi(t_b) = 0$$

Path integral of simple harmonic oscillator

- amplitude can then be written as

$$\begin{aligned} Z(b,a) &= F(T)\exp(iS_{\rm cl}/\hbar) \\ F(T) &= \int_0^0 \mathcal{D}\chi\ \exp\left\{\frac{im}{2\hbar}\int_0^T dt\,(\dot{\chi}^2-\omega^2\chi^2)\right\} \end{aligned}$$

- partition time into discrete steps of length ε and use midpoint prescription

$$\int_0^0 \mathcal{D}\chi = \frac{1}{A}\int_{-\infty}^{\infty}\left(\prod_{l=1}^{N-1}\frac{d\chi_l}{A}\right) \qquad A=\left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{1/2}$$

$$\int_0^T dt(\dot{\chi}^2-\omega^2\chi^2) = \frac{1}{\varepsilon}\sum_{j=0}^{N-1}\left[(\chi_{j+1}-\chi_j)^2-\frac{\varepsilon^2\omega^2}{4}(\chi_{j+1}+\chi_j)^2\right]$$

$$F(T) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2}\int_{-\infty}^{\infty}\left(\prod_{l=1}^{N-1}d\chi_l\right)\exp\left\{\frac{im}{2\hbar\varepsilon}\chi_j M_{jk}\chi_k\right\}$$

Gaussian integration

- a multivariate Gaussian integral remains

$$F(T) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2} \int_{-\infty}^{\infty} \left(\prod_{l=1}^{N-1} d\chi_l\right) \exp\left\{\frac{im}{2\hbar\varepsilon}\chi_j M_{jk}\chi_k\right\}$$

  where M is a symmetric $(N-1)\times(N-1)$ matrix

$$M = \begin{bmatrix} 2 & -1 & 0 & 0 & \cdots \\ -1 & 2 & -1 & 0 & \cdots \\ 0 & -1 & 2 & -1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} - \frac{\varepsilon^2\omega^2}{4} \begin{bmatrix} 2 & 1 & 0 & 0 & \cdots \\ 1 & 2 & 1 & 0 & \cdots \\ 0 & 1 & 2 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

- Gaussian integrals are easily evaluated

$$F(T) = \left(\frac{m}{2\pi i\hbar\varepsilon \det M}\right)^{1/2}$$

Evaluating the determinant

- now must compute $\det M$
- consider $\det(B_n)$ where $n \times n$ matrix B_n has form

$$B_n = \begin{pmatrix} a & b & 0 & 0 & \cdots \\ b & a & b & 0 & \cdots \\ 0 & b & a & b & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}_{n,n}$$

- matches M for $n = N - 1$, $a = 2(1 - \epsilon^2\omega^2/4)$, $b = -(1 + \epsilon^2\omega^2/4)$
- notice that

$$\begin{aligned} \det B_n &= a \det B_{n-1} - b \det \left(\begin{array}{c|cc} b & b & 0 \cdots \\ \hline 0 & & \\ \vdots & & B_{n-2} \end{array}\right) \\ &= a \det B_{n-1} - b^2 \det B_{n-2} \end{aligned}$$

- define $I_n = \det B_n$ to obtain recursion relation

$$I_{n+1} = aI_n - b^2 I_{n-1}, \qquad I_{-1} = 0, \quad I_0 = 1, \qquad n = 0, 1, 2, \ldots$$

Evaluating the determinant (continued)

- rewrite recursion relation as

$$\begin{pmatrix} I_{n+1} \\ I_n \end{pmatrix} = \begin{pmatrix} a & -b^2 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} I_n \\ I_{n-1} \end{pmatrix} = \begin{pmatrix} a & -b^2 \\ 1 & 0 \end{pmatrix}^n \begin{pmatrix} I_1 \\ I_0 \end{pmatrix}$$

- diagonalize

$$\begin{pmatrix} a & -b^2 \\ 1 & 0 \end{pmatrix} = \mathcal{S} \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \mathcal{S}^{-1}$$

$$\lambda_\pm = \frac{1}{2}\left(a \pm \sqrt{a^2 - 4b^2}\right),$$

$$\mathcal{S} = \begin{pmatrix} \lambda_+ & \lambda_- \\ 1 & 1 \end{pmatrix} \quad \mathcal{S}^{-1} = \frac{1}{\lambda_+ - \lambda_-} \begin{pmatrix} 1 & -\lambda_- \\ -1 & \lambda_+ \end{pmatrix}$$

- then we have

$$\begin{pmatrix} I_{n+1} \\ I_n \end{pmatrix} = \mathcal{S} \begin{pmatrix} \lambda_+^n & 0 \\ 0 & \lambda_-^n \end{pmatrix} \mathcal{S}^{-1} \begin{pmatrix} a \\ 1 \end{pmatrix}$$

- thus

$$I_n = \det B_n = \frac{\lambda_+^{n+1} - \lambda_-^{n+1}}{\lambda_+ - \lambda_-} \qquad (\lambda_+ \neq \lambda_-)$$

Amplitude for simple harmonic oscillator

- using $\lambda_\pm = 1 \pm i\omega\epsilon + O(\epsilon^2)$ yields

$$\begin{aligned}
\lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \varepsilon \det M &= \lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \varepsilon \frac{1}{2i\omega\varepsilon}\Big((1+i\omega\varepsilon)^N - (1-i\omega\varepsilon)^N\Big) \\
&= \lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \frac{1}{2i\omega}\left(\left(1+\frac{i\omega T}{N}\right)^N - \left(1-\frac{i\omega T}{N}\right)^N\right) \\
&= \frac{1}{2i\omega}\left(e^{i\omega T} - e^{-i\omega T}\right) = \frac{\sin\omega T}{\omega}.
\end{aligned}$$

- final result for the path integral

$$S_{\rm cl} = \frac{m\omega}{2\sin(\omega T)}\Big[(x_a^2 + x_b^2)\cos(\omega T) - 2x_a x_b\Big]$$

Evolution of gaussian wave packet

- for initial wave packet at time $t_a = 0$ with probability dist.

$$|\phi(x_a, t_a)|^2 = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x_a - \bar{x})^2}{2\sigma^2}\right)$$

- probability amplitude at later time

$$\begin{aligned}\phi(x_b, t_b) &= \int_{-\infty}^{\infty} dx_a \; Z(b,a) \; \phi(x_a, 0) \\ &= \left(\frac{-im\omega(2\pi)^{-3/2}}{\hbar\sigma \sin(\omega t_b)}\right)^{1/2} \int_{-\infty}^{\infty} dx_a \; e^{iS_{\rm cl}/\hbar} \; e^{-(x_a - \bar{x})^2/(4\sigma^2)}\end{aligned}$$

- final result for probability distribution: Gaussian with width s

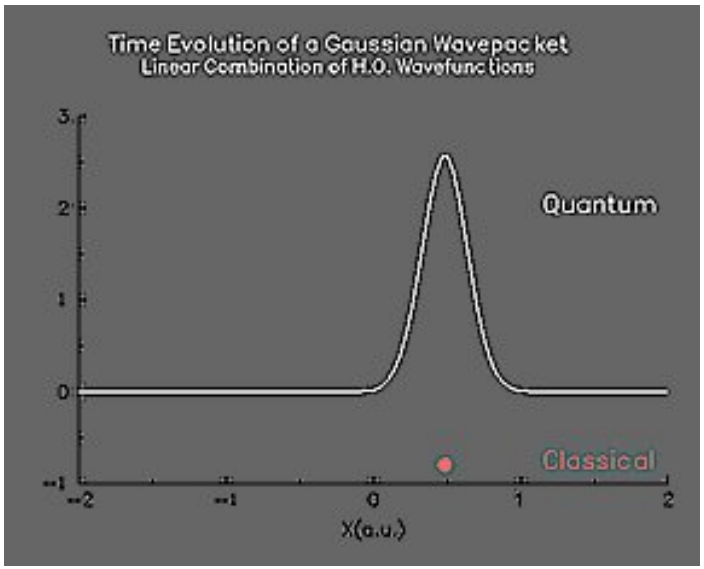
$$|\phi(x_b, t_b)|^2 = \frac{1}{s\sqrt{2\pi}} \exp\left(-\frac{(x_b - \bar{x}\cos(\omega t_b))^2}{2s^2}\right)$$

- new width given by

$$s = \sigma\left\{\cos^2(\omega t_b) + \frac{\hbar^2}{4m^2\omega^2\sigma^4} \sin^2(\omega t_b)\right\}^{1/2}$$

Visualization

- time evolution of a Gaussian wave packet for a simple harmonic oscillator



mass $m = 1\text{g/mol} = 1.66 \times 10^{-27}\text{kg}$
frequency $\omega = 3 \times 10^{14}\text{radians/sec}$
initial wave packet:
center at 0.5 au
RMS spread 0.14 au
1 au (atomic unit) = 0.529 angstrom
probability distribution shown
(in inverse a.u.)

- completely calculated using path integrals $\rightarrow$ did not use Schrodinger equation

Other probability amplitudes

- so path integrals give us simple transition amplitudes

$$\langle x_b(t_b)|x_a(t_a)\rangle = \int_a^b \mathcal{D}x \ \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\ L(x,\dot{x})\right\}$$

- but this important result generalizes to more complicated amplitudes

$$\begin{aligned} &\langle x_b(t_b)|\ x(t_2)\ x(t_1)\ |x_a(t_a)\rangle \\ = &\int_a^b \mathcal{D}x\ x(t_2)x(t_1)\ \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\ L(x,\dot{x})\right\} \end{aligned}$$

for $t_a < t_1 < t_2 < t_b$

Path integrals in imaginary time

- in imaginary time formalism, paths contribute to sum over histories with real exponential weights (not phases)

$$\begin{aligned} &\langle x_b(\tau_b)|\, x(\tau_2)\, x(\tau_1)\, |x_a(\tau_a)\rangle \\ = &\int_a^b \mathcal{D}x\, x(\tau_2)x(\tau_1)\, \exp\left\{-\frac{1}{\hbar}\int_{\tau_a}^{\tau_b} d\tau\, L(x,\dot{x})\right\} \end{aligned}$$

- classical path gets highest weighting
- note that weights are all real and positive since action is real
  - this fact will be crucial for the Monte Carlo method

Vacuum expectation values from path integrals

- obtain correlation functions (vacuum expectation values) from ratios of path integrals

$$\langle 0|x(t_2)x(t_1)|0\rangle = \lim_{T\to\infty} \frac{\langle x_b(T)|x(t_2)x(t_1)|x_a(-T)\rangle}{\langle x_b(T)|x_a(-T)\rangle}$$

$$= \frac{\int_a^b \mathcal{D}x\; x(t_2)x(t_1)\exp\left\{-\frac{1}{\hbar}\int_{-\infty}^{\infty} d\tau L(x,\dot{x})\right\}}{\int_a^b \mathcal{D}x\;\exp\left\{-\frac{1}{\hbar}\int_{-\infty}^{\infty} d\tau L(x,\dot{x})\right\}}$$

- generalizes to more complicated correlation functions
  - any correlation function can be computed using path integrals

Examples for the simple harmonic oscillator

- evaluating path integrals as before, the following correlation functions can be obtained $(\tau_1 \leq \tau_2 \leq \tau_3 \leq \tau_4)$

$$\begin{aligned}
\langle 0|x(\tau_1)|0\rangle &= 0 \\
\langle 0|x(\tau_2)x(\tau_1)|0\rangle &= \frac{\hbar}{2m\omega} e^{-\omega(\tau_2-\tau_1)} \\
\langle 0|x(\tau_4)x(\tau_3)x(\tau_2)x(\tau_1)|0\rangle &= \left(\frac{\hbar}{2m\omega}\right)^2 e^{-\omega(\tau_4-\tau_1)} \\
&\quad \times \left[e^{-\omega(\tau_2-\tau_3)} + 2e^{-\omega(\tau_3-\tau_2)}\right]
\end{aligned}$$

- comparison with spectral representation tells us

$$\langle 0|x(\tau)x(0)|0\rangle = \frac{\hbar}{2m\omega} e^{-\omega\tau}$$

$$\Rightarrow E_1 - E_0 = \hbar\omega \qquad |\langle 1|x(0)|0\rangle|^2 = \frac{\hbar}{2m\omega}$$

Another example in SHO

- excite vacuum with $x(\tau)^2$ operator

$$\langle 0|x^2(\tau)x^2(0)|0\rangle = \left(\frac{\hbar}{2m\omega}\right)^2 \left(1+2e^{-2\omega\tau}\right)$$

- compare with spectral representation at large time separations

$$\begin{aligned}\lim_{\tau\to\infty}\langle 0|x^2(\tau)x^2(0)|0\rangle &= |\langle 0|x^2(0)|0\rangle|^2 \\ &+ |\langle 2|x^2(0)|0\rangle|^2\, e^{-(E_2-E_0)t/\hbar} + \ldots \\ &= \left(\frac{\hbar}{2m\omega}\right)^2 \left(1+2e^{-2\omega\tau}\right)\end{aligned}$$

- interpretation:

$$E_2 - E_0 = 2\hbar\omega$$

$$|\langle 0|x^2(0)|0\rangle|^2 = \left(\frac{\hbar}{2m\omega}\right)^2 \qquad |\langle 2|x^2(0)|0\rangle|^2 = 2\left(\frac{\hbar}{2m\omega}\right)^2$$

One last example in SHO

- to determine expectation value of $x(0)^2$ in first-excited state

$$\langle 0|x(\tau)\, x^2(\tfrac{1}{2}\tau)\, x(0)|0\rangle = 3\left(\frac{\hbar}{2m\omega}\right)^2 e^{-\omega\tau}$$

- compare with spectral interpretation at large times

$$\lim_{\tau\to\infty}\langle 0|x(\tau)x^2(\tfrac{1}{2}\tau)x(0)|0\rangle$$
$$= |\langle 0|x(0)|1\rangle|^2\langle 1|x^2(0)|1\rangle\, e^{-(E_1-E_0)\tau/\hbar} + \cdots$$

  - since $\langle 0|x(0)|0\rangle = \langle 0|x(\tau)|0\rangle = 0$

- by inspection and using previously derived results

$$\langle 1|x^2(0)|1\rangle = \frac{3\hbar}{2m\omega}$$

Pause for reflection

- observables in quantum mechanics can be extracted from the correlation functions (vacuum expectation values)
- imaginary time formalism is a great trick for assisting in such extractions
- correlation functions can be computed via path integrals

$$\langle 0|x(t_2)x(t_1)|0\rangle = \frac{\int_a^b \mathcal{D}x\; x(t_2)x(t_1)\exp\left\{-\frac{1}{\hbar}\int_{-\infty}^{\infty} d\tau L(x,\dot{x})\right\}}{\int_a^b \mathcal{D}x\;\exp\left\{-\frac{1}{\hbar}\int_{-\infty}^{\infty} d\tau L(x,\dot{x})\right\}}$$

Part II

Monte Carlo integration and Markov chains

The die is cast?

- in rare situations, the path integrals can be computed exactly
  - simple harmonic oscillator, free particle
- sometimes the action can be written $S = S_0 + gS_I$
  - S_0 describes the free motion of the particles
  - path integrals using S_0 are Gaussian and can be exactly computed
  - S_I describes the interaction of the particles, but the coupling g is small
  - compute in perturbation theory as expansion in g
- however, if interactions are not weak
  - usually must resort to Monte Carlo methods
    - for example, quantum chromodynamics (QCD)

Simple Monte Carlo integration

- trapezoidal/Simpson's rule not feasible for integrals of very large dimension: too many function evaluations
- must start gambling!
- basic theorem of Monte Carlo integration

$$\int_V f(\vec{x})\, d^D x \approx V\langle f\rangle \pm V\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}}$$

$$\langle f\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i) \qquad \langle f^2\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i)^2$$

- N points $\vec{x}_1, \ldots, \vec{x}_N$ chosen independently and randomly with uniform probability dist. throughout D-dimensional volume V
- justified by the law of large numbers/central limit theorem
- in the limit $N \to \infty$, MC estimate tends to normal distribution, uncertainty tends to standard deviation

Quick review of probabilities

- consider an experiment whose outcome depends on chance
- represent an outcome by X called a random variable
- sample space Ω of experiment is set of all possible outcomes
- X is discrete if Ω is finite or countably infinite, continuous otherwise
- probability distribution for discrete X is real-valued function p_X on domain Ω satisfying $p_X(x) \geq 0$ for all $x \in \Omega$ and $\sum_{x \in \Omega} p_X(x) = 1$
- for any subset E of Ω, probability of E is $P(E) = \sum_{x \in E} p_X(x)$
- a sequence of random variables $X_1, X_2, \ldots, X_N$ that are mutually independent and have same distribution is called an independent trials process

Probability (continued)

- for continuous real-valued X, real-valued function p_X is a probability density and probability of outcome between real values a and b is $P(a \leq X \leq b) = \int_a^b p_X(s)ds$
- cumulative distribution is $F_X(x) = P(X \leq x) = \int_{-\infty}^{x} p_X(s)ds$
- common density: normal $p_X(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu)^2/(2\sigma^2)}$

Review: expected values

- expected value of X is
  $E(X) = \sum_{x \in \Omega} x\, p_X(x) \qquad \left(= \int_{-\infty}^{\infty} s\, p_X(s) ds \right)$
- properties: $E(X+Y) = E(X) + E(Y)$ and $E(cX) = cE(X)$
- for independent random variables X, Y have $E(XY) = E(X)E(Y)$
- can show $E(X)$ is average of outcomes if repeated many times
- for continuous real-valued function f, can show that

$$E(f(X)) = \sum_{x \in \Omega} f(x)\, p_X(x) \qquad \left(= \int_{-\infty}^{\infty} f(s)\, p_X(s)\, ds \right)$$

  - Proof: group together terms in $\sum_x f(x) p_X(x)$ having same $f(x)$ value
  - denote set of different $f(x)$ values by $\mathcal{F}$, and subset of Ω leading to same value of $f(x)$ by $\Omega_{f(x)}$, then

$$\sum_{x \in \Omega} f(x) p_X(x) = \sum_{y \in \mathcal{F}} \sum_{x \in \Omega_{f(x)}} f(x) p_X(x) = \sum_{y \in \mathcal{F}} y \left(\sum_{x \in \Omega_{f(x)}} p_X(x) \right)$$
$$= \sum_{y \in \mathcal{F}} y p(y) = E(f(x))$$

Review: variances

- variance of X is $V(X) = E(\ (X - E(X))^2\ )$
- standard deviation of X is $\sigma(X) = \sqrt{V(X)}$
- properties: $V(cX) = c^2 V(X)$ and $V(X + c) = V(X)$
- for independent random variables X, Y have
  $V(X + Y) = V(X) + V(Y)$ (exercise: prove this)
- let $X_1, \ldots, X_N$ be an independent trials process with $E(X_j) = \mu$ and $V(X_j) = \sigma^2$, and define $A_N = (X_1 + X_2 + \cdots + X_N)/N$, then can show $E(A_N) = \mu, \qquad V(A_N) = \sigma^2/N$

Chebyshev inequality

- Chebyshev inequality: Let X be a discrete random variable with $E(X) = \mu$ and let $\epsilon > 0$ be any positive real number, then

$$P(|X - \mu| \geq \epsilon) \leq \frac{V(X)}{\epsilon^2}$$

- Proof:
  - Let $p_X(x)$ denote distribution of X, then probability that X differs from μ by at least ϵ is $P(|X - \mu| \geq \epsilon) = \sum_{|x-\mu| \geq \epsilon} p_X(x)$
  - considering positive summands and the ranges of summation,

$$V(X) = \sum_x (x - \mu)^2 p_X(x) \geq \sum_{|x-\mu| \geq \epsilon} (x - \mu)^2 p_X(x) \geq \sum_{|x-\mu| \geq \epsilon} \epsilon^2 p_X(x)$$

  - but rightmost expression is

$$\epsilon^2 \sum_{|x-\mu| \geq \epsilon} p_X(x) = \epsilon^2 P(|X - \mu| \geq \epsilon)$$

  - thus, have shown $V(x) \geq \epsilon^2 P(|X - \mu| \geq \epsilon)$

Weak law of large numbers

- Weak law of large numbers: Let $X_1, X_2, \ldots, X_N$ be an independent trials process with $E(X_j) = \mu$ and $V(X_j) = \sigma^2$, where μ, σ are finite, and let $A_N = (X_1 + X_2 + \cdots + X_N)/N$. Then for any $\epsilon > 0$,

$$\lim_{N \to \infty} P(|A_N - \mu| \geq \epsilon) = 0, \qquad \lim_{N \to \infty} P(|A_N - \mu| < \epsilon) = 1$$

- Proof:
  - stated two slides ago that $E(A_N) = \mu$ and $V(A_N) = \sigma^2/N$
  - from Chebyshev inequality

$$P(|A_N - \mu| \geq \epsilon) \leq \frac{V(A_N)}{\epsilon^2} = \frac{\sigma^2}{N\epsilon^2} \overset{N \to \infty}{\longrightarrow} 0$$

- also known as the law of averages
- also applies to continuous random variables

Strong law of large numbers

- Strong law of large numbers: Let $X_1, X_2, \ldots, X_N$ be an independent trials process with $E(X_j) = \mu$ and $E(X_j^4) = K$, where μ, K are finite, then $P\left(\lim_{N\to\infty}(X_1 + X_2 + \cdots + X_N)/N = \mu\right) = 1$
- the finiteness of $E(X_j^4)$ is not needed, but simplifies proof
- Proof:
  - define $Y_j = X_j - \mu$ so $E(Y_j) = 0$ and set $E(Y_j^4) = C < \infty$
  - define $A_N = (Y_1 + Y_2 + \cdots + Y_N)/N$
  - given $E(Y_j) = 0$ and all Y_j are independent,
    $$N^4 E(A_N^4) = NE(Y_j^4) + 6\binom{n}{2}E(Y_i^2 Y_j^2) = NC + 3N(N-1)E(Y_i^2)^2$$
  - since $0 \le V(Y_j^2) = E(Y_j^4) - E(Y_j^2)^2$ then $E(Y_j^2)^2 \le E(Y_j^4) = C$
  - so $E(A_N^4) \le C/N^3 + 3C/N^2$ which means
    $$E(\textstyle\sum_{N=1}^{\infty} A_N^4) = \sum_{N=1}^{\infty} E(A_N^4) \le \sum_{N=1}^{\infty}\left(\frac{C}{N^3} + \frac{3C}{N^2}\right) < \infty$$
  - this implies $\sum_{N=1}^{\infty} A_N^4 < \infty$ with unit probability, and convergence of the series implies $\lim_{N\to\infty} A_N^4 = 0 \quad \Rightarrow \quad \lim_{N\to\infty} A_N = 0$
- proves $E(X)$ is average of outcomes for many repetitions

Application to one-dimensional integral

- if X is a random variable with probability density $p_X(x)$ and f is a well-behaved real-valued function, then $Y = f(X)$ is a random variable
- consider uniform density $p_X(x) = \begin{cases} 1/(b-a) & a \leq x \leq b \\ 0 & \text{otherwise} \end{cases}$
- use this probability density to obtain N outcomes $X_1, X_2, \ldots, X_n$
- apply function f to obtain random variables $Y_j = f(X_j)$
- law of large numbers tell us that

$$\frac{1}{N}\sum_{j=1}^{N} Y_j \overset{N\to\infty}{\longrightarrow} E(Y) = E(f(X)) = \frac{1}{(b-a)}\int_a^b f(s)ds$$

- define $\langle f \rangle \equiv \frac{1}{N}\sum_{j=1}^{N} f(X_j)$ then $(b-a)\lim_{N\to\infty}\langle f \rangle = \int_a^b f(s)ds$
- straightforward generalization to multiple dimensions
- how good is estimate for finite N?

Central limit theorem

- Central limit theorem: Let $X_1, X_2, \ldots, X_N$ be independent random variables with common distribution having $E(X_j) = \mu$ and $V(X_j) = \sigma^2$, where μ, σ are finite, and let $A_N = (X_1 + X_2 + \cdots + X_N)/N$. Then for $a < b$,

$$\lim_{N\to\infty} P\left(\frac{a\sigma}{\sqrt{N}} < (A_N - \mu) < \frac{b\sigma}{\sqrt{N}}\right) = \frac{1}{\sqrt{2\pi}} \int_a^b e^{-x^2/2} dx$$

- alternatively: the distribution of $(X_1 + \cdots + X_N - N\mu)/(\sigma\sqrt{N})$ tends to the standard normal (zero mean, unit variance)
- for proof, consult the literature
- for large N, the central limit theorem tells us that the error one makes in approximating $E(X)$ by A_N is $\sigma/\sqrt{N} = \sqrt{V(X)/N}$
- for $Y = f(X)$ as before, the error in approximating $E(f(X))$ by $\sum_j f(X_j)/N$ is $\sqrt{V(f(X))/N}$
- use Monte Carlo method to estimate $V(f(X))$

$$V(Y) = E((Y - E(Y))^2) \approx \langle (f - \langle f \rangle)^2 \rangle = \langle f^2 \rangle - \langle f \rangle^2$$

Monte Carlo integration

- recap of Monte Carlo integration:

$$\int_V f(\vec{x})\, d^D x \approx V\langle f\rangle \pm V\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}}$$

$$\langle f\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i) \qquad \langle f^2\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i)^2$$

- N points $\vec{x}_1, \ldots, \vec{x}_N$ chosen independently and randomly with uniform probability dist. throughout D-dimensional volume V
- law of large numbers justifies correctness of estimate
- central limit theorem gives estimate of statistical uncertainty
- in the limit $N \to \infty$, MC estimate tends to normal distribution, uncertainty tends to standard deviation

Pseudorandom number generators

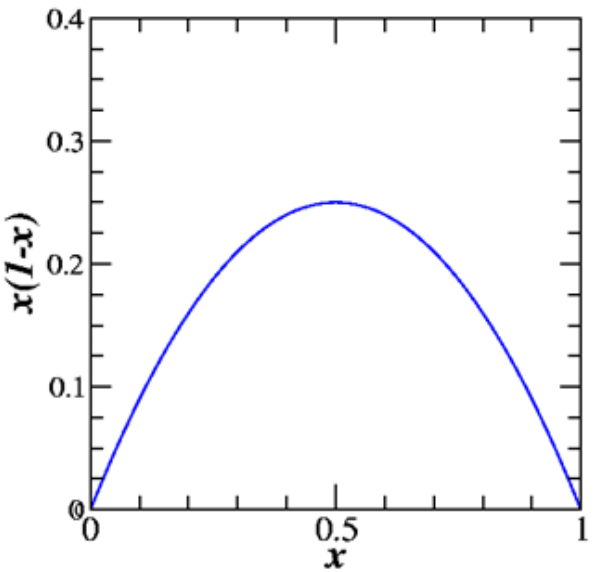
- MC integration requires random numbers
- but computers are deterministic!!
- clever algorithms can produce sequences of numbers which appear to be random (pseudorandom)
  - uniform deviates between 0 and 1
- example: the Mersenne twister
  - *http://www.math.sci.hiroshima-u.ac.jp/∼m-mat/MT/emt.html*
  - currently holds the record for longest period $2^{19937} - 1$
  - very fast, passes all standard tests (Diehard) for good RNG
- devising good RNGs is a science in itself
  - most utilize modulus function, bit shifting, shuffling

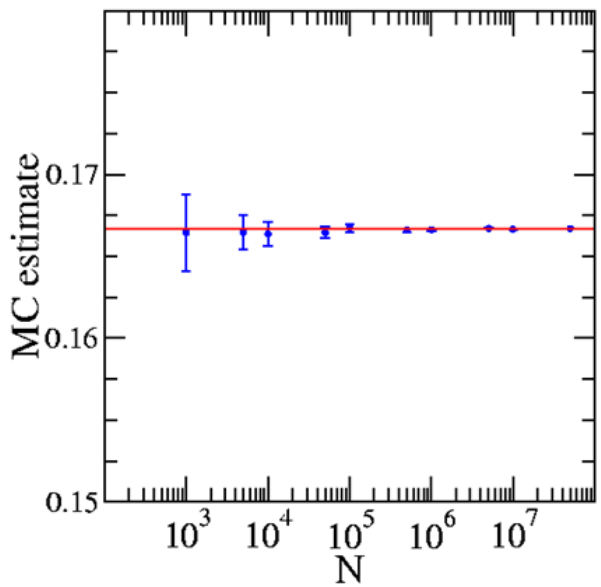
One-dimensional example

- simple example

$$\int_0^1 x(1-x)\,dx = \frac{1}{6} = 0.166666\cdots$$

- plot of integrand and some Monte Carlo estimates





- not efficient for 1-dim integrals!

Importance sampling

- Monte Carlo method works best for flat functions, problems when integrand sharply peaked
- importance sampling can greatly improve efficiency of Monte Carlo integration $\rightarrow$ variance reduction
- recall simple integration

$$\int_a^b f(x)\,dx \approx \frac{(b-a)}{N}\sum_{j=1}^{N} f(x_j)$$

x_j chosen with uniform probability between a and b

- choose function $g(x) > 0$ with $\int_a^b g(x)dx = 1$ so $h(x) = \frac{f(x)}{g(x)}$ is as close as possible to a constant

$$\int_a^b f(x)dx = \int_a^b h(x)g(x)dx \approx \frac{(b-a)}{N}\sum_{j=1}^{N} h(x_j)$$

where x_j now chosen with probability density $g(x)$

- must be able to sample with probability density $g(x)$
- how to choose $g(\vec{x})$ for complicated multi-dimensional integral?

Sampling non-uniform distributions

- random number generators sample the uniform distribution
- to sample other densities, apply transformation method
- random variable U with uniform density $p_U(u) = 1$ for $0 \leq x \leq 1$
- transform to new random variable $Y = \phi(U)$ where ϕ is a strictly increasing function
  - strictly increasing function ensures inverse function is single-valued
  - also ensures that if $u + du > u$ then $y + dy > y$ for $y = \phi(u)$
- what is density p_Y?
- from conservation of probability

$$p_Y(y)dy = p_U(u)du \qquad p_Y(y) = p_U(u)\frac{du}{dy} = p_U(\phi^{-1}(y))\frac{d\phi^{-1}(y)}{dy}$$

Sampling non-uniform distributions (continued)

- desired density p_Y is usually known, so must determine ϕ

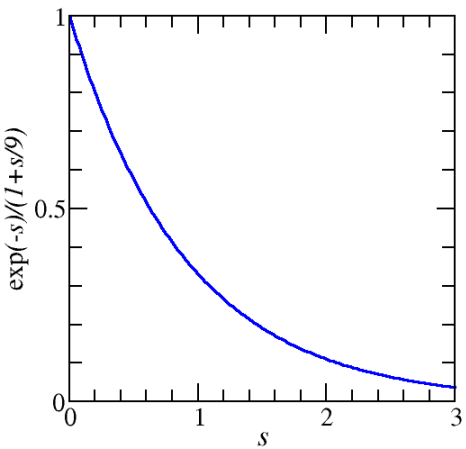
$$\int_0^u du' = \int_{\phi(0)}^{\phi(u)} p_Y(y)dy \quad \Rightarrow \quad u = F_Y(\phi(u)) \quad \Rightarrow \quad \phi(u) = F_Y^{-1}(u)$$

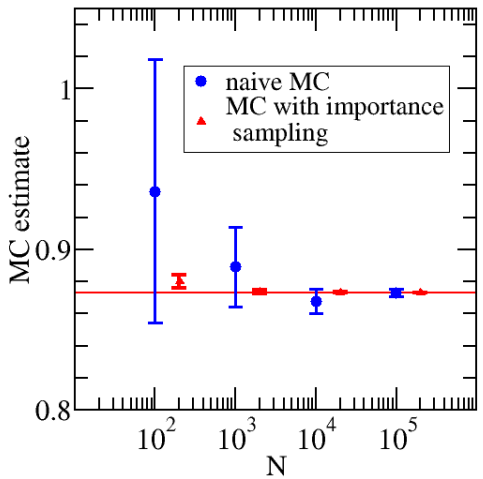
- F^{-1} unique since F is strictly increasing function
- summary: random variable Y with density $p_Y(y)$ and cumulative distribution $F_Y(y) = \int_{-\infty}^{y} p_Y(s)ds$ can be sampled by sampling with uniform deviate U then applying transformation

$$Y = F_Y^{-1}(U)$$

Exponential density

- transformation method requires density whose indefinite integral can be obtained and inverted
- method useful for only a handful of density functions
- one example: the exponential $p_Y(y) = e^{-y}/(1-e^{-b})$ for $0 \le y \le b$
  - cumulative distribution $F_Y(y) = \int_0^y p_Y(s)ds = (1-e^{-y})/(1-e^{-b})$
  - inverse $F_Y^{-1}(u) = -\ln\left(1-(1-e^{-b})u\right)$
- example integral: $\displaystyle\int_0^3 \frac{e^{-s}\,ds}{1+s/9} \approx 0.873109$



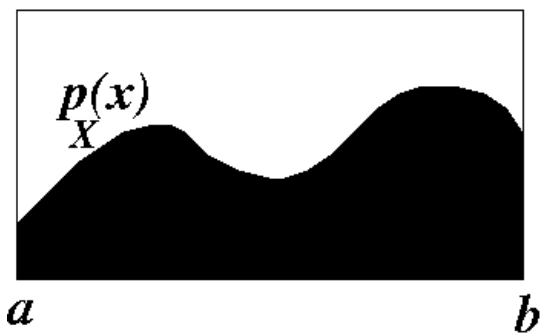


plot of integrand (left); dramatic improvement using importance sampling (right)

Rejection method

- can sample from probability density whose cumulative distribution is not easily calculable and invertible using the rejection method
- sampling from density $p_X(x)$ for $a \leq x \leq b$

  $\Rightarrow$ equivalent to choosing a random point in two dimensions with uniform probability in the area under curve $p_X(x)$
- simplest method: pick random point with uniform probability in box $a \leq x \leq b$ horizontally and $0 \leq y \leq \max(p_X(x))$ vertically
  - accept if below curve
  - reject if above curve, repeat until acceptance



- if $p_X(x)$ sharply peaked, use a comparison function $f(x)$ satisfying $f(x) \geq p_X(x)$ for all $a \leq x \leq b$ and which can be sampled by transformation method

Integrals of very high dimension

- sampling methods described so far work well in one-dimension
- for multi-dimensional integrals, transformation and rejection methods not feasible
- use of Markov chains to handle highly multi-dimensional integrals

А. А. Марков (1886).

- Markov chains were introduced by the Russian mathematician Andrei Markov (1856-1922) in 1906

Markov chains

- discrete Markov chain: stochastic process which generates a sequence of states with probabilities depending only on current state
  - consider a system which can be in one of R states $s_1, s_2, \ldots, s_R$
  - system moves successively from one state to another
  - each move is called a step (discrete "time")
  - if current state is s_i, then chain moves to state s_j at next step with probability p_{ij} which does not depend on previous states of chain
  - probabilities p_{ij} are called transition probabilities
  - the square $R \times R$ real-valued matrix $\mathbf{P}$ whose elements are p_{ij} is called the transition matrix or the Markov matrix
- time homogeneous if transition probabilities p_{ij} independent of "time" or position in chain
- definition generalizes to continuous set of states
  - leads to matrix of transition densities
- will not deal with continuous-time chains here

Some basic properties of Markov chains

- transition matrix $\mathbf{P}$ has non-negative entries $p_{ij} \geq 0$
- since probability of going from s_i to any state must be unity, then matrix elements must satisfy $\sum_{j=1}^{R} p_{ij} = 1$ (rows sum to unity)
- if columns also sum to unity, $\mathbf{P}$ is called doubly stochastic matrix
- if $\mathbf{P}_1$ and $\mathbf{P}_2$ are Markov matrices, then the matrix product $\mathbf{P}_1\mathbf{P}_2$ is also a Markov matrix
- every eigenvalue λ of a Markov matrix satisfies $|\lambda| \leq 1$
- every Markov matrix has at least one eigenvalue equal to unity

Eigenvalues/eigenvectors of real square matrices

- for a square matrix $\mathbf{P}$, a nonzero column vector $\mathbf{v}$ which satisfies $\mathbf{P}\mathbf{v} = \lambda\mathbf{v}$ for complex scalar λ is known as a right eigenvector corresponding to eigenvalue λ
  - often, “right eigenvectors" are simply called “eigenvectors"
- a nonzero vector $\mathbf{v}$ satisfying $\mathbf{v}^T\mathbf{P} = \lambda\mathbf{v}^T$, where T indicates transpose, is known as a left eigenvector
- every square $R \times R$ matrix has R complex eigenvalues, counting multiple roots according to their multiplicity
- for a real square matrix, the eigenvalues are either real or come in complex conjugate pairs
- eigenvectors for distinct eigenvalues are linearly independent
- a degenerate eigenvalue may not have distinct eigenvectors
- R linearly independent eigenvectors guaranteed only if all R eigenvalues distinct
- a matrix $\mathbf{P}$ and its transpose $\mathbf{P}^T$ have the same eigenvalues

Properties of Markov matrices (continued)

- every eigenvalue λ of Markov matrix $\mathbf{P}$ satisfies $|\lambda| \leq 1$
  - Proof: suppose complex number λ is an eigenvalue of $\mathbf{P}$ with corresponding eigenvector $\mathbf{v}$ so that $\mathbf{P}\mathbf{v} = \lambda\mathbf{v}$
  - let k be such that $|v_k| \geq |v_j|$ for all j
  - k-th component of eigenvalue equation gives us $\sum_j p_{kj} v_j = \lambda v_k$
  - use generalized triangle inequality for complex numbers $|\sum_k z_k| \leq \sum_k |z_k|$ to show
    $$|\lambda v_k| = |\sum_j p_{kj} v_j| \leq \sum_j p_{kj} |v_j| \leq \sum_j p_{kj} |v_k| = |v_k|$$
  - thus, $|\lambda v_k| = |\lambda||v_k| \leq |v_k| \quad \rightarrow \quad |\lambda| \leq 1$
- every Markov matrix $\mathbf{P}$ has a least one eigenvalue equal to unity
  - Proof: let $\mathbf{v}$ be a vector satisfying $v_j = 1$ for all j
  - then $\sum_j p_{ij} v_j = \sum_j p_{ij} = 1 = v_i$
  - hence, $\mathbf{v}$ is an eigenvector corresponding to eigenvalue 1

Multi-step probabilities

- n-step transition probability: ij-th element $p_{ij}^{(n)}$ of matrix $\mathbf{P}^n$ is probability that Markov chain, starting in state s_i, will be in state s_j after n steps
  - probability to go from s_i to s_j in 2 steps is $\sum_{k=1}^{R} p_{ik}p_{kj}$
  - generalizes to n-steps
- for starting probability vector $\mathbf{u}$, probability that chain in state s_j after n steps is $u_j^{(n)} = \sum_{i=1}^{R} u_i p_{ij}^{(n)}$
  - u_i is probability starting state is s_i, matrix form $\mathbf{u}^{(n)T} = \mathbf{u}^T\mathbf{P}^n$
- first visit probability: the probability that a Markov chain, starting in state s_i, is found for the first time in state s_j after n steps $\rightarrow$ denoted by $f_{ij}^{(n)}$
  - define $f_{ij}^{(0)} = 0$ one step, $f_{ij}^{(1)} = p_{ij}$, two steps, $f_{ij}^{(2)} = \sum_{k\neq j} p_{ik}p_{kj}$
  - generalize $f_{ij}^{(n)} = \sum_{k\neq j} p_{ik}\, f_{kj}^{(n-1)}$
- important relation for later user: $p_{ij}^{(n)} = \sum_{m=1}^{n} f_{ij}^{(m)} p_{jj}^{(n-m)}$

Mean first passage and mean recurrence times

- total visit probability: probability that, starting from state s_i, chain will ever visit state s_j:
$$f_{ij} = \sum_{n=1}^{\infty} f_{ij}^{(n)}$$
- mean first passage time from s_i to s_j is expected number of steps to reach state s_j in an ergodic Markov chain for the first time, starting from state $s_i \rightarrow$ denoted by m_{ij} (by convention, $m_{ii} = 0$)
$$m_{ij} = \sum_{n=1}^{\infty} n\, f_{ij}^{(n)}$$
- mean recurrence time μ_i of state s_i is expected number of steps to return to state s_i for the first time in an ergodic Markov chain starting from s_i
$$\mu_i = \sum_{n=1}^{\infty} n\, f_{ii}^{(n)}$$

Classes

- state s_j is accessible from state s_i if $p_{ij}^{(n)} > 0$ for some finite n
  - often denoted by $s_i \longrightarrow s_j$
  - if $s_i \longrightarrow s_j$ and $s_j \longrightarrow s_k$, then $s_i \longrightarrow s_k$
- states s_i and s_j communicate if $s_i \longrightarrow s_j$ and $s_j \longrightarrow s_i$
  - denoted by $s_i \longleftrightarrow s_j$
  - $s_i \longleftrightarrow s_j$ and $s_j \longleftrightarrow s_k$ implies $s_i \longleftrightarrow s_k$
- class = a set of states that all communicate with one another
- if C_1 and C_2 are communicating classes, then either $C_1 = C_2$ or C_1, C_2 are disjoint
  - if C_1 and C_2 have a common state s_i, then $s_i \longleftrightarrow s_{j1}$ for all $s_{j1} \in C_1$ and $s_i \longleftrightarrow s_{j2}$ for all $s_{j2} \in C_2$, so $s_{j1} \longleftrightarrow s_{j2}$ implying $C_1 = C_2$
- set of all states can be partitioned into separate classes
  - if transition from class C_1 to different class C_2 is possible, then transition from C_2 to C_1 not possible, otherwise $C_1 = C_2$

Irreducible Markov chains

- a Markov chain is called irreducible if the probability to go from every state to every state (not necessarily in one step) is greater than zero
- all states in irreducible chain are in one single communicating class

Classification of states in Markov chains

- states in a Markov chain are
  - (a) recurrent (persistent) or transient
    - recurrent states are either positive or null
  - (b) periodic (cyclic) or aperiodic
- recurrent or persistent state has $f_{ii} = \sum_{n=1}^{\infty} f_{ii}^{(n)} = 1$
  - unit probability of returning to state after a finite length

  transient state has $f_{ii} = \sum_{n=1}^{\infty} f_{ii}^{(n)} < 1$
- recurrent state is positive if mean recurrence time finite $\mu_i < \infty$

  otherwise, called null
- the period of a state in a Markov chain is the greatest common divisor of all $n \geq 0$ for which $p_{ii}^{(n)} > 0$
  - transition s_i to s_i not possible except for multiples of period $d(i)$
- periodic state s_i has period $d(i) > 1$

  aperiodic state s_i has period $d(i) = 1$

Recurrent and transient states

- for a recurrent state, $\sum_{n=1}^{\infty} p_{ii}^{(n)} = \infty$, whereas

  for a transient state, $\sum_{n=1}^{\infty} p_{ii}^{(n)} < \infty$
- proof:
  - we start with the following:

$$\sum_{n=1}^{N} p_{ij}^{(n)} = \sum_{n=1}^{N} \sum_{m=1}^{n} f_{ij}^{(m)} p_{jj}^{(n-m)} = \sum_{m=1}^{N} f_{ij}^{(m)} \sum_{n=0}^{N-m} p_{jj}^{(n)} \leq \sum_{m=1}^{N} f_{ij}^{(m)} \sum_{n=0}^{N} p_{jj}^{(n)}$$

  - but for $N > N'$ we also have

$$\sum_{n=1}^{N} p_{ij}^{(n)} = \sum_{m=1}^{N} f_{ij}^{(m)} \sum_{n=0}^{N-m} p_{jj}^{(n)} \geq \sum_{m=1}^{N'} f_{ij}^{(m)} \sum_{n=0}^{N-m} p_{jj}^{(n)} \geq \sum_{m=1}^{N'} f_{ij}^{(m)} \sum_{n=0}^{N-N'} p_{jj}^{(n)}$$

  - putting together above results:

$$\sum_{m=1}^{N'} f_{ij}^{(m)} \sum_{n=0}^{N-N'} p_{jj}^{(n)} \leq \sum_{n=1}^{N} p_{ij}^{(n)} \leq \sum_{m=1}^{N} f_{ij}^{(m)} \sum_{n=0}^{N} p_{jj}^{(n)}$$

  - take $N \to \infty$ first, then $N' \to \infty$ to get

$$f_{ij} \sum_{n=0}^{\infty} p_{jj}^{(n)} \leq \sum_{n=1}^{\infty} p_{ij}^{(n)} \leq f_{ij} \sum_{n=0}^{\infty} p_{jj}^{(n)} \quad \Rightarrow \quad f_{ij} \sum_{n=0}^{\infty} p_{jj}^{(n)} = \sum_{n=1}^{\infty} p_{ij}^{(n)}$$

Recurrent and transient states (continued)

- for a recurrent state, $\sum_{n=1}^{\infty} p_{ii}^{(n)} = \infty$, whereas

  for a transient state, $\sum_{n=1}^{\infty} p_{ii}^{(n)} < \infty$
- proof (continued):
  - so far have shown $f_{ij} \sum_{n=0}^{\infty} p_{jj}^{(n)} = \sum_{n=1}^{\infty} p_{ij}^{(n)}$
  - set $i = j$ then $f_{ii}(1 + \sum_{n=1}^{\infty} p_{ii}^{(n)}) = \sum_{n=1}^{\infty} p_{ii}^{(n)}$
  - so finally
    $$\sum_{n=1}^{\infty} p_{ii}^{(n)} = \frac{f_{ii}}{1 - f_{ii}}$$
  - $f_{ii} = 1$ for a recurrent state and $f_{ii} < 1$ for a transient state, which proves the above statements
- note that the above results also imply
  $$\sum_{n=1}^{\infty} p_{ij}^{(n)} = \frac{f_{ij}}{1 - f_{ii}}$$

Recurrent and transient states (furthermore)

- a Markov chain returns to a recurrent state infinitely often and returns to a transient state only a finite number of times
- proof:
  - let $g_{ij}(m)$ denote probability that chain enters state s_j at least m times, starting from s_i
  - clearly $g_{ij}(1) = f_{ij}$
  - one also sees $g_{ij}(m+1) = f_{ij} g_{jj}(m)$ so $g_{ij}(m) = (f_{ij})^m$
  - probability of entering s_j infinitely many times is $g_{ij} = \lim_{m\to\infty} g_{ij}(m) = \lim_{m\to\infty} (f_{ij})^m$
  - so starting in s_j then

$$g_{jj} = \lim_{m\to\infty} (f_{jj})^m = \begin{cases} 1 & \text{for recurrent state } f_{jj} = 1 \\ 0 & \text{for transient state } f_{jj} < 1 \end{cases}$$

A crucial theorem about two sequences

- important theorem: (the basic limit theorem)
  given a sequence $f_0, f_1, f_2, \ldots$ such that
  $$f_0 = 0, \qquad f_n \geq 0, \qquad \sum_{n=0}^{\infty} f_n = 1$$
  and greatest common divisor of those n for which $f_n > 0$ is $d \geq 1$
  and another sequence $u_0, u_1, u_2, \ldots$ defined by
  $$u_0 = 1, \qquad u_n = \sum_{m=1}^{n} f_m u_{n-m} \quad (n \geq 1)$$
  then
  $$\lim_{n\to\infty} u_{nd} = \begin{cases} d\mu^{-1} & \text{if } \mu = \sum_{n=1}^{\infty} n f_n < \infty \\ 0 & \text{if } \mu = \infty \end{cases}$$
- proof:
  - that will cost extra! please upgrade to the premium lectures

Asymptotic behavior of $p_{jj}^{(n)}$

- asymptotic behavior of $p_{jj}^{(n)}$ can be summarized as

$$\lim_{n\to\infty} p_{jj}^{(dn)} = \begin{cases} 0 & s_j \text{ transient or null recurrent} \\ \mu_j^{-1} & s_j \text{ aperiodic positive recurrent} \\ d\mu_j^{-1} & s_j \text{ positive recurrent with period } d \end{cases}$$

- proof:
  - if s_j transient, $\sum_n p_{jj}^{(n)}$ finite (converges) requiring $p_{jj}^{(n)} \to 0$
  - for recurrent s_j, let $f_n = f_{jj}^{(n)}$ and $u_n = p_{jj}^{(n)}$
  - sequences f_n, u_n so defined satisfy conditions of basic limit theorem
  - basic limit theorem gives $p_{jj}^{(dn)} \to d\mu_j^{-1}$ where $\mu_j = \sum_n n f_{jj}^{(n)}$ is mean recurrence time
  - aperiodic case when $d = 1$
  - null recurrent s_j has $\mu_j = \infty$ so $p_{jj}^{(n)} \to \mu_j^{-1} = 0$

Asymptotic behavior of $p_{ij}^{(n)}$

- asymptotic behavior of $p_{ij}^{(n)}$ can be summarized as

$$\lim_{n\to\infty} p_{ij}^{(n)} = \begin{cases} 0 & s_j \text{ transient or null recurrent} \\ f_{ij}\mu_j^{-1} & s_j \text{ aperiodic positive recurrent} \end{cases}$$

- ignore periodic case here
- proof:
  - $p_{ij}^{(n)} = \sum_{m=1}^{n} f_{ij}^{(m)} p_{jj}^{(n-m)} = \sum_{m=1}^{n'} f_{ij}^{(m)} p_{jj}^{(n-m)} + \sum_{m=n'+1}^{n} f_{ij}^{(m)} p_{jj}^{(n-m)} \quad (n' < n)$
  - since $0 \le \sum_{m=n'+1}^{n} f_{ij}^{(m)} p_{jj}^{(n-m)} \le \sum_{m=n'+1}^{n} f_{ij}^{(m)}$ then

$$0 \le \left(p_{ij}^{(n)} - \sum_{m=1}^{n'} f_{ij}^{(m)} p_{jj}^{(n-m)} \right) \le \sum_{m=n'+1}^{n} f_{ij}^{(m)} \quad (n' < n)$$

  - take $n \to \infty$, then $n' \to \infty$ above, denote $p_{jj} = \lim_{n\to\infty} p_{jj}^{(n)}$

$$0 \le \left(\lim_{n\to\infty} p_{ij}^{(n)} - p_{jj} f_{ij} \right) \le 0 \quad \Rightarrow \quad \lim_{n\to\infty} p_{ij}^{(n)} = p_{jj} f_{ij}$$

  - for s_j transient or null recurrent, $p_{jj} = 0$ and f_{ij} finite, so $\lim_{n\to\infty} p_{ij}^{(n)} = 0$
  - for s_j aperiod positive recurrent, $p_{jj} = \mu_j^{-1}$ so $p_{ij}^{(n)} \to f_{ij}\mu_j^{-1}$

Important result for recurrent states

- if s_i is recurrent and $s_i \rightarrow s_j$, then $f_{ji} = 1$
- proof:
  - let $\alpha > 0$ denote probability to reach s_j from s_i without previously returning to s_i
  - probability of never returning to s_i from s_j is $1 - f_{ji}$
  - probability of never returning to s_i from s_i is at least $\alpha(1 - f_{ji})$
  - but s_i is recurrent so probability of no return is zero
  - thus, $f_{ji} = 1$
- for two communicating states $s_i \leftrightarrow s_j$ that are each recurrent, it follows that $f_{ij} = f_{ji} = 1$

Similarity of states in a class

- all states in a class of a Markov chain are of the same type, and if periodic, all have the same period
- proof:
  - for any two states s_i and s_j in a class, there exists integers r and s such that $p_{ij}^{(r)} = \alpha > 0$ and $p_{ji}^{(s)} = \beta > 0$ so
    $$p_{ii}^{(n+r+s)} = \sum_{kl} p_{ik}^{(r)} p_{kl}^{(n)} p_{li}^{(s)} \geq \sum_{k} p_{ik}^{(r)} p_{kk}^{(n)} p_{ki}^{(s)} \geq p_{ij}^{(r)} p_{jj}^{(n)} p_{ji}^{(s)} = \alpha\beta p_{jj}^{(n)}$$
  - suppose s_i has period t, then for $n = 0$, the right-hand side is positive, so $p_{ii}^{(r+s)} > 0$ which means that $r + s$ must be a multiple of t
  - hence, left-hand side vanishes unless n is multiple of t, so $p_{jj}^{(n)}$ can be nonzero only if n is multiple of t, so s_i and s_j have same period
  - if s_i is transient, then left-hand side is a term of a convergent series, so the same is true for $p_{jj}^{(n)}$, and if $p_{ii}^{(n)} \to 0$, then $p_{jj}^{(n)} \to 0$
  - the same statements remain true if the roles of i and j are reversed, so either both s_i and s_j are transient, or neither is; also, if one is a null state, then so is the other
- chain aperiodic if $p_{ii} > 0$ for at least one s_i

Fact concerning finite Markov chains

- in an irreducible chain having finite number R of states, there are no null states and it is impossible that all states are transient
- proof:
  - all rows of the matrix $\mathbf{P}^n$ must add to unity
  - since each row contains finite number of non-negative elements, it is impossible that $p_{ij}^{(n)} \to 0$ for all i, j pairs
  - thus, impossible that all states are transient
  - so at least one state must be non-null
  - but since irreducible (one class), all states must be non-null
- in an R-state irreducible Markov chain, it is possible to go from any state to any other state in at most $R - 1$ steps

Fixed-point or stationary distributions

- a probability vector $\mathbf{w}$ is called stationary or invariant or a fixed-point if $\mathbf{w}^T = \mathbf{w}^T\mathbf{P}$
- clearly, one also has $\mathbf{w}^T = \mathbf{w}^T\mathbf{P}^n$
- the probability vector is always the same (stationary) for the chain
- when this occurs, the Markov chain is said to be in equilibrium

Fatou's lemma

- lemma: let $a_n(t)$ for $n = 1, 2, \ldots$ be a function on a discrete set $T = \{1, 2, \ldots\}$, assume $\lim_{n\to\infty} a_n(t)$ exists for each t in T, and suppose $a_n(t) \geq 0$ for all t, n, then

$$\sum_{t\in T} \left(\lim_{n\to\infty} a_n(t) \right) \leq \lim_{n\to\infty} \sum_{t\in T} a_n(t)$$

- proof:
  - for any integer M

$$\sum_{t=1}^{M} \left(\lim_{n\to\infty} a_n(t) \right) = \lim_{n\to\infty} \sum_{t=1}^{M} a_n(t) \leq \lim_{n\to\infty} \sum_{t=1}^{\infty} a_n(t)$$

    since all $a_n(t) \geq 0$
  - take limit $M \to \infty$ to obtain required result
- example: $a_n(t) = \dfrac{n}{n^2 + t^2}$
  - for $n > t$ then $\lim_{n\to\infty} a_n(t) = 0$ so $\sum_{t=1}^{\infty} \left(\lim_{n\to\infty} a_n(t) \right) = 0$
  - $\sum_{t=1}^{\infty} a_n(t) = \dfrac{\pi}{2} \coth(n\pi) - \dfrac{1}{2n}$ so $\lim_{n\to\infty} \sum_{t=1}^{\infty} a_n(t) = \dfrac{\pi}{2}$

Dominated convergence theorem

- theorem: let $a_n(t)$ for $n = 1, 2, \ldots$ be a function on a discrete set $T = \{1, 2, \ldots\}$, assume $\lim_{n\to\infty} a_n(t)$ exists for each t in T, and suppose a function $B(t)$ exists such that $|a_n(t)| \leq B(t)$ for all t, n and $\sum_{t\in T} B(t) < \infty$, then

$$\sum_{t\in T} \left(\lim_{n\to\infty} a_n(t) \right) = \lim_{n\to\infty} \sum_{t\in T} a_n(t)$$

- proof:
  - let $a(t) = \lim_{n\to\infty} a_n(t)$ and since $|a(t)| \leq B(t)$ then $\sum_{t=1}^{\infty} a(t)$ converges
  - for any integer M

$$\left| \sum_{t=1}^{\infty} a_n(t) - \sum_{t=1}^{\infty} a(t) \right| \leq \sum_{t=1}^{M} |a_n(t) - a(t)| + \sum_{t=M+1}^{\infty} \left(|a_n(t)| + |a(t)| \right)$$

  - now $\lim_{n\to\infty} \sum_{t=1}^{M} |a_n(t) - a(t)| = \sum_{t=1}^{M} \left(\lim_{n\to\infty} |a_n(t) - a(t)| \right) = 0$

$$\sum_{t=M+1}^{\infty} \left(|a_n(t)| + |a(t)| \right) \leq 2 \sum_{t=M+1}^{\infty} B(t)$$

  - so for any integer M

$$\left| \lim_{n\to\infty} \sum_{t=1}^{\infty} a_n(t) - \sum_{t=1}^{\infty} \lim_{n\to\infty} a_n(t) \right| \leq 2 \sum_{t=M+1}^{\infty} B(t)$$

  - right-hand side is remainder of convergent series so equals zero in $M \to \infty$ limit

Fundamental limit theorem for ergodic Markov chains

- Theorem: an irreducible aperiodic Markov chain with transition matrix $\mathbf{P}$ has a stationary distribution $\mathbf{w}$ satisfying $w_j > 0$, $\sum_j w_j = 1$, and $\mathbf{w}^T = \mathbf{w}^T\mathbf{P}$ if, and only if, all its states are positive recurrent, and this stationary distribution is unique and identical to the limiting distribution $w_j = \lim_{n\to\infty} p_{ij}^{(n)}$ independent of initial state s_i
- Proof:
  - for irreducible aperiodic chain, the following possibilities exist:
    (a) all states are positive recurrent
    (b) all states are null recurrent
    (c) all states are transient
  - if all states transient or null recurrent, $\lim_{n\to\infty} p_{ij}^{(n)} = 0$
  - if all states positive recurrent, then since all states communicate, $f_{ij} = 1$ for all i, j and previous result becomes $\lim_{n\to\infty} p_{ij}^{(n)} = \mu_j^{-1}$
  - can define $w_j = \lim_{n\to\infty} p_{ij}^{(n)}$ which is independent of initial state s_i
  - for all states positive recurrent, then $0 < \mu_j < \infty$ so $w_j > 0$ for all j

Fundamental limit theorem (2)

- Theorem: an irreducible aperiodic Markov chain with transition matrix $\mathbf{P}$ has a stationary distribution $\mathbf{w}$ satisfying $w_j > 0$, $\sum_j w_j = 1$, and $\mathbf{w}^T = \mathbf{w}^T\mathbf{P}$ if, and only if, all its states are positive recurrent, and this stationary distribution is unique and identical to the limiting distribution $w_j = \lim_{n\to\infty} p_{ij}^{(n)}$ independent of initial state s_i
- Proof (continued):
  - we have $p_{ij}^{(m+n)} = \sum_{k=1}^{\infty} p_{ik}^{(n)} p_{kj}^{(m)}$ so using Fatou's lemma:
    $$\lim_{n\to\infty} p_{ij}^{(m+n)} = \lim_{n\to\infty} \sum_{k=1}^{\infty} p_{ik}^{(n)} p_{kj}^{(m)} \geq \sum_{k=1}^{\infty} \lim_{n\to\infty} p_{ik}^{(n)} p_{kj}^{(m)}$$
  - taking the limit $n \to \infty$ yields $w_j \geq \sum_{k=1}^{\infty} w_k \, p_{kj}^{(m)}$
  - define $s \equiv \sum_{k=1}^{\infty} w_k$ then sum above equation over j:
    $$s = \sum_{j=1}^{\infty} w_j \geq \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} w_k \, p_{kj}^{(m)} = \sum_{k=1}^{\infty} w_k \sum_{j=1}^{\infty} p_{kj}^{(m)} = \sum_{k=1}^{\infty} w_k = s$$
    interchanging order of the two infinite summations is possible since all summands non-negative (Fubini's theorem)
  - since $s \geq s$, equality must hold for all j: $$w_j = \sum_{k=1}^{\infty} w_k \, p_{kj}^{(m)}$$

Fundamental limit theorem (3)

- Theorem: an irreducible aperiodic Markov chain with transition matrix $\mathbf{P}$ has a stationary distribution $\mathbf{w}$ satisfying $w_j > 0$, $\sum_j w_j = 1$, and $\mathbf{w}^T = \mathbf{w}^T\mathbf{P}$ if, and only if, all its states are positive recurrent, and this stationary distribution is unique and identical to the limiting distribution $w_j = \lim_{n\to\infty} p_{ij}^{(n)}$ independent of initial state s_i
- Proof (continued):
  - have shown $w_j = \sum_{k=1}^{\infty} w_k\, p_{kj}^{(m)}$
  - for $m = 1$, we see the limiting vector $\mathbf{w}$ is stationary!!
  - next, from $\sum_{j=1}^{\infty} p_{ij}^{(n)} = 1$ then use Fatou:
    $$1 = \lim_{n\to\infty} \sum_{j=1}^{\infty} p_{ij}^{(n)} \geq \sum_{j=1}^{\infty} \lim_{n\to\infty} p_{ij}^{(n)} = \sum_{j=1}^{\infty} w_j$$
  - given $\sum_j w_j \leq 1$ then consider the limit $m \to \infty$ of
    $$w_j = \lim_{m\to\infty} \sum_{k=1}^{\infty} w_k\, p_{kj}^{(m)}$$
  - since $0 \leq p_{kj}^{(m)} \leq 1$ then $|w_k p_{kj}^{(m)}| \leq w_k$ and $\sum_{k=1}^{\infty} w_k < \infty$ so the dominated convergence theorem can be applied
    $$w_j = \lim_{m\to\infty} \sum_{k=1}^{\infty} w_k\, p_{kj}^{(m)} = \sum_{k=1}^{\infty} w_k \lim_{m\to\infty} p_{kj}^{(m)} = \left(\sum_{k=1}^{\infty} w_k\right) w_j$$
  - can at last conclude $\sum_{j=1}^{\infty} w_j = 1$

Fundamental limit theorem (4)

- Theorem: an irreducible aperiodic Markov chain with transition matrix $\mathbf{P}$ has a stationary distribution $\mathbf{w}$ satisfying $w_j > 0$, $\sum_j w_j = 1$, and $\mathbf{w}^T = \mathbf{w}^T\mathbf{P}$ if, and only if, all its states are positive recurrent, and this stationary distribution is unique and identical to the limiting distribution $w_j = \lim_{n\to\infty} p_{ij}^{(n)}$ independent of initial state s_i
- Proof (continued):
  - only uniqueness of stationary state to show
  - if another stationary vector $\mathbf{v}$ existed, it would have to satisfy $v_j > 0$, $\sum_{j=1}^{\infty} v_j = 1$, and $v_j = \sum_{i=1}^{\infty} v_i p_{ij}^{(n)}$
  - conditions for dominated convergence theorem again apply, so taking $n \to \infty$ limit gives

$$v_j = \lim_{n\to\infty} \sum_{i=1}^{\infty} v_i p_{ij}^{(n)} = \sum_{i=1}^{\infty} v_i \lim_{n\to\infty} p_{ij}^{(n)} = \left(\sum_{i=1}^{\infty} v_i\right) w_j = w_j$$

  - since $\mathbf{v} = \mathbf{w}$, then $\mathbf{w}$ is unique

An example

- consider the following transition matrix $\mathbf{P} = \begin{bmatrix} \frac{3}{4} & \frac{1}{4} & 0 \\ 0 & \frac{2}{3} & \frac{1}{3} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{bmatrix}$
- $\mathbf{P}^2$ all positive entries, so chain is irreducible
- eigenvalues are $1, \frac{1}{2}, \frac{5}{12}$
- right and left eigenvectors (unnormalized) are

$$\text{right:} \quad \overset{1}{\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}} \quad \overset{\frac{1}{2}}{\begin{bmatrix} 2 \\ -2 \\ 1 \end{bmatrix}} \quad \overset{\frac{5}{12}}{\begin{bmatrix} 3 \\ -4 \\ 3 \end{bmatrix}} \qquad \text{left:} \quad \overset{1}{\begin{bmatrix} 2 \\ 3 \\ 2 \end{bmatrix}} \quad \overset{\frac{1}{2}}{\begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}} \quad \overset{\frac{5}{12}}{\begin{bmatrix} -3 \\ -1 \\ 4 \end{bmatrix}}$$

- left fixed-point probability vector

$$\mathbf{w} = \frac{1}{7} \begin{bmatrix} 2 \\ 3 \\ 2 \end{bmatrix} \qquad \lim_{n \to \infty} \mathbf{P}^n = \mathbf{W} = \frac{1}{7} \begin{bmatrix} 2 & 3 & 2 \\ 2 & 3 & 2 \\ 2 & 3 & 2 \end{bmatrix}$$

Summary of results

- positive recurrent chain guarantees existence of at least one invariant probability vector
- irreducibility guarantees uniqueness of invariant probability vector
- aperiodicity guarantees limit distribution coincides with invariant distribution

Equilibrium in Markov chains

- suppose a Markov chain is started with probability vector given by $\mathbf{w}$, the left fixed-point vector of the transition matrix $\mathbf{P}$
- this means the probability of starting in state s_i is w_i
- the probability of being in state s_j after n steps is $\left(\mathbf{w}^T\mathbf{P}^n\right)_j$, but $\mathbf{w}^T\mathbf{P}^n = \mathbf{w}^T$, so this probability is w_j
- thus, the probability vector is always the same, that is, it is stationary or invariant
- when this occurs, the Markov chain is said to be in equilibrium
- recall that an ergodic Markov chain which starts in any probability vector $\mathbf{y}$ eventually tends to equilibrium
- the process of bringing the chain into equilibrium from a random starting probability vector in known as thermalization

Reversibility in Markov chains

- an ergodic Markov chain is reversible if the probability of going from state s_i to s_j is the same as that for going from state s_j to s_i once the chain is in equilibrium
- the probability that a transition from s_i to s_j occurs is the probability w_i of finding the chain in state s_i in equilibrium times the transition probability p_{ij}
- reversibility occurs when $w_i p_{ij} = w_j p_{ji}$
- the above condition is often referred to as detailed balance
- note that detailed balance guarantees the fixed-point condition: since $\sum_j p_{ij} = 1$ then

$$\sum_j w_j p_{ji} = \sum_j w_i p_{ij} = w_i$$

Law of large numbers for Markov chains

- consider an R-state ergodic Markov chain which starts in state s_i
- define $X_j^{(m)} = \begin{cases} 1 & \text{if chain in state } s_j \text{ after } m \text{ steps} \\ 0 & \text{otherwise} \end{cases}$
- define $N_j^{(n)}$ as number of times chain in state s_j in first n steps

$$N_j^{(n)} = X_j^{(1)} + X_j^{(2)} + \cdots + X_j^{(n)}$$

- often called occupation times
- expected value $E(X_j^{(m)}) = p_{ij}^{(m)}$ so

$$E(N_j^{(n)}) = \sum_{h=1}^{n} p_{ij}^{(h)}$$

- it can be shown that

$$\lim_{n\to\infty} E(N_j^{(n)})/n = w_j$$

- can show law of large numbers for ergodic Markov chain:

$$P(|N_j^{(n)}/n - w_j| > \varepsilon) \to 0 \text{ as } n \to \infty$$

- also require $\sum_{n=1}^{\infty} n^2 p_{ii}^{(n)} < \infty$

Central limit and ergodic theorem for Markov chains

- can show a central limit holds

$$\lim_{n\to\infty} P\left(\frac{a\sigma_j}{\sqrt{n}} < \left(\frac{N_j^{(n)}}{n} - w_j\right) < \frac{b\sigma_j}{\sqrt{n}}\right) = \frac{1}{\sqrt{2\pi}}\int_a^b e^{-x^2/2}dx$$

  where σ_j depends on w_j
- distributions of random variables $N_j^{(n)}$ tend to normal distributions
- let $X_1, X_2, \ldots, X_n$ be the actual outcomes that make up an ergodic R-state Markov chain
- from the definition of $X_j^{(n)}$, it follows that $\sum_{j=1}^{R} X_j^{(n)} = 1$ so

$$\frac{1}{n}\sum_{h=0}^{n-1} f(X_h) = \frac{1}{n}\sum_{h=0}^{n-1}\sum_{j=1}^{R} X_j^{(h)} f(s_j) = \sum_{j=1}^{R} N_j^{(n)} f(s_j) \to \sum_{j=1}^{R} w_j f(s_j)$$

- Markov-chain “time"-average approaches required ensemble average!!

Monte Carlo integration

- recap of Markov-chain Monte Carlo integration:

$$\int_V f(\vec{x})\, d^D x \approx V\langle f\rangle \pm V\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}}$$

$$\langle f\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i) \qquad \langle f^2\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i)^2$$

- each point in D-dimensional volume V is a state of a Markov chain
- N points $\vec{x}_1, \ldots, \vec{x}_N$ are elements in an ergodic Markov chain
- law of large numbers justifies correctness of estimate
- central limit theorem gives estimate of statistical uncertainty
  - above formula for error assumes the $\vec{x}_j$ are statistically independent

What's the catch?

- Monte Carlo estimates require statistically independent random configurations
- configurations generated by Markov process depend on previous elements in the chain
- this dependence known as autocorrelation
- this autocorrelation can actually be measured!
- for any observable (integrand) O_i, autocorrelation $\varrho(\tau)$ defined by

$$\frac{\langle O_i O_{i+\tau} \rangle - \langle O_i \rangle^2}{\langle O_i^2 \rangle - \langle O_i \rangle^2}$$

  - highly correlated $\longrightarrow$ value near 1
  - independent $\longrightarrow$ value near 0
- dependence decreases as distance between elements in chain increases
  - do not use every element in chain for "measurements"
  - skip some number of elements between measurements

Constructing the transition probability

- generally know probability density $\pi(\phi)$ we need to sample
- for our path integrals, we need to generate paths with probability distribution

$$\pi(\phi) = \frac{e^{-S[\phi]/\hbar}}{\int_a^b \mathcal{D}\phi'\ e^{-S[\phi']/\hbar}}$$

- in imaginary time formalism, path integral weight is real and positive $\longrightarrow$ probability interpretation for Monte Carlo
- how do we construct the Markov transition matrix $P(\widetilde{\phi} \leftarrow \phi)$?
  - change to quantum mechanical notation of putting earlier states on right, later states on left
- simplest answer to this question is

  the Metropolis-Hastings method

- useful for local updating so changes to action are small
- probability normalization never enters in the calculation!

The Metropolis-Hastings algorithm

- this method uses an auxiliary proposal density $R(\widetilde{\phi} \leftarrow \phi)$ which
  - must be normalized
  - can be evaluated for all $\phi, \widetilde{\phi}$
  - can be easily sampled
  - no relationship to the fixed-point probability density $\pi(\phi)$ needed
- given this proposal density, the Metropolis-Hastings method updates $\phi \to \widetilde{\phi}$ as follows:
  1. use $R(\widetilde{\phi} \leftarrow \phi)$ to propose new value $\widetilde{\phi}$ from current value ϕ
  2. accept the new value with probability
  $$P_{\text{acc}}(\widetilde{\phi} \leftarrow \phi) = \min\left(1, \frac{R(\phi \leftarrow \widetilde{\phi})\pi(\widetilde{\phi})}{R(\widetilde{\phi} \leftarrow \phi)\pi(\phi)}\right)$$
  3. if rejected, the original value ϕ is retained
- if proposal density satisfies reversibility $R(\widetilde{\phi} \leftarrow \phi) = R(\phi \leftarrow \widetilde{\phi})$, then acceptance probability reduces to $\min(1, \pi(\widetilde{\phi})/\pi(\phi))$
  - original Metropolis method

Detailed balance in Metropolis-Hastings

- Metropolis-Hastings satisfies detailed balance
- proof:
  - (normalized) transition probability density is

$$W(\widetilde{\phi} \leftarrow \phi) = P_{\rm acc}(\widetilde{\phi} \leftarrow \phi) R(\widetilde{\phi} \leftarrow \phi)$$
$$+\delta(\widetilde{\phi} - \phi) \left(1 - \int \mathcal{D}\overline{\phi}\, P_{\rm acc}(\overline{\phi} \leftarrow \phi) R(\overline{\phi} \leftarrow \phi) \right)$$

  - define

$$\begin{aligned} A(\widetilde{\phi} \leftarrow \phi) &\equiv P_{\rm acc}(\widetilde{\phi} \leftarrow \phi) R(\widetilde{\phi} \leftarrow \phi) \pi(\phi) \\ &= \min\left(1, \frac{R(\phi \leftarrow \widetilde{\phi})\pi(\widetilde{\phi})}{R(\widetilde{\phi} \leftarrow \phi)\pi(\phi)}\right) R(\widetilde{\phi} \leftarrow \phi)\pi(\phi) \\ &= \min\left(R(\widetilde{\phi} \leftarrow \phi)\pi(\phi),\ R(\phi \leftarrow \widetilde{\phi})\pi(\widetilde{\phi})\right) \end{aligned}$$

    where last line follows from $R(\widetilde{\phi} \leftarrow \phi)\pi(\phi) \geq 0$
  - symmetric: $A(\widetilde{\phi} \leftarrow \phi) = A(\phi \leftarrow \widetilde{\phi})$.

Detailed balance in Metropolis-Hastings (continued)

- so we have

$$
\begin{aligned}
W(\widetilde{\phi} \leftarrow \phi)\pi(\phi) &= P_{\text{acc}}(\widetilde{\phi} \leftarrow \phi) R(\widetilde{\phi} \leftarrow \phi)\pi(\phi) \\
&+ \quad \delta(\widetilde{\phi} - \phi)\left(1 - \int \mathcal{D}\overline{\phi}\, P_{\text{acc}}(\overline{\phi} \leftarrow \phi) R(\overline{\phi} \leftarrow \phi)\right)\pi(\phi) \\
&= \quad A(\widetilde{\phi} \leftarrow \phi) + \delta(\widetilde{\phi} - \phi)\left(\pi(\phi) - \int \mathcal{D}\overline{\phi}\, A(\overline{\phi} \leftarrow \phi)\right) \\
&= \quad A(\widetilde{\phi} \leftarrow \phi) + \delta(\widetilde{\phi} - \phi)\, K(\phi)
\end{aligned}
$$

  where

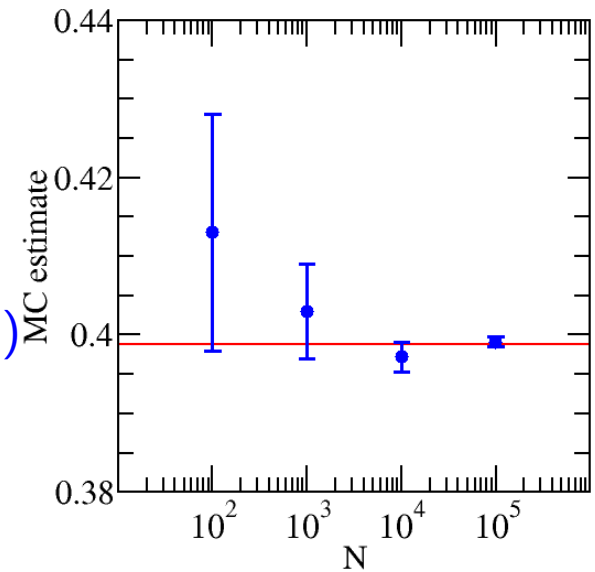
$$K(\phi) = \pi(\phi) - \int \mathcal{D}\overline{\phi} A(\overline{\phi} \leftarrow \phi)$$

- given symmetry of A and Dirac δ-function, then detailed balance holds

$$W(\widetilde{\phi} \leftarrow \phi)\pi(\phi) = W(\phi \leftarrow \widetilde{\phi})\pi(\widetilde{\phi})$$

A one dimensional example

- does this really work?
- let $g(x) = \cos(\sqrt{1+x^2})$ and $h(x) = e^{-x^2}/(x^2+2)$
- $g(x)$ changes sign, $h(x) \geq 0$
- consider ratio of integrals $I = \dfrac{\int_{-\infty}^{\infty} g(x)h(x)dx}{\int_{-\infty}^{\infty} h(x)dx} = 0.3987452$
- sampling density $\pi(x) = Z^{-1}h(x)$ where $Z = \int_{-\infty}^{\infty} h(x)dx$
- algorithm:
  - choose δ uniform probability for $-\Delta \leq \delta \leq \Delta$
  - propose $\widetilde{x} = x + \delta$
  - acceptance probability $\min(1, \pi(\widetilde{x})/\pi(x)) = \min(1, h(\widetilde{x})/h(x))$
- $\Delta = 1.5$ for acceptance $\sim 50\%$
- never needed Z



Part III

Monte Carlo study of the simple harmonic oscillator

Discretization of SHO action

- action of harmonic oscillator (imaginary time formalism)

$$S[x(\tau)] = \int_{\tau_a}^{\tau_b} d\tau \ \left(\tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}m\omega^2 x^2\right)$$

- discretize time $N\varepsilon = \tau_b - \tau_a$ for Monte Carlo evaluation

$$\frac{S}{\hbar} = \frac{m\varepsilon}{2\hbar}\sum_{j=0}^{N-1}\left[\left(\frac{x_{j+1}-x_j}{\varepsilon}\right)^2 + \omega^2\left(\frac{x_{j+1}+x_j}{2}\right)^2\right]$$

- choose ε so discretization errors sufficiently small
- introduce dimensionless parameters

$$x_k = d_k\sqrt{\frac{\varepsilon\hbar}{m}} \qquad \kappa = \frac{1}{4}\varepsilon^2\omega^2$$

$$\frac{S}{\hbar} = \frac{1}{2}\sum_{j=0}^{N-1}\left[(d_{j+1}-d_j)^2 + \kappa(d_{j+1}+d_j)^2\right]$$

Discretization of action (continued)

- a few more manipulations produce

$$\frac{S}{\hbar} = \frac{1}{2}(1+\kappa)(d_0^2 + d_N^2) + (1+\kappa)\left[\sum_{j=1}^{N-1} d_j^2\right] - (1-\kappa)\left[\sum_{j=0}^{N-1} d_j d_{j+1}\right]$$

- first constant irrelevant (set to zero), then one last rescaling

$$u_j = d_j\sqrt{1+\kappa} \quad g = \frac{1-\kappa}{1+\kappa} \quad d_0 = d_N = 0$$

- final result for action

$$\frac{S}{\hbar} = \left[\sum_{j=1}^{N-1} u_j^2\right] - g\left[\sum_{j=0}^{N-1} u_j u_{j+1}\right]$$

Metropolis updating of path

- to update location (at a single time)
  - propose random shift $-\Delta \leq \delta \leq \Delta$ with uniform probability
  - calculate change to the action
$$\delta S/\hbar = \delta \ (\delta + 2u_j - g(u_{j-1} + u_{j+1}))$$
  - accept $u_j^{\text{new}} = u_j + \delta$ with probability $\min(1, e^{-\delta S/\hbar})$
  - rule of thumb: fix Δ for about 50% acceptance rate
    - lower rate = wasting too much time with rejections
    - higher rate = moving through phase space too slowly
- repeat for each u_j for $j = 1, \ldots, N-1$ (this is called one sweep)
- repeat for certain number of sweeps
  - until autocorrelations sufficiently small

Actual C++ code

- here is actual C++ code which does the updating

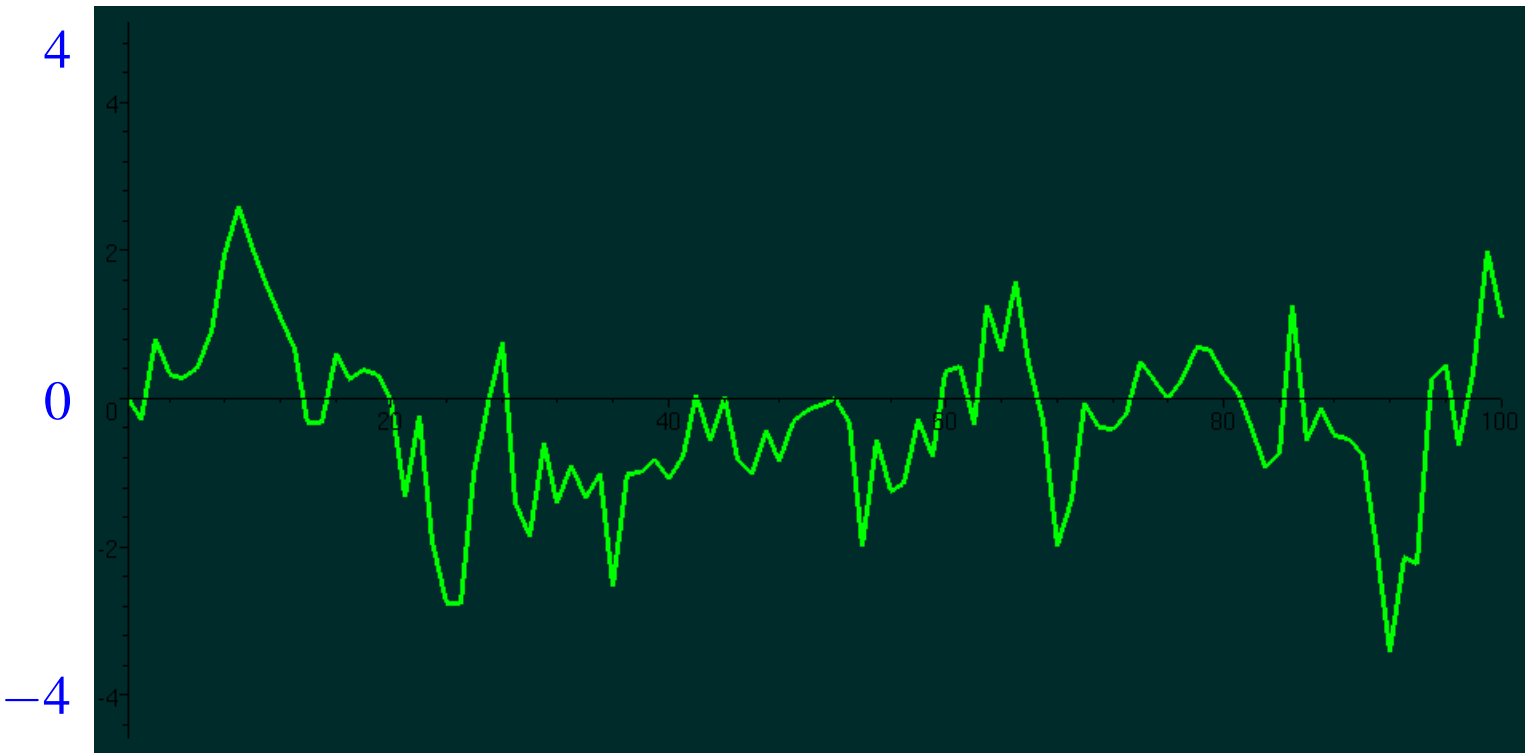
```
void markov::update()
{
 double shift,deltaS;
 for (int i=1;i<=Nsweeps;i++)
   for (int t=1;t<Ntimesteps;t++){
            // propose shift in location[t]
    shift=2.0*max_shift_per_instance*(rng.generate()-0.5);

            // compute change in action
    deltaS=shift*(shift+2.0*locations[t]
              -hop_param*(locations[t-1]+locations[t+1]));

            // Metropolis accept or reject
    if (deltaS<0.0) accept=1;
    else accept=(rng.generate()<=exp(-deltaS));
    if (accept) locations[t]+=shift;
       }
}
```

Simulation guidelines

- to start Markov chain
  - choose a random path (hot start)
  - or choose $u_j = 0$ for all j (cold start)
  - update N_{therm} sweeps until fixed point of chain achieved (thermalization) $\longrightarrow$ check some simple observable
- once thermalized, begin “measurements"
- must choose
  - ε so discretization errors sufficiently small
  - Δ for adequate acceptance rate
  - N_{sweeps} for sufficiently small autocorrelations
  - N_{meas} for desired precision of results

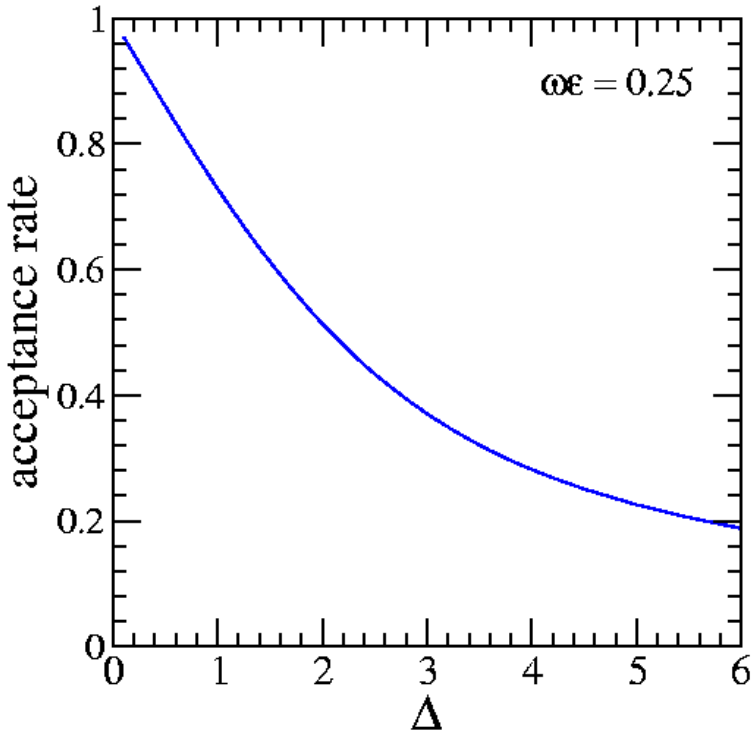
Path animation

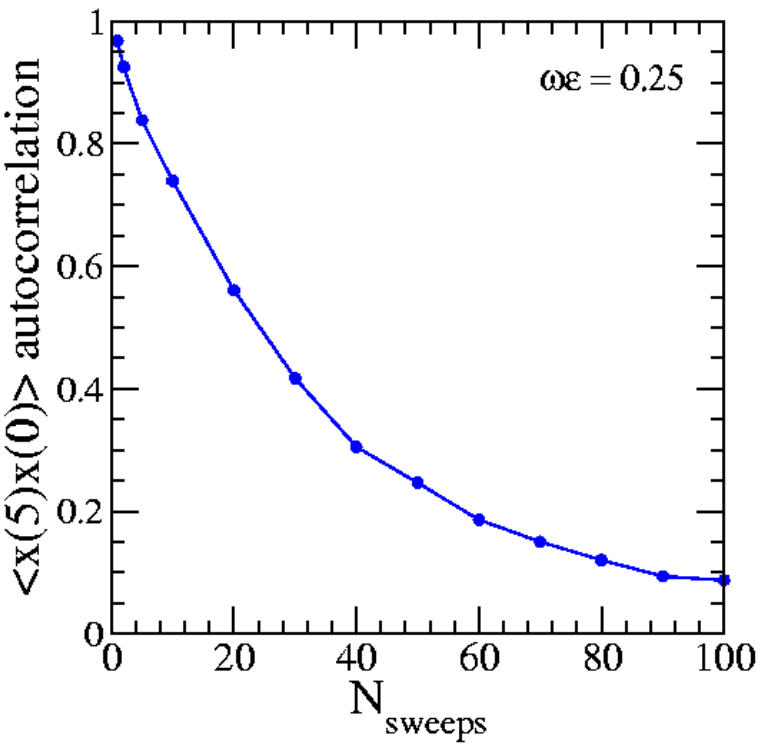
- animation of first 100 time slices of u_j path



Acceptance rate and autocorrelations

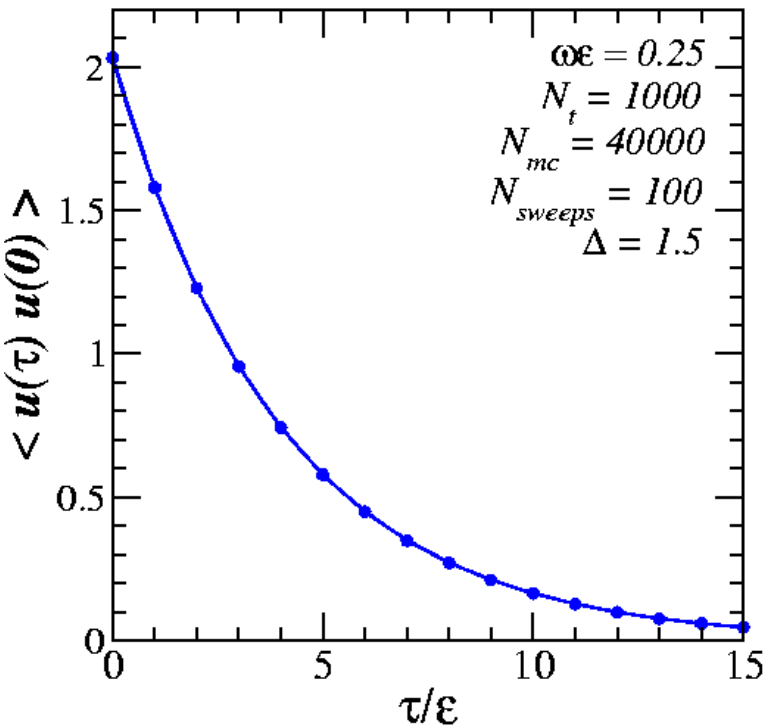
- choose Δ so acceptance rate near 0.5
- choose N_{sweeps} so autocorrelations near 0.1





Correlation function

- comparison of final Monte Carlo estimates with exact results



- exact result shown as curve
- Monte Carlo estimates shown by circles (statistical uncertainties too small to see)

Part IV

Monte Carlo calculations in real scalar field theory in 2+1 dimensions

Action in continuous space-time

- action in continuous Euclidean D-dimensional space-time (imaginary time formalism) given by

$$S = \int d^D x \left(\frac{1}{2} \partial_\mu \varphi(x) \partial_\mu \varphi(x) + \frac{1}{2} m^2 \varphi(x)^2 + \frac{g}{4!} \varphi(x)^4 \right).$$

- action must be dimensionless (natural units $\hbar = c = 1$)
- m has units of a derivative ∂_μ, that is, of a mass
- units of field $[\phi] = [m]^{\frac{1}{2}D-1}$
- coupling g has units $[g] = [m]^{4-D}$
  - coupling dimensionless in 4 space-time dimensions
  - has units of mass in 3 space-time dimensions so g/m dimensionless

Quantization

- quantization using path integrals
- generalize notion of "path": a path here is a field configuration
- path integral is now integrations over all field configurations
- for real scalar field, integral $-\infty \leq \phi(x) \leq \infty$ at every space-time point x
- time-ordered two-point function given by

$$\langle T\phi(x_1)\phi(x_2)\rangle = \frac{\int \mathcal{D}\phi\ \phi(x_1)\phi(x_2)\exp(-S[\phi])}{\int \mathcal{D}\phi\ \exp(-S[\phi])}.$$

- generalizes to n-point functions: time-ordered product of n fields

Discretization of action

- Monte Carlo study requires action on a space-time lattice
- use anisotropic cubic lattice with temporal lattice spacing a_t and spatial lattice spacing a_s
- use simplest finite difference for the field derivatives
- action is given by

$$\begin{aligned} S &= a_s^{D-1} a_t \sum_x \left(\sum_\mu \frac{(\varphi(x+a_\mu\hat{\mu})-\varphi(x))^2}{2a_\mu^2} + \frac{1}{2}m^2\varphi(x)^2 + \frac{g}{4!}\varphi(x)^4 \right) \\ &= a_s^{D-1} a_t \sum_x \left(-\sum_\mu \frac{\varphi(x+a_\mu\hat{\mu})\varphi(x)}{a_\mu^2} + \frac{1}{2}\left(m^2 + \sum_\nu \frac{2}{a_\nu^2} \right)\varphi(x)^2 + \frac{g}{4!}\varphi(x)^4 \right) \end{aligned}$$

- redefine the field: $\sqrt{a_s^{D-3} a_t}\ \varphi(x) = \sqrt{2\kappa_s}\ \phi(x)$

  where κ_s is dimensionless number, new field $\phi(x)$ is dimensionless

Action on lattice

- a few more dimensionless parameters:

$$a_s/a_t = \zeta, \quad \lambda = \frac{g\zeta\kappa_s^2}{6a_s^{D-4}},$$
$$\kappa_s(a_s^2 m^2 + 2\zeta^2 + 2D - 2) = 1 - 2\lambda, \quad \kappa = \zeta\kappa_s$$

- final form for lattice action

$$S = \sum_x \left(-\frac{2\kappa}{\zeta} \sum_{j=1}^{D-1} \phi(x)\phi(x+a_s\hat{j}) - 2\kappa\zeta\, \phi(x)\phi(x+a_t\hat{t}) + (1-2\lambda)\phi(x)^2 + \lambda\phi(x)^4 \right)$$

- hopping parameter κ essentially sets mass parameter, λ is interaction coupling

Exact results in free field theory

- the free field theory $\lambda = 0$ is exactly soluable
- path integrals are multivariate gaussians
- free action can be written in form

$$S[\phi] = \tfrac{1}{2} \sum_{xy} \phi(x) M(x,y) \phi(y)$$

- for N lattice sites, M is real and symmetric $N \times N$ matrix having positive eigenvalues
- this matrix given by

$$\begin{aligned} M(x,y) \quad = \quad & -\frac{2\kappa}{\zeta} \sum_{j=1}^{D-1} \left(\delta(y, x + a_s \hat{j}) + \delta(x, y + a_s \hat{j}) \right) \\ & -2\kappa\zeta \left(\delta(y, x + a_t \hat{t}) + \delta(x, y + a_t \hat{t}) \right) + 2\delta(x,y) \end{aligned}$$

Gaussian integrals in free theory

- N-dimensional multivariate Gaussian integral of form

$$\prod_{i=1}^{N}\left(\int_{-\infty}^{\infty}d\phi_i\right)\exp(-\tfrac{1}{2}\phi_j M_{jk}\phi_k + J_n\phi_n)$$

$$= \left(\det\left(\frac{M}{2\pi}\right)\right)^{-1/2}\exp\left(\tfrac{1}{2}J_j M^{-1}_{jk}J_k\right)$$

- J-trick: use derivatives wrt to J_k, followed by $J_k \to 0$ to evaluate all integrals involving any number of products of the fields

$$\prod_{i=1}^{N}\left(\int_{-\infty}^{\infty}d\phi_i\right)\phi_{m_1}\phi_{m_2}\ldots\phi_{m_r}\ \exp(-\tfrac{1}{2}\phi_j M_{jk}\phi_k)$$

$$= \frac{\delta}{\delta J_{m_1}}\cdots\frac{\delta}{\delta J_{m_r}}\prod_{i=1}^{N}\left(\int_{-\infty}^{\infty}d\phi_i\right)\ \exp(-\tfrac{1}{2}\phi_j M_{jk}\phi_k + J_n\phi_n)$$

- does Wick contractions automagically!

Two-point function

- two-point function given by $\langle T\phi(x_1)\phi(x_2)\rangle = M^{-1}(x_1,x_2)$
- invert M by method of Green functions and use Fourier series
- for $L_x \times L_y \times L_t$ lattice, result is

$$M^{-1}(x,y) = \frac{\zeta}{2\kappa L_x L_y L_t} \sum_{k_\mu} \frac{\cos(k\cdot(x-y))}{(a_s^2 m^2 + 4\sum_{j=1}^{2} \sin^2(\tfrac{1}{2}k_j) + 4\zeta^2 \sin^2(\tfrac{1}{2}k_t))}$$

  where $k_\mu = 2\pi n_\mu / L_\mu$ for $n_\mu = 0, 1, 2, \ldots, L_\mu - 1$
- pole gives energy $a_t E_p$ of single particle of momentum $a_s p$

$$a_t E_p = 2\sinh^{-1}\left(\frac{1}{2\zeta}\sqrt{a_s^2 m^2 + 4\sin^2(\tfrac{1}{2}a_s p_x) + 4\sin^2(\tfrac{1}{2}a_s p_y)}\right)$$

- for small a_t, a_s this becomes $E_p = \sqrt{m^2 + p_x^2 + p_y^2}$
- spectrum is sum of free particle energies

Single-site Monte Carlo updating

- Metropolis-Hastings method needs acceptable acceptance rate
- changing all field values at once generally leads to large changes in action $\longrightarrow$ near zero acceptance rate
- reasonable acceptance rate achieved by updating field at a single lattice site at any given time
- ergodicity ensured by sweeping through lattice, updating each and every site one at a time
- in battle against autocorrelations, expect
  - small wavelength modes updated well
  - long wavelength modes updated not so well

δS for single-site update

- recall action is

$$S = \sum_x \left(-\frac{2\kappa}{\zeta} \sum_{j=1}^{D-1} \phi(x)\phi(x+a_s\hat{j}) - 2\kappa\zeta\, \phi(x)\phi(x+a_t\hat{t}) + (1-2\lambda)\phi(x)^2 + \lambda\phi(x)^4 \right)$$

- for $\widetilde{\phi} \leftarrow \phi$, change in action is $\delta S = S[\widetilde{\phi}] - S[\phi]$
- define neighborhood

$$N(x) = -\frac{2\kappa}{\zeta} \sum_{j=1}^{D-1} \left(\phi(x+a_s\hat{j}) + \phi(x-a_s\hat{j}) \right) - 2\kappa\zeta \left(\phi(x+a_t\hat{t}) + \phi(x-a_t\hat{t}) \right)$$

- if field at one site x changed $\phi(x) \to \phi(x) + \Delta$, then

$$\delta S = \Delta \left(N(x) + (\Delta + 2\phi(x)) \left(1 + \lambda \left((\Delta + 2\phi(x))\Delta + 2(\phi(x)^2 - 1) \right) \right) \right)$$

δS for single-site update (continued)

- change in action can also be written

$$\begin{aligned}
\delta S &= \Delta\left(a_0 + a_1\Delta + a_2\Delta^2 + a_3\Delta^3\right), \\
a_0 &= N(x) + 2\phi(x)(1 + 2\lambda(\phi(x)^2 - 1)) \\
a_1 &= 1 + 2\lambda(3\phi(x)^2 - 1) \\
a_2 &= 4\lambda\phi(x) \\
a_3 &= \lambda
\end{aligned}$$

Metropolis sweeps

- single-site updates involve a single continuous real variable ϕ
- use simplest proposal density

$$R(\widetilde{\phi} \leftarrow \phi) = \begin{cases} \dfrac{1}{\Delta_0} & -\frac{1}{2}\Delta_0 \leq (\widetilde{\phi} - \phi) \leq \frac{1}{2}\Delta_0 \\ 0 & |\widetilde{\phi} - \phi| > \frac{1}{2}\Delta_0 \end{cases}$$

- width Δ_0 chosen for acceptance probability around 50%
- proposed new value accepted with probability $\min(1, \exp(-\delta S))$
- if rejected, keep current field value
- sweeping through lattice ensures ergodicity
- in sweeping through the lattice in predetermined order, detailed balance no longer holds
  - not a problem since the fixed-point stability condition still holds
  - detailed balance maintained by updating sites in random order

Battling autocorrelations

- when the single particle mass $a_t m_{\text{gap}}$ is small, the coherence length $\xi = 1/(a_t m_{\text{gap}})$ becomes large
- $\xi \to \infty$ signals continuum limit
- $\xi \to \infty$ occurs near critical point (2nd order phase transition)
- we will see that autocorrelations with Metropolis updating become long ranged as ξ becomes large

  $\to$ known as critical slowing down
- autocorrelations problematic even for $\xi \approx 5$ with Metropolis
- need help to better update long wavelength modes

Microcanonical updating

- long wavelength modes are associated with lower frequencies, lower energies
- in other words, long-wavelength modes associated with very small changes to the action
- possible way to improve autocorrelations:

  $\rightarrow$ make large but action preserving $\delta S = 0$ changes

  to field at one site
- call this a microcanonical update
  - often referred to as overrelaxation
- local updating is so easy, don't want to give up on it yet!
- must still update in such a way to satisfy detailed balance
- not ergodic, so microcanonical sweeps must be used in combination with ergodic scheme, such as Metropolis sweeps

Microcanonical updating (2)

- we know Metropolis-Hasting method satisfies detailed balance
- choose proposal density strongly peaked about action-preserving value of field, then carefully take δ-function limit
- revisit Metropolis-Hastings with sharply-peaked Breit-Wigner proposal probability density

$$R_f(\widetilde{\phi} \leftarrow \phi) = \frac{1}{\pi} \frac{\varepsilon}{\left(\widetilde{\phi} - f(\phi)\right)^2 + \varepsilon^2}$$

where ε is a constant and $f(\phi)$ is well-behaved, single-valued, invertible function

- acceptance probability

$$P_{\rm acc}(\widetilde{\phi} \leftarrow \phi) = \min\left(1, \frac{R_f(\phi \leftarrow \widetilde{\phi})\pi(\widetilde{\phi})}{R_f(\widetilde{\phi} \leftarrow \phi)\pi(\phi)}\right) = \min\left(1, \frac{\left((\widetilde{\phi} - f(\phi))^2 + \varepsilon^2\right)\pi(\widetilde{\phi})}{\left((\phi - f(\widetilde{\phi}))^2 + \varepsilon^2\right)\pi(\phi)}\right)$$

Microcanonical updating (3)

- carefully take $\varepsilon \to 0$ limit: $R_f(\widetilde{\phi} \leftarrow \phi) \to \delta(\widetilde{\phi} - f(\phi))$
- determining acceptance probability is tricky
- probability of proposing a value between $f(\phi) - \sqrt{\varepsilon} \leq \widetilde{\phi} \leq f(\phi) + \sqrt{\varepsilon}$ is

$$\int_{f(\phi)-\sqrt{\varepsilon}}^{f(\phi)+\sqrt{\varepsilon}} d\widetilde{\phi}\, R_f(\widetilde{\phi} \leftarrow \phi) = \frac{2}{\pi} \tan^{-1}\left(\frac{1}{\sqrt{\varepsilon}}\right)$$

  which does tends to unity as $\varepsilon \to 0$
- if $f(\phi)$ more than $\sqrt{\varepsilon}$ away from ϕ, probability transition is actually made is

$$\int_{f(\phi)-\sqrt{\varepsilon}}^{f(\phi)+\sqrt{\varepsilon}} d\widetilde{\phi}\, W_f(\widetilde{\phi} \leftarrow \phi) = \int_{f(\phi)-\sqrt{\varepsilon}}^{f(\phi)+\sqrt{\varepsilon}} d\widetilde{\phi}\, P_{\rm acc}(\widetilde{\phi} \leftarrow \phi) R_f(\widetilde{\phi} \leftarrow \phi)$$

$$= \min\left(\frac{2}{\pi} \tan^{-1}\left(\frac{1}{\sqrt{\varepsilon}}\right), \frac{1}{\pi} \int_{f(\phi)-\sqrt{\varepsilon}}^{f(\phi)+\sqrt{\varepsilon}} d\widetilde{\phi} \frac{\varepsilon\, \pi(\widetilde{\phi})}{\left((\phi - f(\widetilde{\phi}))^2 + \varepsilon^2\right)\pi(\phi)}\right)$$

Microcanonical updating (4)

- write $\widetilde{\phi} = f(\phi) + y$, then remaining integral becomes

$$\frac{1}{\pi}\int_{-\sqrt{\varepsilon}}^{\sqrt{\varepsilon}} dy \frac{\varepsilon\, \pi(f(\phi)+y)}{\Big((\phi - f(f(\phi)+y))^2 + \varepsilon^2\Big)\pi(\phi)}$$

- if $f(f(\phi)) \neq \phi$, can show this integral goes to zero as $\varepsilon \to 0$
- for self-inverse function $f(f(\phi)) = \phi$, expansion about $y = 0$ must be carefully done, integral has form

$$\frac{\varepsilon}{\pi}\int_{-\sqrt{\varepsilon}}^{\sqrt{\varepsilon}} dy \frac{(a_0 + a_1 y + a_2 y^2 + \dots)}{(\varepsilon^2 + b_2 y^2 + b_3 y^3 + b_4 y^4 \dots)}$$

- must retain $b_2 y^2$ in denominator, expand rest about $y = 0$:

$$\frac{\varepsilon}{\pi}\int_{-\sqrt{\varepsilon}}^{\sqrt{\varepsilon}} dy \frac{a_0}{(\varepsilon^2 + b_2 y^2)} \left\{1 + \frac{a_1}{a_0} y + \frac{a_2}{a_0} y^2 + \left(\frac{a_3}{a_0} - \frac{b_3}{\varepsilon^2}\right) y^3 \dots\right\}$$

- for $b_2 > 0$, result of integration is

$$\frac{2a_0}{\pi\sqrt{b_2}} \tan^{-1}\left(\sqrt{\frac{b_2}{\varepsilon}}\right) \left\{1 + d_1\sqrt{\varepsilon} + d_2\varepsilon + d_3\varepsilon^{3/2} + \cdots\right\}$$

Microcanonical updating (5)

- acceptance probability in limit $\varepsilon \to 0$ given by

$$P_{\text{acc}} = \min\left(1, \frac{a_0}{\sqrt{b_2}}\right)$$

- here $a_0 = \pi(f(\phi))/\pi(\phi)$ and $b_2 = (f'(f(\phi)))^2$
- differentiate both sides of $f(f(\phi)) = \phi$ with respect to ϕ, so for self-inverse function

$$1 = \frac{d}{d\phi}\Big(f(f(\phi))\Big) = f'(f(\phi))\, f'(\phi)$$

$$\frac{1}{(f'(f(\phi)))^2} = \left|\frac{f'(\phi)}{f'(f(\phi))}\right| \qquad \text{(self-inverse function)}$$

- take limit $\varepsilon \to 0$ acceptance probability goes to

$$P_{\text{acc}}(\widetilde{\phi} \leftarrow \phi) = \min\left(1, \frac{\sqrt{|f'(\phi)|}\,\pi(\widetilde{\phi})}{\sqrt{|f'(\widetilde{\phi})|}\,\pi(\phi)}\right)$$

Microcanonical updating (6)

- specialize to action preserving function $f(\phi)$
- for infinitesimal change $\phi \to \phi + \delta\phi$

$$S(\phi + \delta\phi) = S(f(\phi + \delta\phi))$$

- expand both sides

$$\begin{aligned} S(\phi) + S'(\phi)\delta\phi + O(\delta\phi^2) &= S(f(\phi) + f'(\phi)\delta\phi + O(\delta\phi^2)) \\ &= S(f(\phi)) + S'(f(\phi))\, f'(\phi)\delta\phi + O(\delta\phi^2) \\ &= S(\phi) + S'(f(\phi))\, f'(\phi)\delta\phi + O(\delta\phi^2). \end{aligned}$$

- solve order by order in $\delta\phi$

$$S'(\phi) = S'(f(\phi))\, f'(\phi) \;\to\; f'(\phi) = \frac{S'(\phi)}{S'(f(\phi))}, \quad f'(f(\phi)) = \frac{S'(f(\phi))}{S'(\phi)}$$

- proposal and acceptance probability densities are

$$R_f(\widetilde{\phi} \leftarrow \phi) = \delta\Big(\widetilde{\phi} - f(\phi)\Big), \qquad f(f(\phi)) = \phi, \quad S(f(\phi)) = S(\phi),$$

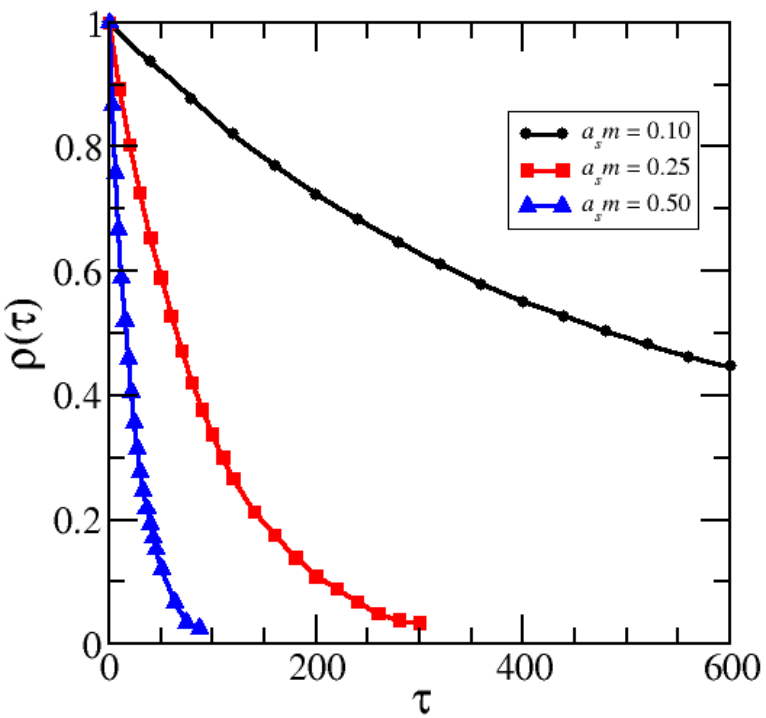
$$P_{\rm acc}(\widetilde{\phi} \leftarrow \phi) = \min\left(1, \left|\frac{S'(\phi)}{S'(\widetilde{\phi})}\right|\right), \quad \pi(\phi) = \frac{\exp(-S[\phi])}{\displaystyle\int \mathcal{D}\widetilde{\phi}\, \exp(-S[\widetilde{\phi}])}$$

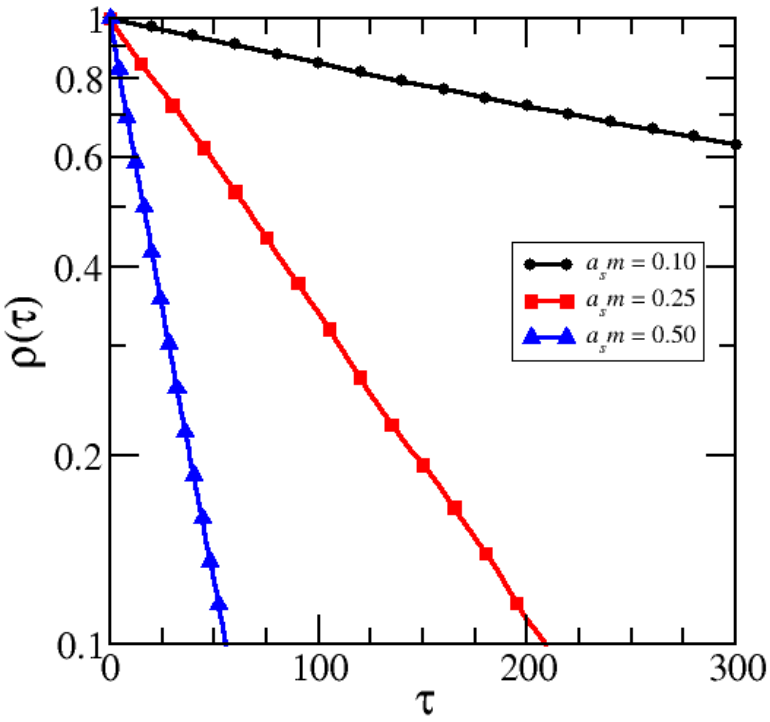
Microcanonical updating (7)

- generalize to multiple self-inverse functions
  - for ϕ^4 at most four field values with same local action
- generalize to probability μ of proposing a change
  - sometimes need $\mu < 1$ to prevent (damped) oscillations in autocorrelation function
- summary of microcanonical updating process:
  1. decide to propose new field value with probability μ (skip steps below if no proposal)
  2. solve $\delta S(\phi) = 0$, let ϕ_j denote real solutions different from ϕ
     - these are roots of a cubic polynomial
  3. randomly choose one of the ϕ_j with equal probability, let $\widetilde{\phi}$ denote the chosen value
  4. accept with probability
     $$P_{\text{acc}}(\widetilde{\phi} \leftarrow \phi) = \min\left(1, \left|\frac{S'(\phi)}{S'(\widetilde{\phi})}\right|\right)$$
     if rejected, original value ϕ retained

Autocorrelations

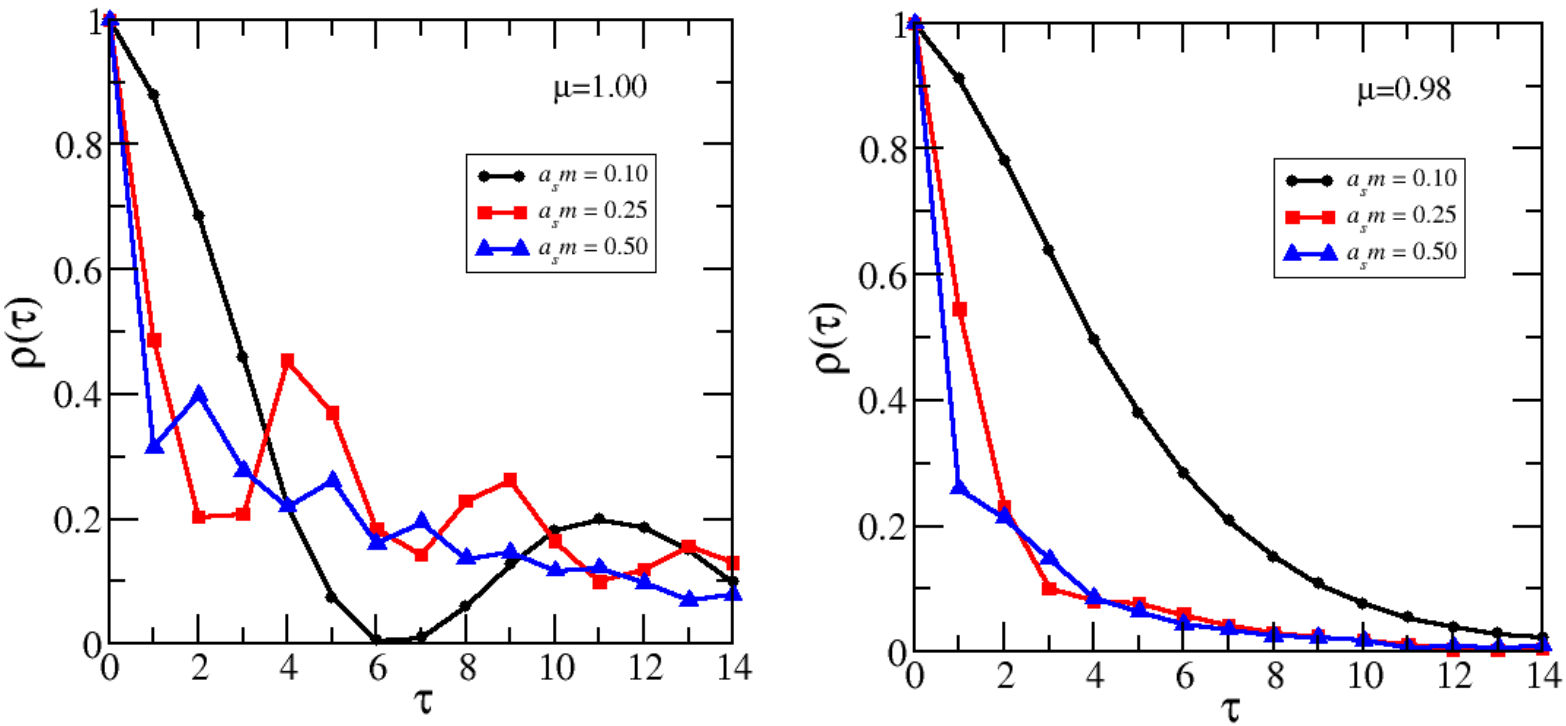
- studied autocorrelation function $\rho(\tau)$ of $\langle \Phi(t)\Phi(0)\rangle$ for $t = 1/(2a_s m)$ and $\Phi(t) = \sum_{xy} \phi(x,y,t)$
- τ is number of Metropolis sweeps in plots below
- $a_s m = 0.10, 0.25, 0.50$ for $\lambda = 0$ on 24^3 isotropic lattice
- 2200 sweeps to reduce autocorrelations to 0.1 for $a_s m = 0.10$





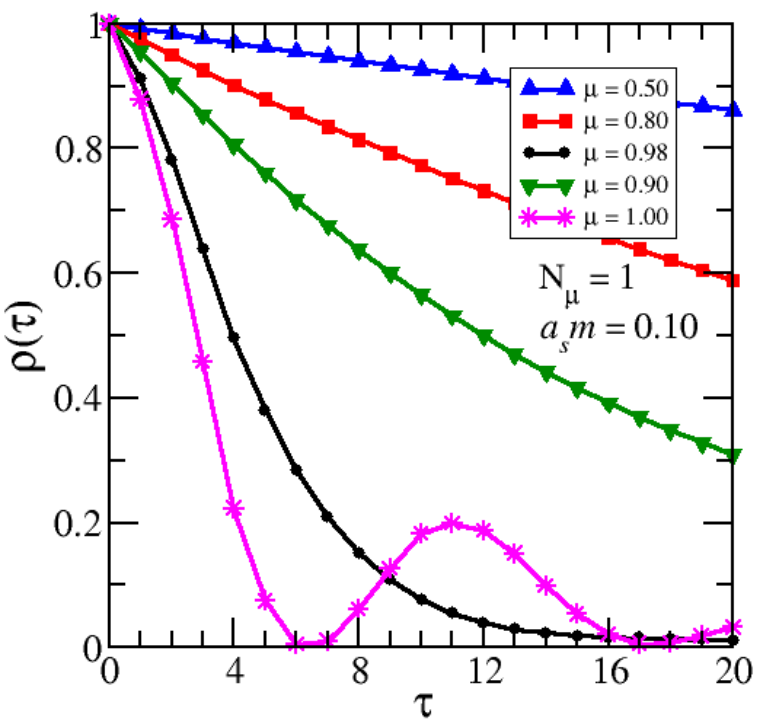
Autocorrelations

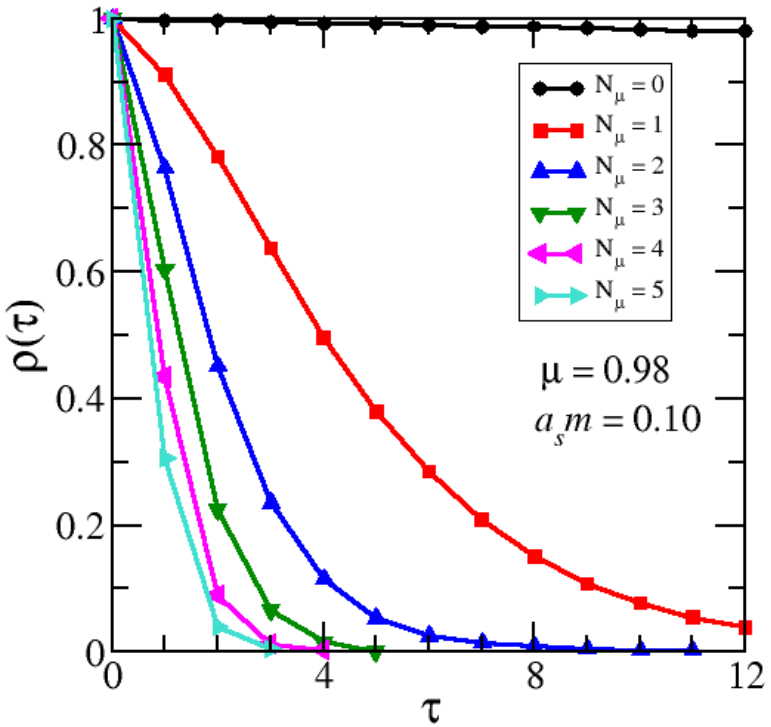
- autocorrelations $\rho(\tau)$ of $\langle \Phi(t)\Phi(0)\rangle$ for $t = 1/(2a_s m)$
- τ is number of compound sweeps,
- compound sweep = 1 Metropolis + 1 microcanonical sweep
- μ is probability of proposing change in microcanonical updates
- $a_s m = 0.10, 0.25, 0.50$ for $\lambda = 0$ on 24^3 isotropic lattice
- undesirable oscillations on left removed using $\mu = 0.98$ or updating sites in random order



Autocorrelations

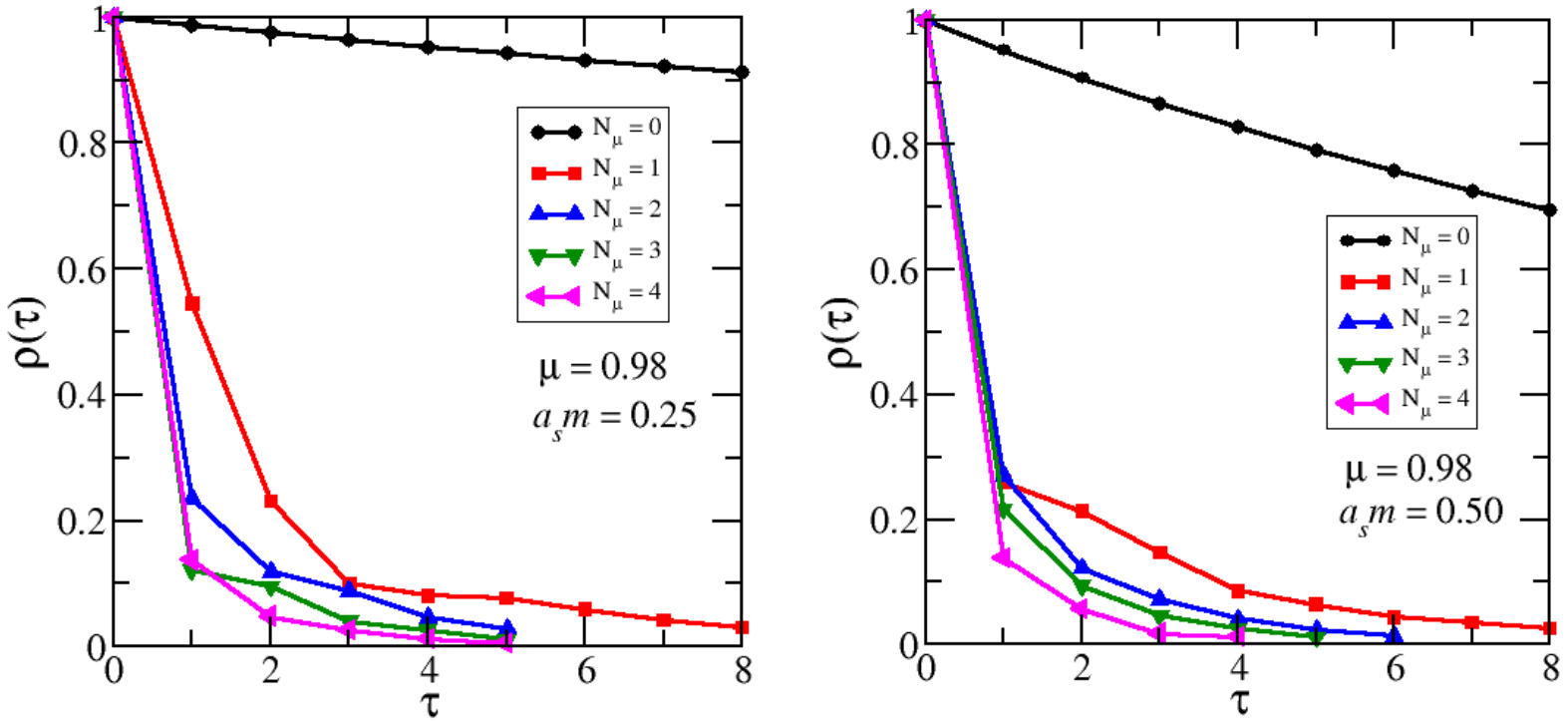
- autocorrelations $\rho(\tau)$ of $\langle \Phi(t)\Phi(0)\rangle$ for $t = 1/(2a_s m)$
- τ is number of compound sweeps
- compound sweep = 1 Metropolis + N_μ microcanonical sweeps
- μ is probability of proposing change in microcanonical updates
- $a_s m = 0.10$ for $\lambda = 0$ on 24^3 isotropic lattice
- left-hand plot, $N_\mu = 1$ and μ is varied
- right-hand plot, $\mu = 0.98$ and N_μ is varied





Autocorrelations

- autocorrelations $\rho(\tau)$ of $\langle \Phi(t)\Phi(0)\rangle$ for $t = 1/(2a_s m)$
- τ is number of compound sweeps
- compound sweep = 1 Metropolis + N_μ microcanonical sweeps
- $\mu = 0.98$ probability of proposing change in microcanonical
- $a_s m = 0.25, 0.50$ for $\lambda = 0$ on 24^3 isotropic lattice



Calculating the spectrum

- stationary-state energies extracted from asymptotic decay rates of temporal correlations of the fields
- temporal evolution of field as Heisenberg-picture quantum operator

$$\phi(t) = e^{Ht}\phi(0)e^{-Ht}$$

- under certain general assumptions and ignoring temporal boundary conditions, then for $t \geq 0$

$$\begin{aligned}\langle 0|\phi(t)\phi(0)|0\rangle &= \sum_n \langle 0|e^{Ht}\phi(0)e^{-Ht}|n\rangle\langle n|\phi(0)|0\rangle, \\ &= \sum_n \left|\langle n|\phi(0)|0\rangle\right|^2 e^{-(E_n-E_0)t} = \sum_n A_n e^{-(E_n-E_0)t},\end{aligned}$$

- where complete set of (discrete) eigenstates of H satisfying $H|n\rangle = E_n|n\rangle$ inserted
- if $\langle 1|\phi(0)|0\rangle \neq 0$, then A_1 and $E_1 - E_0$ can be extracted as t becomes large, assuming $\langle 0|\phi(0)|0\rangle = 0$
- can use any operator $O(t)$ which is a function of the field $\phi(t)$ only on a time slice t

Calculating the spectrum (2)

- extraction of A_1 and $E_1 - E_0$ done using correlated$-\chi^2$

$$\chi^2 = \sum_{tt'} \Big(C(t) - M(t,\alpha) \Big) \sigma_{tt'}^{-1} \Big(C(t') - M(t',\alpha) \Big)$$

  where $C(t)$ represents Monte Carlo estimates of correlation function with covariance matrix $\sigma_{tt'}$ and model function is $M(t,\alpha) = \alpha_1 e^{-\alpha_0 t}$.
- minimize expression with respect to the model parameters α_0, α_1
- uncertainties in the best-fit parameters $\alpha_0 = E_1 - E_0$ and $\alpha_1 = A_1$ are obtained by a jackknife or bootstrap procedure
- fit must be done for a time range $t_{\text{min}} \leq t \leq t_{\text{max}}$ such that an acceptable fit quality is obtained, that is, $\chi^2/\text{dof} \approx 1$
- sum of two-exponentials as model function can be used to minimize sensitivity to t_{min}
  - but fit parameters associated with faster-decaying exponential generally *not* good estimates of gap to next energy level and should be discarded

Jackknife resampling

- return to independent trials process $X_1, X_2, \ldots, X_N$
- expected value $E(f(X))$ estimated using $\langle f \rangle = \frac{1}{N} \sum_{k=1}^{N} f(X_k)$
- sometimes f is a very complicated function, or it could be a function of the expected value!
- propagation of errors often not possible $\rightarrow$ resampling schemes
- let $\langle f \rangle$ denote Monte Carlo estimate of some quantity f using all X_k for $k = 1, 2, \ldots, N$
- let $\langle f \rangle_J$ denote Monte Carlo estimate of f omitting X_J (so use the other $N-1$ values X_k)
- jackknife error estimate given by

$$\sigma^{(J)} = \left(\frac{N-1}{N} \sum_{J=1}^{N} (\langle f \rangle_J - \langle f \rangle)^2 \right)^{1/2}$$

- Monte Carlo error formula can be used to determine covariance matrix $\sigma_{tt'}$ for correlation function itself in χ^2
- jackknife gives errors in model fit parameters

Bootstrap resampling

- another resampling scheme is the bootstrap
- again, let $\langle f \rangle$ denote Monte Carlo estimate of some quantity f using all X_k for $k = 1, 2, \ldots, N$
- let $\langle f \rangle_b$ denote Monte Carlo estimate of f using a new set $\widehat{X}_k$ for $k = 1, 2, \ldots, N$ where each $\widehat{X}_k$ is one of the original X_j chosen randomly with equal probability (a bootstrap sample)
- a given X_j can occur multiple times in the bootstrap sample
- obtain large number B of such estimates
- let $\widehat{\langle f \rangle} = (1/B) \sum_{b=1} \langle f \rangle_b$
- bootstrap error given by

$$\sigma^{(B)} = \left(\frac{1}{B-1} \sum_{b=1}^{B} (\langle f \rangle_b - \widehat{\langle f \rangle})^2 \right)^{1/2}$$

- plot of probability distribution from bootstrap estimates

The effective mass

- particularly good visual tool to see how well energy extracted is so-called effective mass
- for correlator $C(t)$, effective mass defined by

$$m_{\text{eff}}(t) = \ln\left(\frac{C(t)}{C(t+a_t)}\right)$$

- function which tends to $E_1 - E_0$ as t becomes large

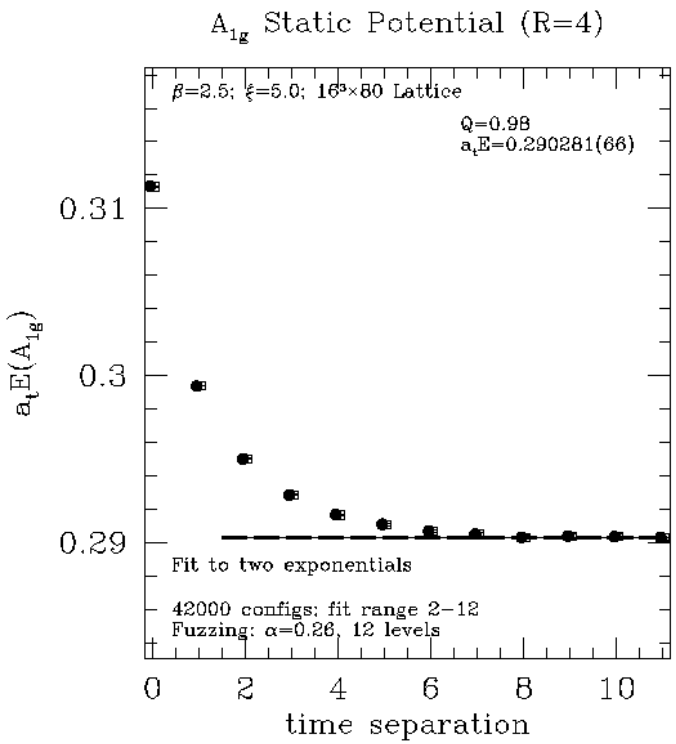
$$\lim_{t\to\infty} m_{\text{eff}}(t) = \lim_{t\to\infty} \ln\left(\frac{A_1 e^{-(E_1-E_0)t}\left(1+(A_2/A_1)e^{-(E_2-E_1)t}+\ldots\right)}{A_1 e^{-(E_1-E_0)(t+a_t)}\left(1+(A_2/A_1)e^{-(E_2-E_1)(t+a_t)}+..\right)}\right)$$

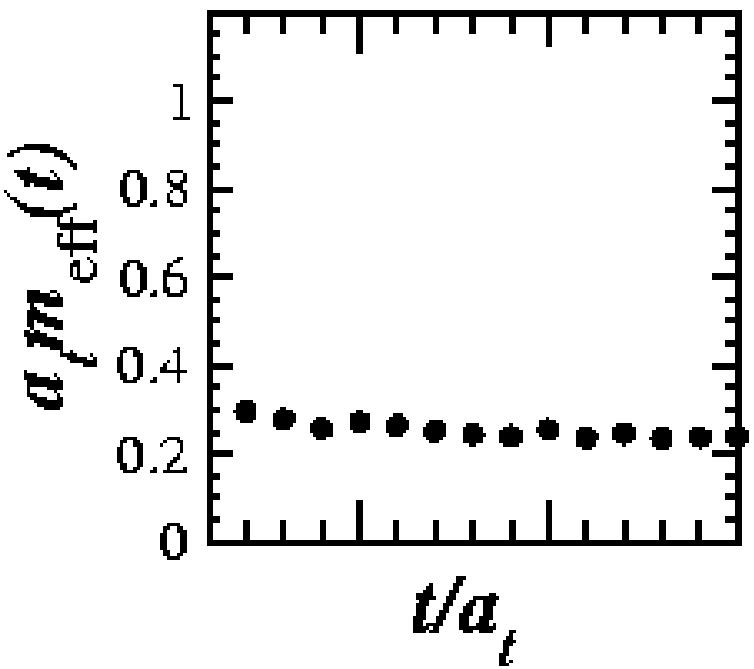
$$= \ln\left(e^{(E_1-E_0)a_t}\right) = a_t(E_1-E_0).$$

- value $E_1 - E_0$ seen as large-time plateau in effective mass
- contributions from faster-decaying exponentials seen as deviations of the effective mass from its asymptotic plateau value
- "good" operator with little coupling to higher-lying states = rapid onset of plateau
- statistically noise generally grows with t

The effective mass (continued)

- two examples of effective masses
- left: static quark-antiquark potential for separation 0.5 fm
- right: nucleon





Excited states from correlation matrices

- extracting more than just the lowest energy in a symmetry channel requires a hermitiam matrix of correlation functions $C_{ij}(t)$
- let $\lambda_n(t,t_0)$ denote eigenvalues of $C(t_0)^{-1/2}\,C(t)\,C(t_0)^{-1/2}$, for t_0 some fixed reference time
- these eigenvalues can be viewed as principal correlators
- ordered such that $\lambda_0 \geq \lambda_1 \geq \cdots$ as t becomes large
- can show that

$$\begin{aligned} \lim_{t\to\infty} \lambda_n(t,t_0) &= e^{-E_n(t-t_0)}\Big(1+O(e^{-\Delta_n(t-t_0)})\Big), \\ \Delta_n &= \min_{k\neq n} |E_k - E_n|. \end{aligned}$$

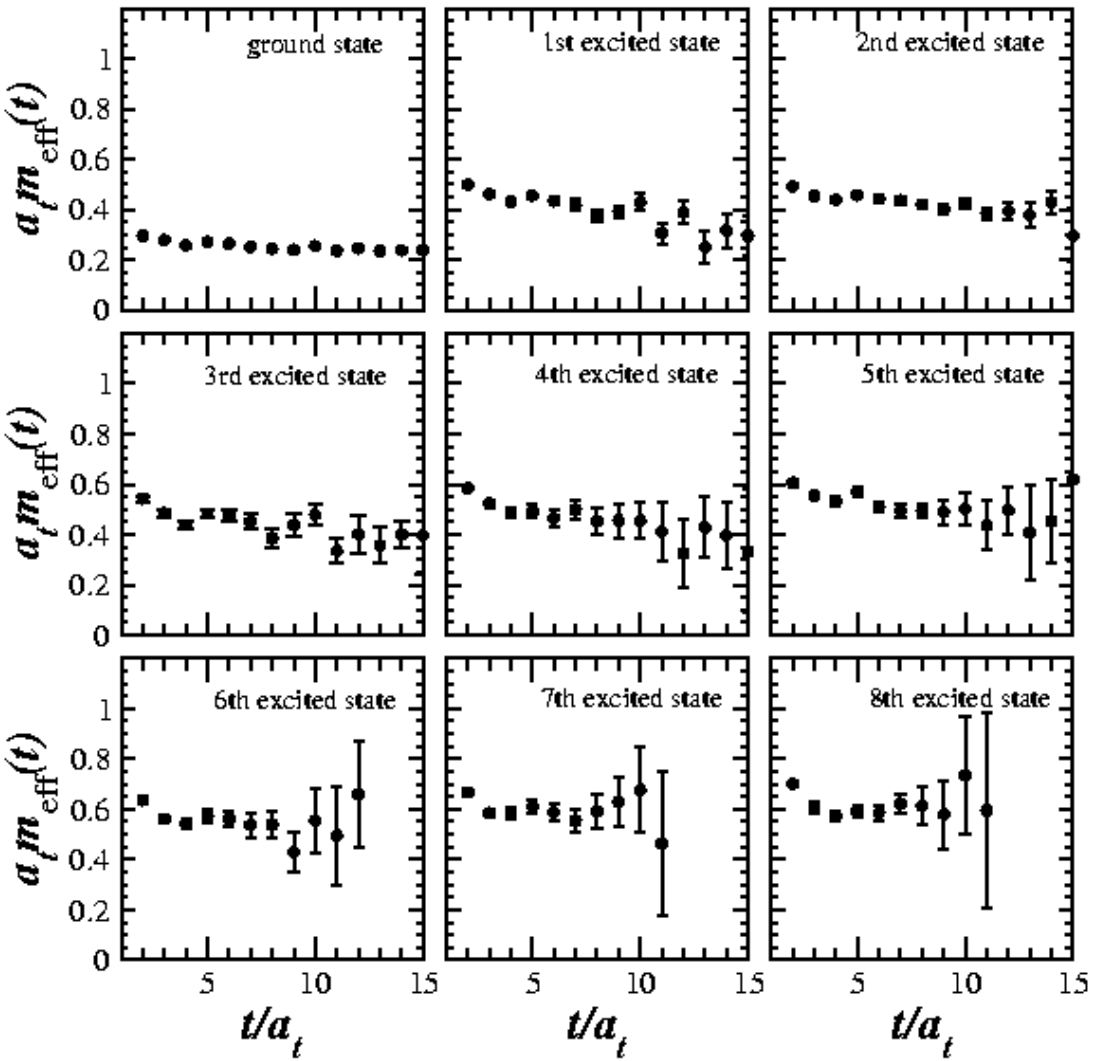
- principal effective masses associated with principal correlators

$$m_{\rm eff}^{(n)}(t) = \ln\left(\frac{\lambda_n(t,t_0)}{\lambda_n(t+a_t,t_0)}\right)$$

- for $N\times N$ correlation matrix, these functions plateau to N lowest lying energies

Principal effective masses

- LHPC currently holds world record for most energy levels extracted in any lattice QCD computation: 9 in nucleon channel



Spectrum for free scalar field theory

- for free-field case on $N_x \times N_y \times N_t$ lattice, define

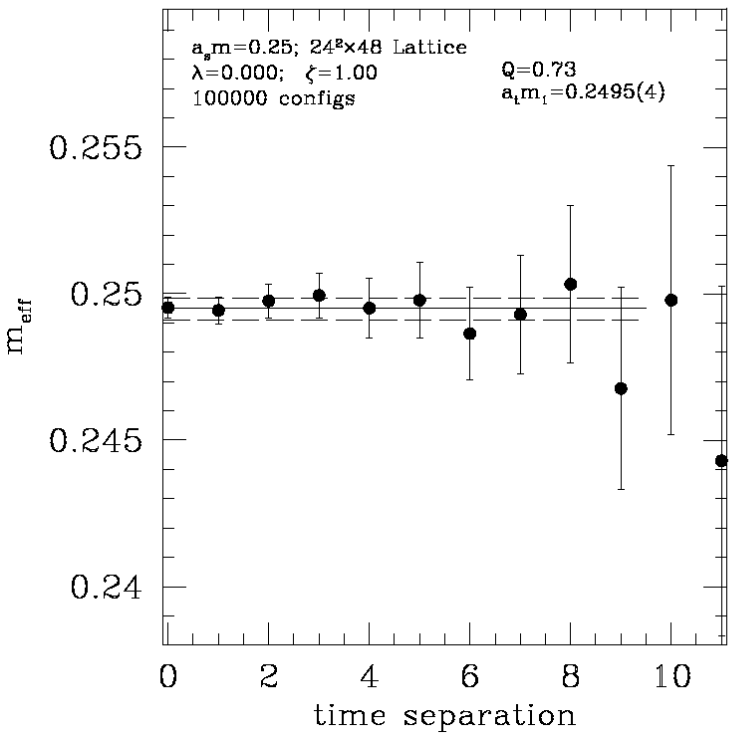
$$\Phi(t, n_x, n_y) = \sum_{x,y} \phi(x, y, t)\ e^{2\pi i x n_x / N_x + 2\pi i n_y / N_y}$$

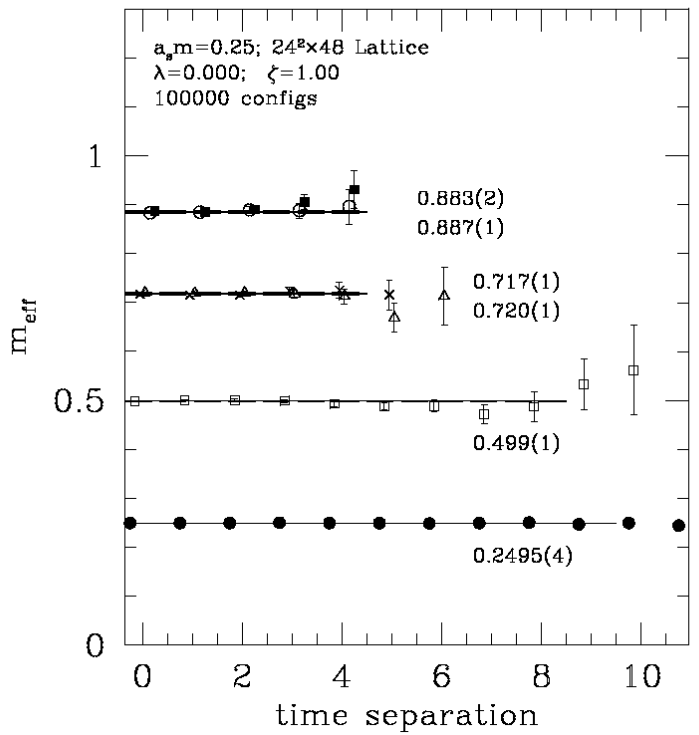
- lowest six levels having total zero momentum can be extracted using the following set of six operators:

$$\begin{aligned}
O_0(t) &= \Phi(t,0,0) \\
O_1(t) &= \Phi(t,0,0)\ \Phi(t,0,0) \\
O_2(t) &= \Phi(t,1,0)\ \Phi(t,-1,0) \\
O_3(t) &= \Phi(t,0,1)\ \Phi(t,0,-1) \\
O_4(t) &= \Phi(t,1,1)\ \Phi(t,-1,-1) \\
O_5(t) &= \Phi(t,1,-1)\ \Phi(t,-1,1)
\end{aligned}$$

Spectrum for $\lambda = 0$

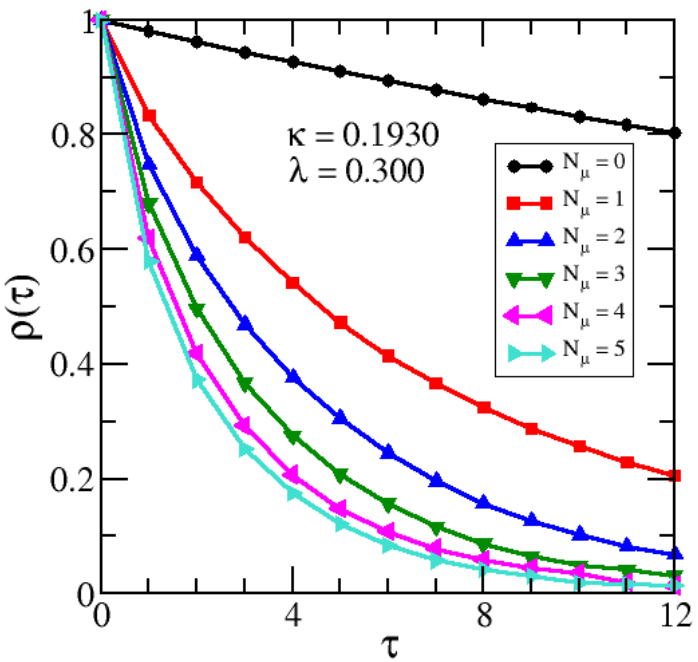
- extracted six lowest-lying levels in $\lambda = 0$ scalar field theory
- $24^2 \times 48$ isotropic lattice with $a_s m = 0.25$
- exact results: 0.24935 for the mass, 0.49871 for twice the mass, 0.71903 for the two states having minimal relative momenta, and 0.88451 for the next two states

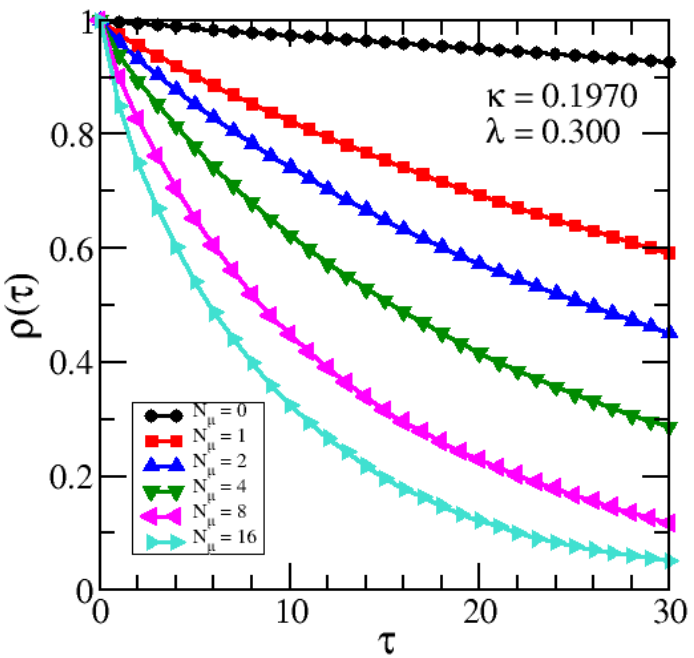




Autocorrelations in the interacting theory

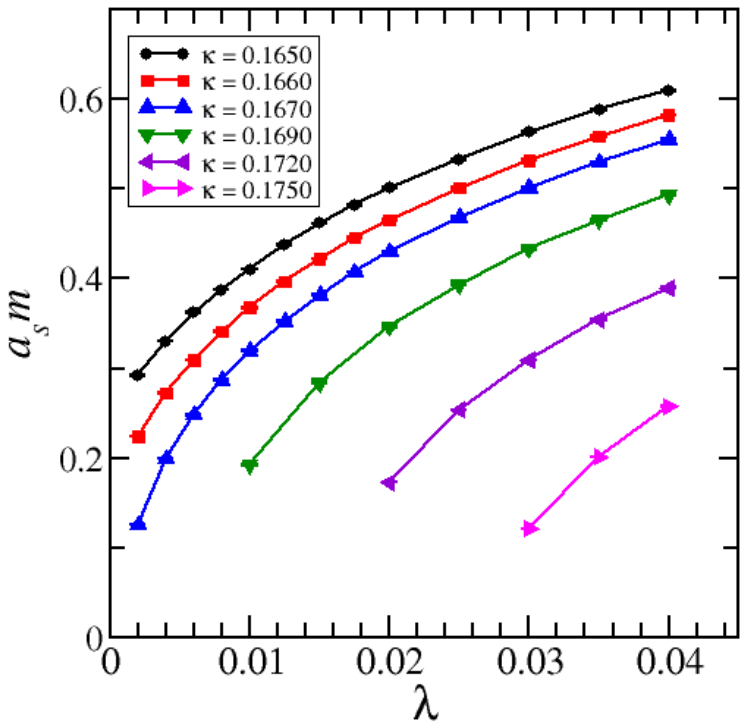
- autocorrelations $\rho(\tau)$ of $\langle \Phi(t)\Phi(0)\rangle$ for $t \sim 1/(2a_s m_{\rm gap})$
- compound sweep = 1 Metropolis + N_μ microcanonical sweep
- $\mu = 1$ is probability of proposing change in microcanonical
- left plot: $t = 2a_t$ used with $\kappa = 0.1930$ and $\lambda = 0.300$ on $24^2 \times 48$ isotropic lattice and $a_s m_{\rm gap} \sim 0.25$
- right plot: $t = 5a_t$ used with $\kappa = 0.1970$ and $\lambda = 0.300$ on $32^2 \times 96$ isotropic lattice and $a_s m_{\rm gap} \sim 0.10$
- microcanonical acceptance rate about 80% in both cases

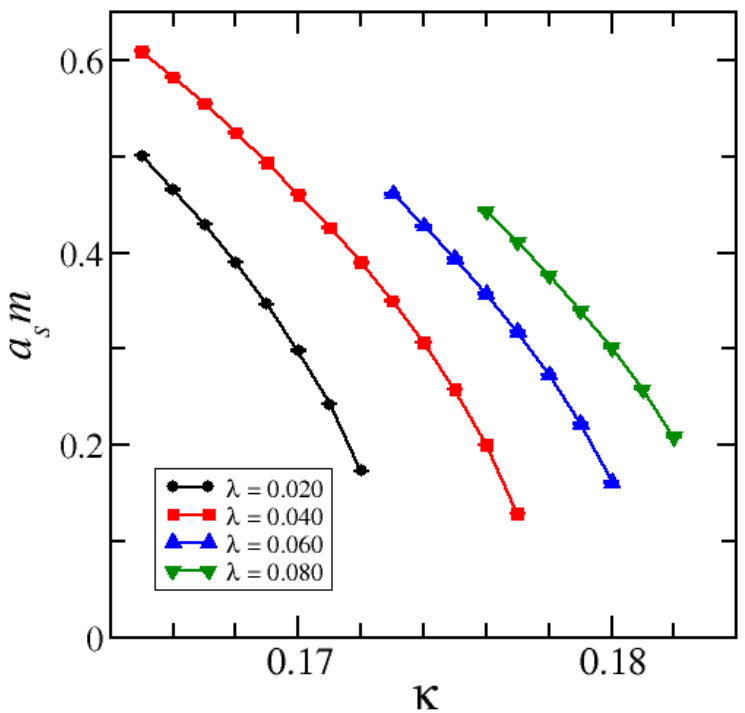




Mass gaps

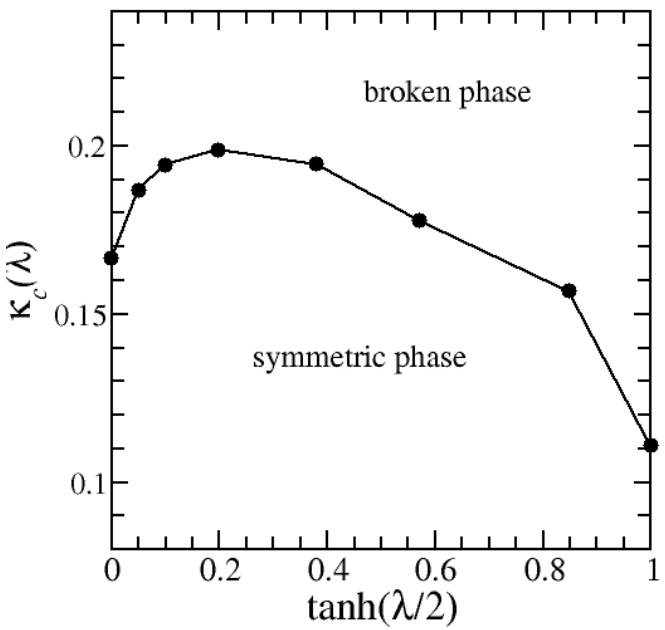
- various single particle masses on 24^3 isotropic lattice





Phase structure

- theory has two phases separated by a line of critical points
- for each value of λ, there exists a critical value $\kappa_c(\lambda)$ at which mass gap goes to zero
- symmetric phase for $\kappa < \kappa_c(\lambda)$
  - $\phi \to -\phi$ symmetry holds, $\langle \phi \rangle = 0$
- broken phase for $\kappa > \kappa_c(\lambda)$
  - $\phi \to -\phi$ spontaneously broken, $\langle \phi \rangle \neq 0$



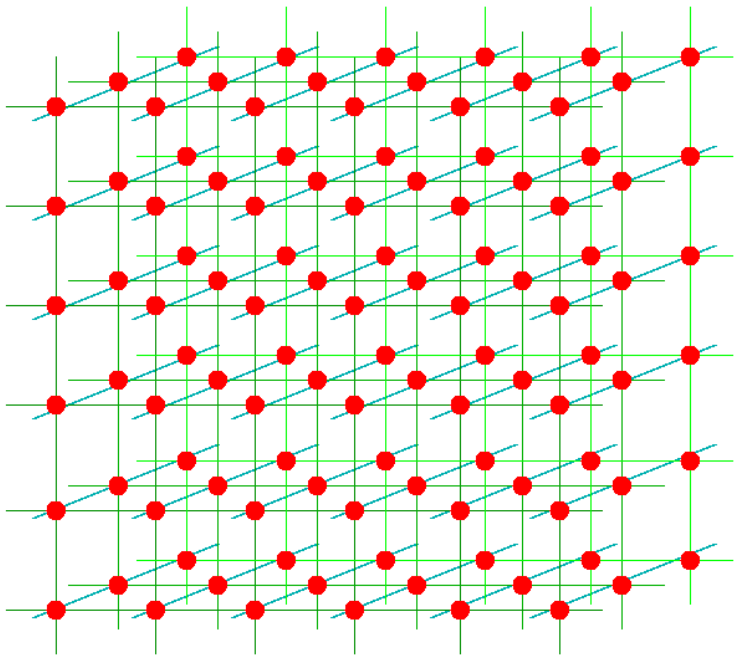
Part V

Monte Carlo calculations in lattice Quantum Chromodynamics

Lattice QCD

- hypercubic space-time lattice
- quarks reside on sites, gluons reside on links between sites
- for gluons, 8 dimensional integral on each link

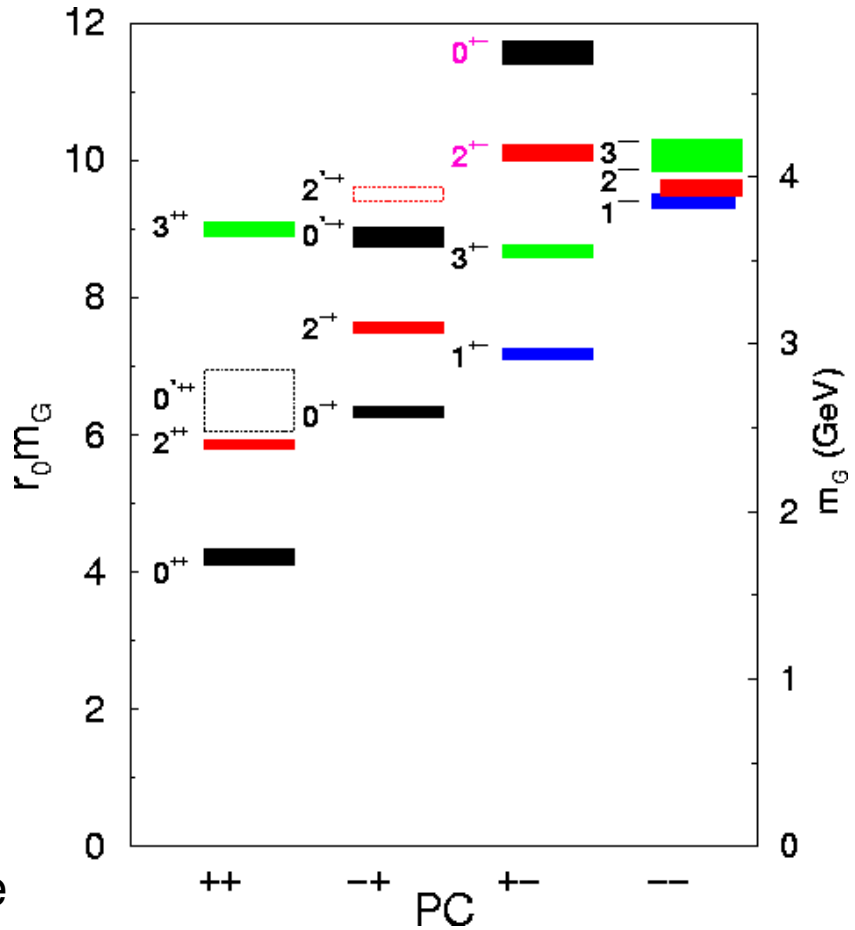
- path integral has dimension $32N_xN_yN_zN_t$
  - 10.6 million for 24^4 lattice
- more sophisticated updating algorithms
- systematic errors
  - discretization
  - finite volume



Glueball spectrum in pure gauge theory

- gluons can bind to form glueballs
  - e.m. analogue: massive globules of pure light!
- states labeled by J^{PC}
- scale set by $r_0^{-1} = 410(20)$ MeV
- computed using pseudo-heatbath and microcanonical
- 24×24 correlation matrix in each symmetry channel
- spin identification
- mass gap with a bounty
  - Clay mathematics institute will pay $ 1 million

C. Morningstar and M. Peardon, Phys. Rev. D 60, 034509 (1999)



Conclusion

- observables in quantum mechanical systems can be extracted from the correlation functions of the theory
- correlation functions can be computed using path integrals
- path integrals in the imaginary time formalism can be evaluated using the Monte Carlo method
- importance sampling from Markov chains
- Metropolis-Hastings method
- microcanonical updating
- 1-dimensional simple harmonic oscillator was first example
- calculations in real scalar ϕ^4 theory in $2+1$ dimensions

For Further Reading

- C.M. Grinstead and J.L. Snell,
  Introduction to Probability
- E. Parzen,
  Stochastic Processes
  (Holden-Day, San Francisco, 1962).
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  Stochastic Processes
  (Macmillan, New York, 1965).
- I. Montvay and G. Münster
  Quantum Fields on a Lattice
  (Cambridge Press, 1994).