

Stochastic Simulation

Aiichiro Nakano

*Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Chemical Engineering & Materials Science
Department of Quantitative & Computational Biology
University of Southern California*

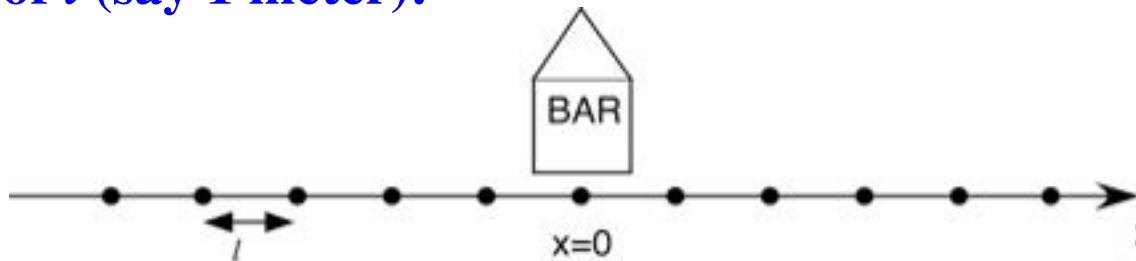
Email: anakano@usc.edu

Goal: Random walk,
central limit theorem,
diffusion equation



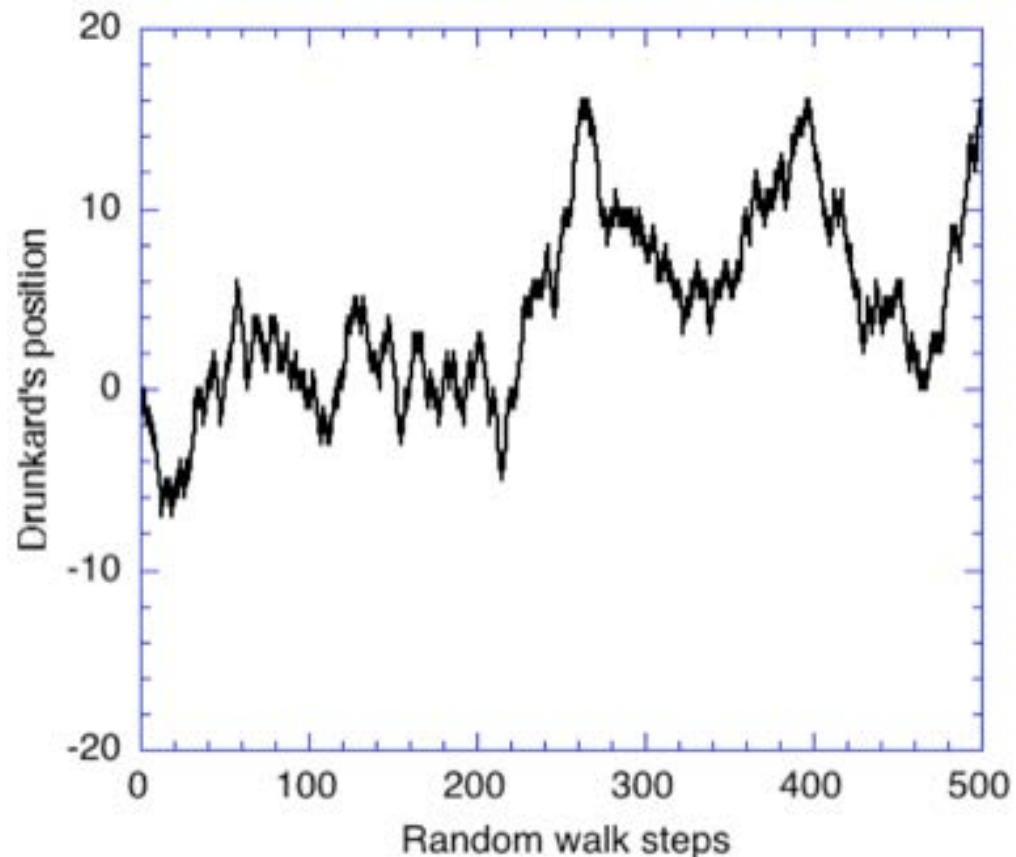
Random Walk

- **Drunkard's walk problem:** A drunkard starts from a bar ($x = 0$) & at every time interval τ (say 1 second) moves randomly either to the right or to the left by a step of l (say 1 meter).



- **Program diffuse.c**

```
initialize a random number sequence
for walker = 1 to N_walker
    position = 0
    for step = 1 to Max_step
        if rand() > RAND_MAX/2 then
            increment position by 1
        else
            decrement position by 1
        endif
    endfor step
endfor walker
```



Applications of Random Walk

Applications in Phys 516

- $x = \text{stock price}$: Stochastic simulation of a stock
- $x = 1\text{D coordinate, histogram of the walkers} = \text{probability to find a quantum particle}$: Quantum Monte Carlo (QMC) simulation

What to learn

- Probability: Central limit theorem
- Partial differential equation (PDE): Diffusion equation

Historical origin

- Einstein's theorem of Brownian motion (1905)



from Prof. Paul Newton's
homepage



5. Über die von der molekularkinetischen Theorie
der Wärme geforderte Bewegung von in ruhenden
Flüssigkeiten suspendierten Teilchen;
von A. Einstein.

In dieser Arbeit soll gezeigt werden, daß nach der molekularkinetischen Theorie der Wärme in Flüssigkeiten suspendierte Körper von mikroskopisch sichtbarer Größe infolge der Molekularbewegung der Wärme Bewegungen von solcher Größe ausführen müssen, daß diese Bewegungen leicht mit dem Mikroskop nachgewiesen werden können. Es ist möglich, daß die hier zu behandelnden Bewegungen mit der sogenannten „Brownschen Molekularbewegung“ identisch sind; die mir erreichbaren Angaben über letztere sind jedoch so ungenau, daß ich mir hierüber kein Urteil bilden konnte.

Wenn sich die hier zu behandelnde Bewegung samt den für sie zu erwartenden Gesetzmäßigkeiten wirklich beobachten läßt, so ist die klassische Thermodynamik schon für mikroskopisch unterscheidbare Räume nicht mehr als genau gültig anzusehen und es ist dann eine exakte Bestimmung der wahren Atomgröße möglich. Erwiese sich umgekehrt die Voraussage dieser Bewegung als unzutreffend, so wäre damit ein schwerwiegendes Argument gegen die molekularkinetische Auffassung

Diffusion Equation

558

A. Einstein.

und indem wir

$$\frac{1}{\tau} \int_{-\infty}^{+\infty} \frac{\Delta^2}{2} \varphi(\Delta) d\Delta = D$$

Diffusion constant

$$D = \left\langle \frac{\Delta^2}{2\tau} \right\rangle_{\text{avg}}$$

setzen und nur das erste und dritte Glied der rechten Seite berücksichtigen:

(1)

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}.$$

Histogram, $f(x,t)$, of random walkers follows a partial differential equation

Dies ist die bekannte Differentialgleichung der Diffusion, und man erkennt, daß D der Diffusionskoeffizient ist.

A. Einstein, Ann. Phys. 17, 549-560 (1905)

Stochastic Model of Stock Prices

Fluctuation in stock price

Market Summary > Apple Inc

NASDAQ: AAPL

+ Follow

132.05 USD +1.13 (0.86%) ↑

Closed: Jan 8, 7:59 PM EST · Disclaimer

After hours 131.75 -0.30 (0.23%)

1 day

5 days

1 month

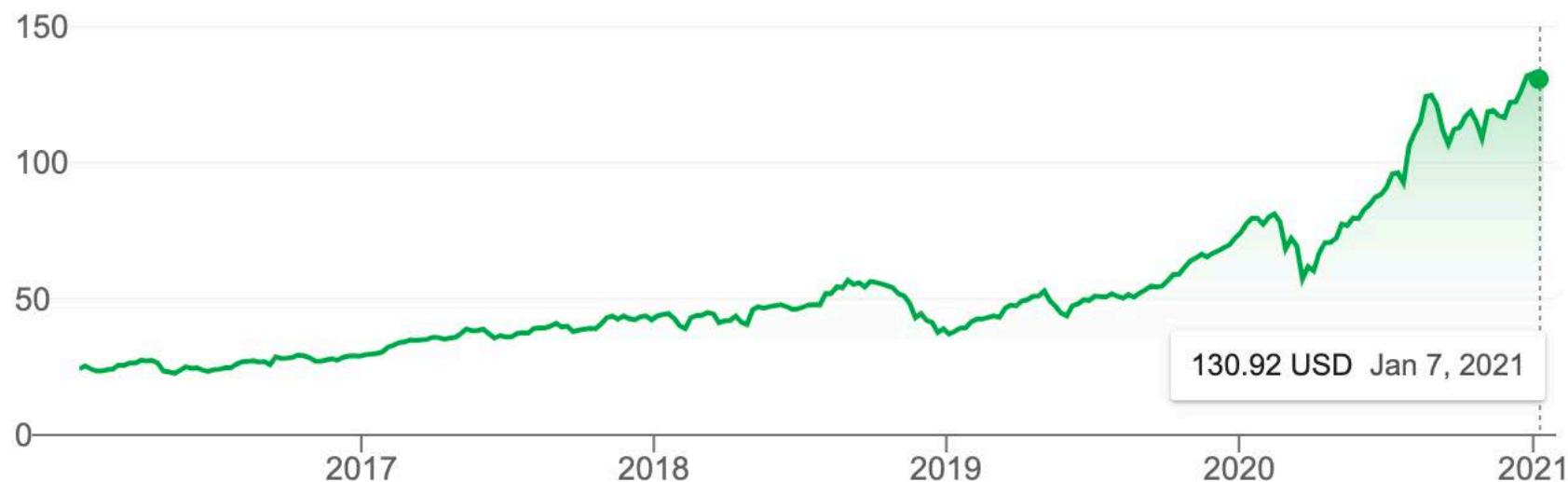
6 months

YTD

1 year

5 years

Max



Stochastic Model of Stock Prices

Basis of Black-Scholes analysis of option prices

$$dS = \mu S dt + \sigma S \varepsilon \sqrt{dt}$$



The Bank of Sweden Prize in Economic Sciences in Memory of Alfred Nobel
1997

"for a new method to determine the value of derivatives"



Robert C. Merton

1/2 of the prize
USA

Harvard University
Cambridge, MA, USA
b. 1944

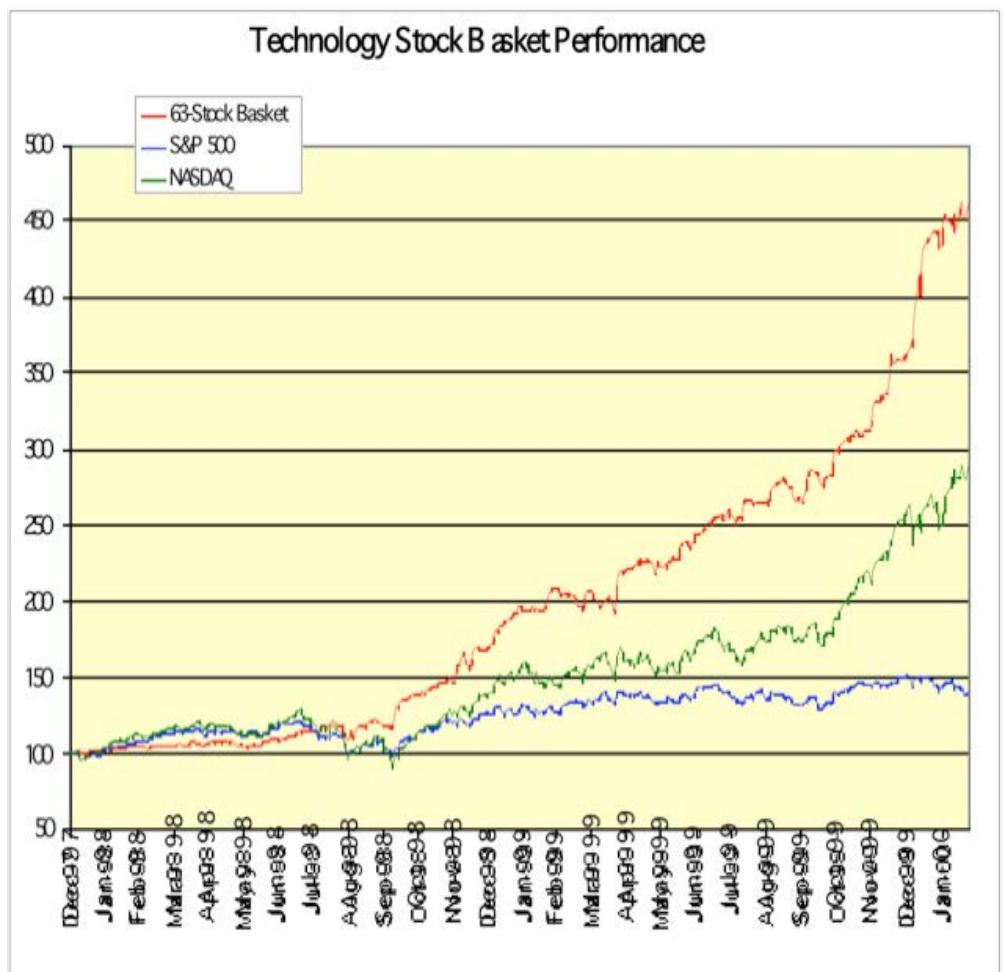


Myron S. Scholes

1/2 of the prize
USA

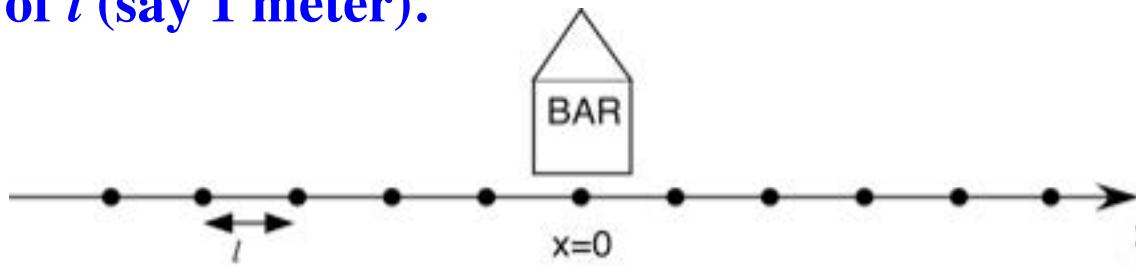
Long Term Capital Management
Greenwich, CT, USA
b. 1941
(in Timmins, ON, Canada)

Computational stock portfolio trading



Random Walk

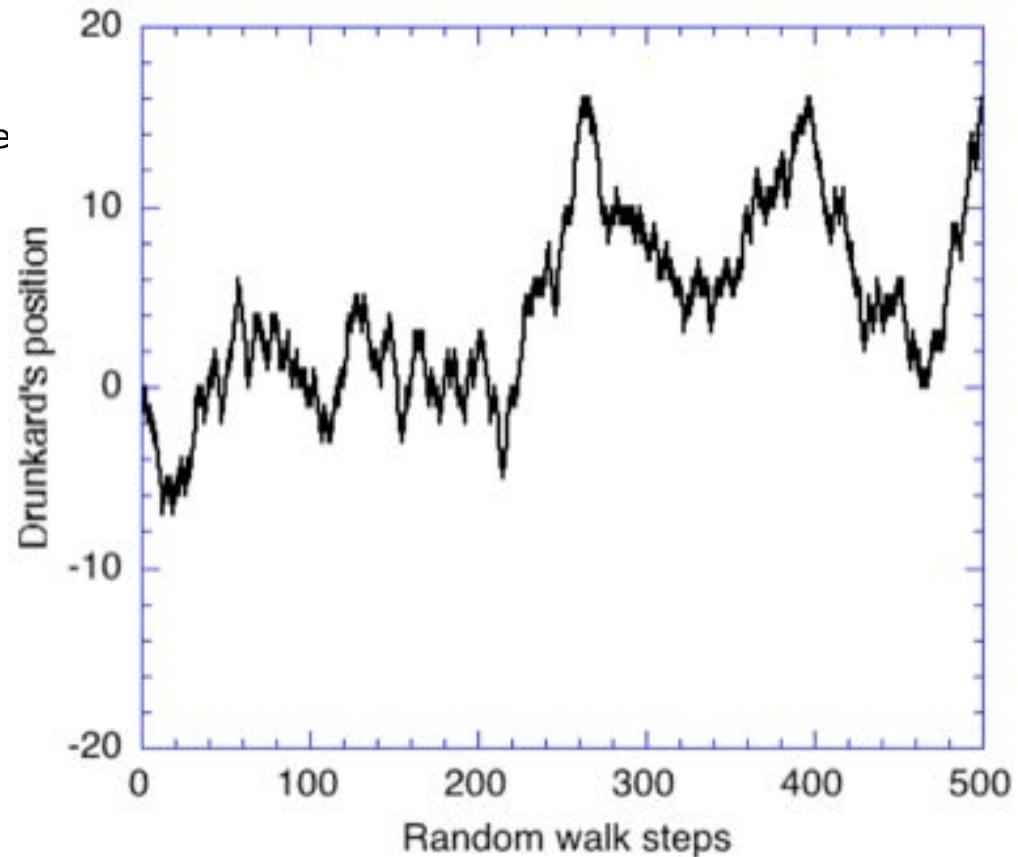
- **Drunkard's walk problem:** A drunkard starts from a bar ($x = 0$) & at every time interval τ (say 1 second) moves randomly either to the right or to the left by a step of l (say 1 meter).



- Program [diffuse.c](#)

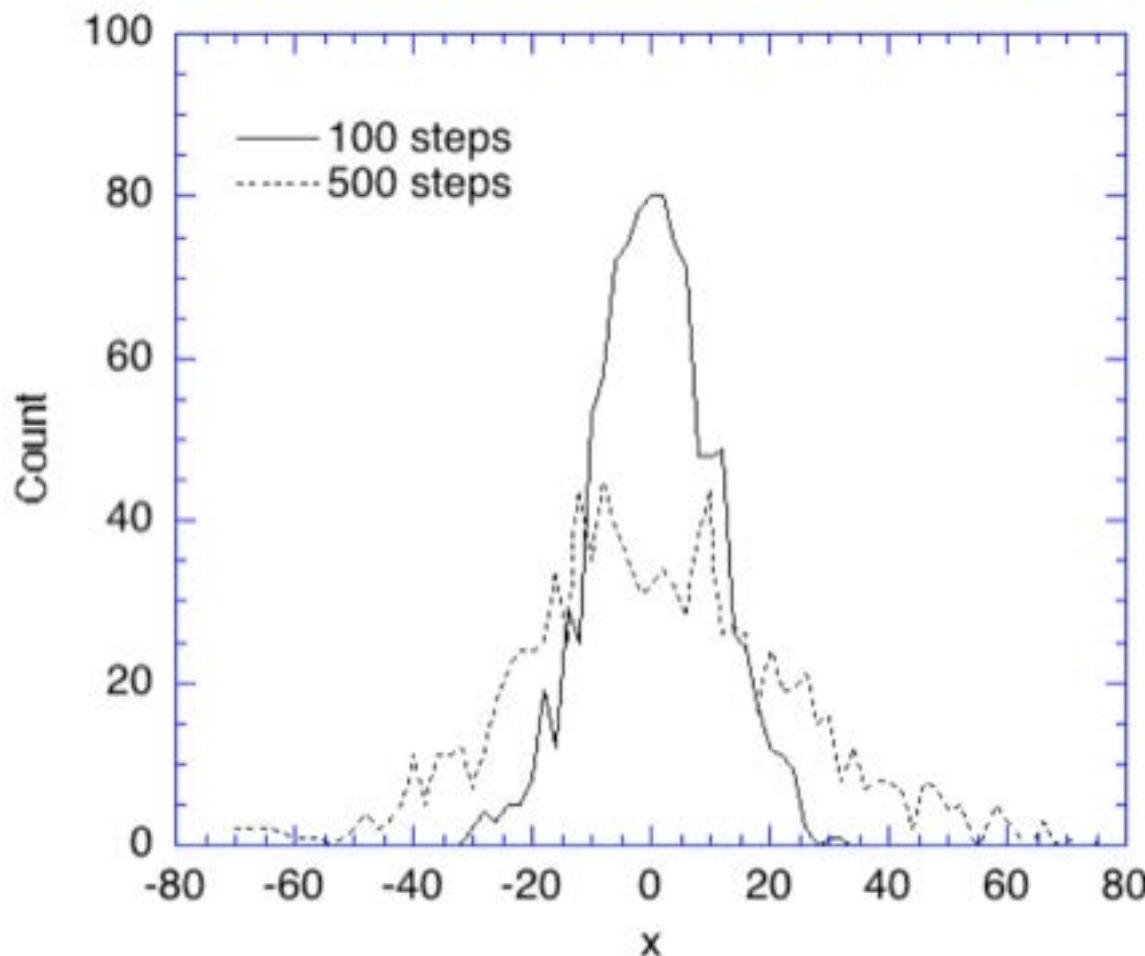
```
initialize a random number sequence
for walker = 1 to N_walker
    position = 0
    for step = 1 to Max_step
        if rand() > RAND_MAX/2 then
            increment position by 1
        else
            decrement position by 1
        endif
    endfor step
endfor walker
```

Outer loop over walkers
to take statistics



Probability Distribution

- **Probability distribution, $P(x, t)$:** Histogram of the positions of many drunkards (with different random-number seeds)



See `hist[]` in [diffuse.c](#)

Binomial Distribution

$$P_n(x = (n_{\rightarrow} - n_{\leftarrow})l) = \frac{n!}{n_{\rightarrow}! n_{\leftarrow}!} p^{n_{\rightarrow}} (1-p)^{n_{\leftarrow}}$$

- Generating function

$$\sum_{n_{\rightarrow}=0}^n \frac{n!}{n_{\rightarrow}! n_{\leftarrow}!} p^{n_{\rightarrow}} q^{n_{\leftarrow}} = (p+q)^n$$

- Differentiate w.r.t. p & multiply by p (then w.r.t. q),

$$\langle x_n \rangle = \sum_{n_{\rightarrow}=0}^n \frac{n!}{n_{\rightarrow}! n_{\leftarrow}!} p^{n_{\rightarrow}} (1-p)^{n_{\leftarrow}} (n_{\rightarrow} - n_{\leftarrow})l = n(p-q)l$$

$$\begin{aligned}\langle x_n^2 \rangle - \langle x_n \rangle^2 &= [n(n-1)(p-q)^2 + n]l^2 - [n(p-q)l]^2 \\ &= [1 - (p-q)^2]nl^2 \\ &= [(p+q)^2 - (p-q)^2]nl^2 \\ &= 4pqnl^2.\end{aligned}$$

- For $p = q = 1/2$, $\text{Var}[x_n] = nl^2$

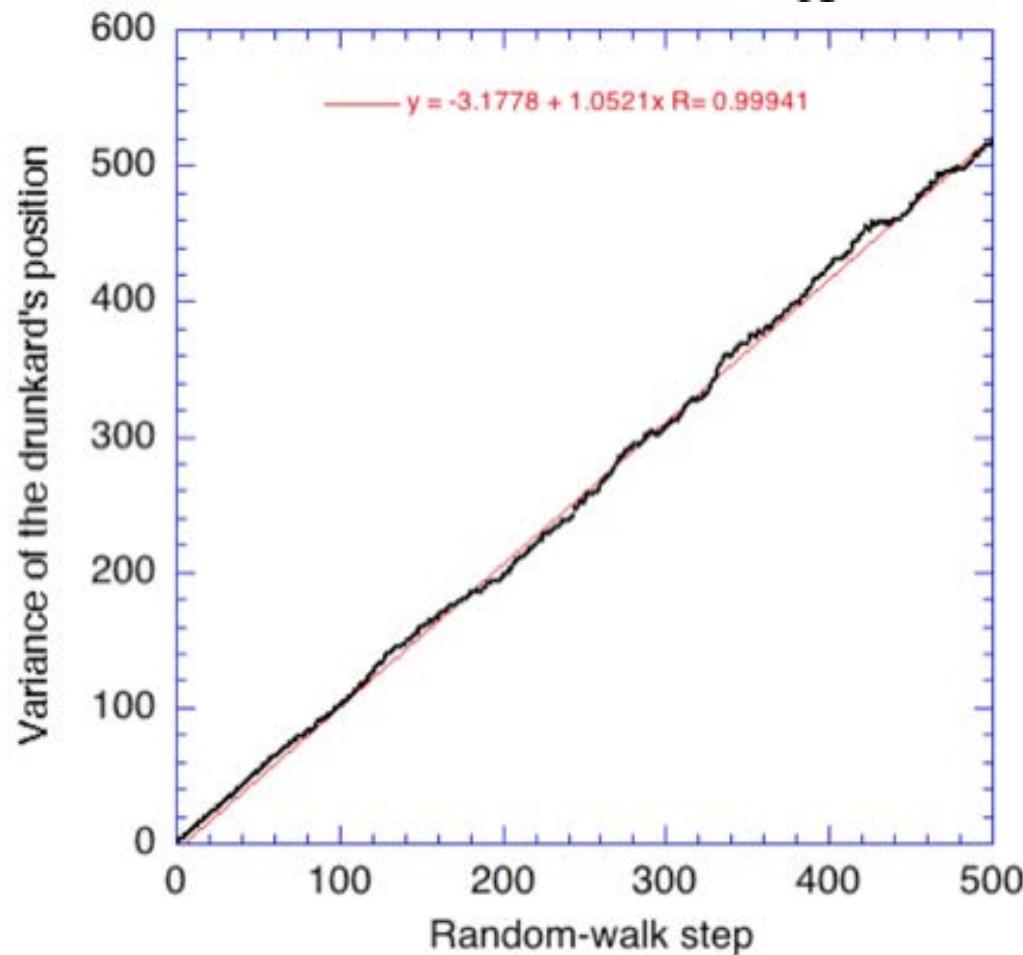
See [lecture note](#) (p. 3) for proof

Diffusion Law

$$\langle x(t = n\tau)^2 \rangle = nl^2 = 2 \left(\frac{l^2}{2\tau} \right) t$$

\cancel{D}

$$\frac{1}{\tau} \int_{-\infty}^{+\infty} \frac{\Delta^2}{2} \varphi(\Delta) d\Delta = D$$



Continuous Limit: Diffusion Equation

- Recursive relation

$$P(x,t) = \frac{1}{2} P(x-l,t-\tau) + \frac{1}{2} P(x+l,t-\tau)$$

$$\frac{P(x,t) - P(x,t-\tau)}{\tau} = \frac{l^2}{2\tau} \frac{P(x-l,t-\tau) - 2P(x,t-\tau) + P(x+l,t-\tau)}{l^2}$$

- $\tau \rightarrow 0, l \rightarrow 0, l^2/2\tau = D = \text{constant}$

$$\frac{\partial}{\partial t} P(x,t) = D \frac{\partial^2}{\partial x^2} P(x,t)$$

- Schrödinger equation in imaginary time $it \equiv \tau \rightarrow$ basis of Quantum Monte Carlo simulation

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}.$$

Analytic Solution of Diffusion Equation

- Formal solution

$$P(x,t) = \exp\left(tD \frac{\partial^2}{\partial x^2}\right) P(x,0) \quad \text{←} \quad \frac{\partial}{\partial t} P = D \frac{\partial^2}{\partial x^2} P$$

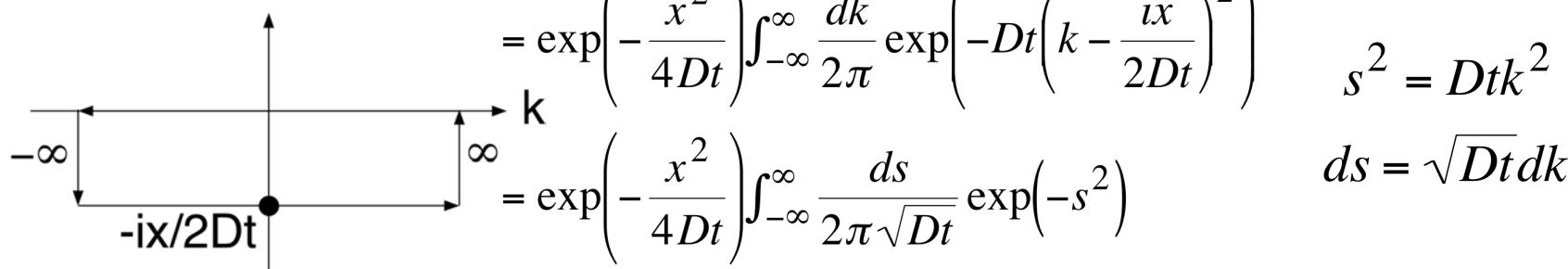
- Initial condition: delta function

$$P(x,0) = \delta(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp(ikx)$$

$$P(x,t) = \exp\left(tD \frac{\partial^2}{\partial x^2}\right) \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp(ikx) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp(-Dtk^2 + ixk)$$

$$= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp\left(-Dt\left(k - \frac{ix}{2Dt}\right)^2 + \frac{x^2}{4D^2t^2}\right)$$

$$= \exp\left(-\frac{x^2}{4Dt}\right) \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp\left(-Dt\left(k - \frac{ix}{2Dt}\right)^2\right) \quad s^2 = Dtk^2$$



$$\oint dz = 0$$

$$= \exp\left(-\frac{x^2}{4Dt}\right) \frac{\sqrt{\pi}}{2\pi\sqrt{Dt}} = \boxed{\frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{x^2}{2\sigma^2}\right)} \quad \sigma^2 = 2Dt$$

Delta Function

- Orthonormal basis set: Plane waves

$$\left\{ \frac{1}{\sqrt{N}} \exp(ik_m x) \mid k_m = \frac{2\pi m}{L} \quad (m = 0, \dots, N-1) \right\}$$

- Completeness

$$\psi_j = \sum_{l=0}^{N-1} \frac{1}{N} \sum_{m=0}^{N-1} \exp(ik_m(x_j - x_l)) \psi_l$$

- $\Delta x \rightarrow 0$

$$\psi(x_j) = \int_0^L \frac{dx}{\Delta x} \frac{1}{N} \sum_{m=0}^{N-1} \exp(ik_m(x_j - x)) \psi(x) = \int_0^L \frac{dx}{L} \sum_{m=0}^{N-1} \exp(ik_m(x_j - x)) \psi(x)$$

$$\therefore \delta(x_j - x) = \frac{1}{L} \sum_{m=0}^{N-1} \exp(ik_m(x_j - x))$$

$$\delta(x_j - x) = \frac{1}{2\pi} \frac{2\pi}{L} \sum_{m=0}^{N-1} \exp(ik_m(x_j - x))$$

$$= \frac{1}{2\pi} \Delta k \sum_{m=0}^{N-1} \exp(ik_m(x_j - x)) \rightarrow \frac{1}{2\pi} \int dk \exp(ik(x_j - x))$$

$$\boxed{\Delta k = \frac{2\pi}{L} \rightarrow 0}$$

Big Picture: Closing the Loop

drunkard's walk

↓ binomial
distribution

$$P_N(x) = \frac{N!}{N_{\rightarrow}! N_{\leftarrow}!} p^{N_{\rightarrow}} q^{N_{\leftarrow}}$$

$$\xrightarrow{\tau, l \rightarrow 0 \quad l^2/\tau = \text{cnst} \equiv 2D}$$

$$\xrightarrow{N \rightarrow \infty}$$

central limit theorem

$$\frac{\partial}{\partial t} P = D \frac{\partial^2}{\partial x^2} P$$

↓ exact
solution

$$P(x,t) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

$$\sigma = l\sqrt{N}$$

$$\sigma^2 = 2Dt = 2\frac{l^2}{2\tau}t = Nl^2$$

Central Limit Theorem

$$P_N(x) = \frac{N!}{\left(\frac{N+x}{2}\right)!\left(\frac{N-x}{2}\right)!} \left(\frac{1}{2}\right)^N \quad x = (n_{\rightarrow} - n_{\leftarrow})$$

Here, we set $l = 1$

- For $N \rightarrow \infty$,

$$\lim_{N \rightarrow \infty} P_N(x) = P(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right) \quad \sigma = \sqrt{N}$$

where we have used Stirling's formula

$$N! = \sqrt{2\pi} N^{N+1/2} e^{-N} \left(1 + \frac{1}{12N} + \dots\right)$$

- **Central limit theorem:** Sum of any random variables, $Y = (y_1 + \dots + y_N)$, itself is a random variable that follows the normal (Gaussian) distribution for large N

Stirling's Formula

- **Gamma function:** $\Gamma(z) \equiv \int_0^\infty e^{-t} t^{z-1} dt \quad (z \in C; \operatorname{Re} z > 0)$

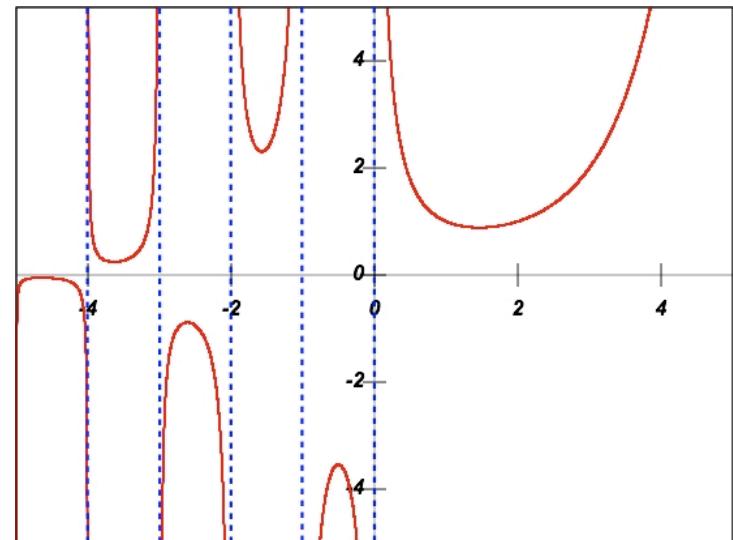
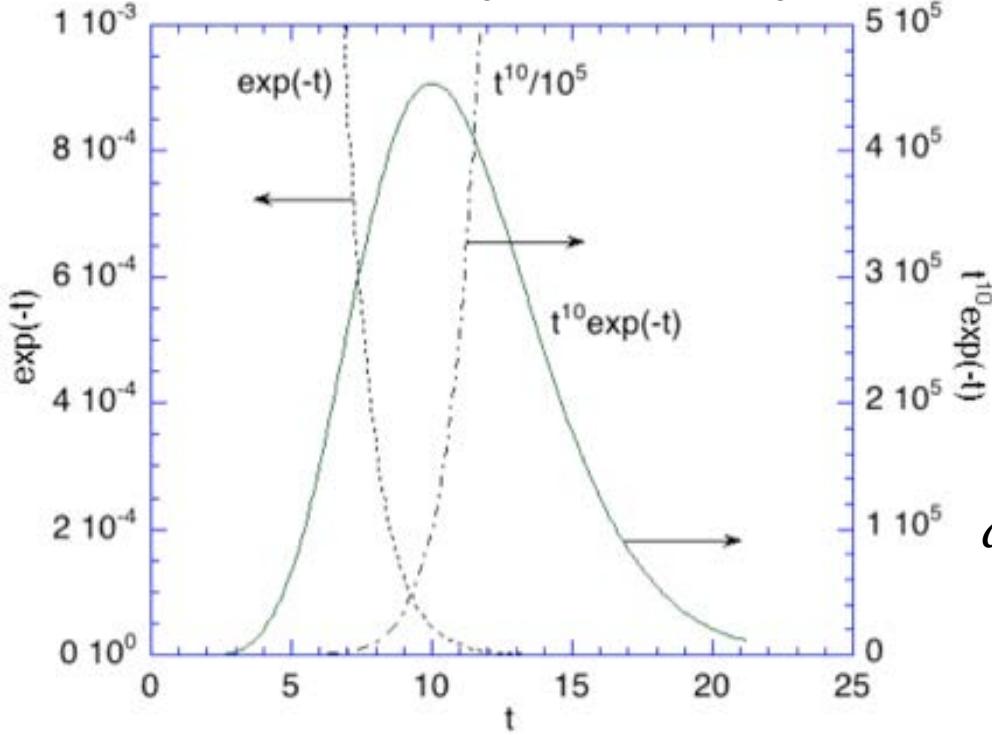
1. $\Gamma(z+1) = \int_0^\infty e^{-t} t^z dt = \left[-e^{-t} t^z \right]_0^\infty - \int_0^\infty (-e^{-t}) z t^{z-1} dt = z\Gamma(z)$

2. $\Gamma(0) = \int_0^\infty e^{-t} dt = \left[-e^{-t} \right]_0^\infty = 1$ Integration by parts

$$\therefore \Gamma(N+1) = N\Gamma(N) = N(N-1)\Gamma(N-1) = \dots = N!$$

- **Asymptotic expansion strategy**

$$\Gamma(z+1) = \int_0^\infty e^{-t} t^z dt = \int_0^\infty f(t) dt$$



$$df/dt = e^{-t} t^{z-1} (-t + z) = 0$$



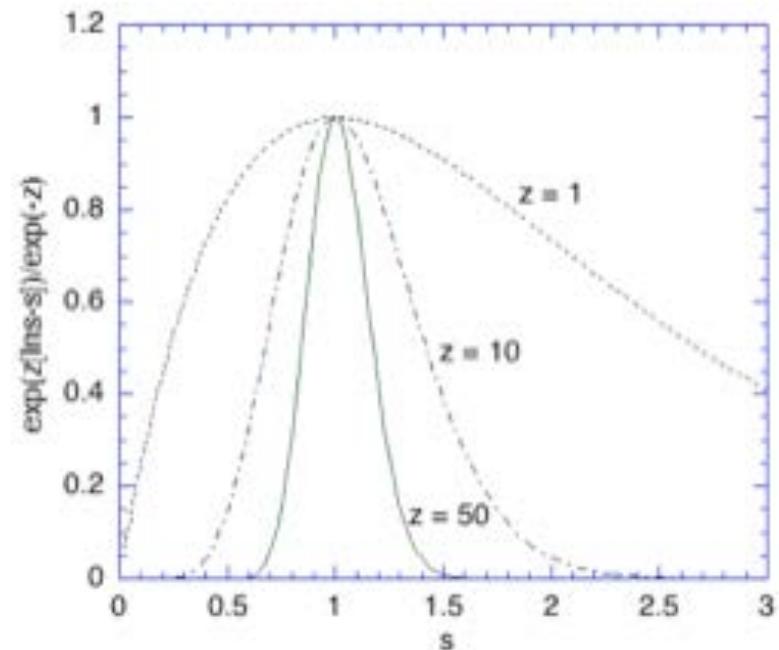
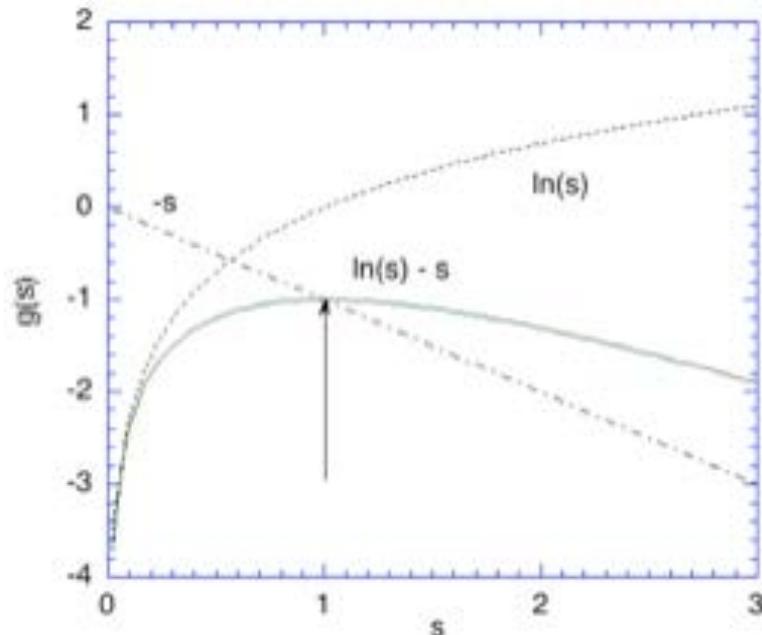
$$t = z$$

Saddle-Point Method

- $t \equiv sz$ — factor out explicit z dependence:

$$\Gamma(z+1) = \int_0^\infty e^{-zs} (zs)^z z ds = z^{z+1} \int_0^\infty e^{-zs} \exp(z \ln s) ds = z^{z+1} \int_0^\infty \exp(z(\ln s - s)) ds$$

- $g(s) = \ln s - s$, is peaked at $s = 1$ ($dg/ds = 1/s - 1 = 0$ at $s = 1$)



- Taylor expansion at the maximum

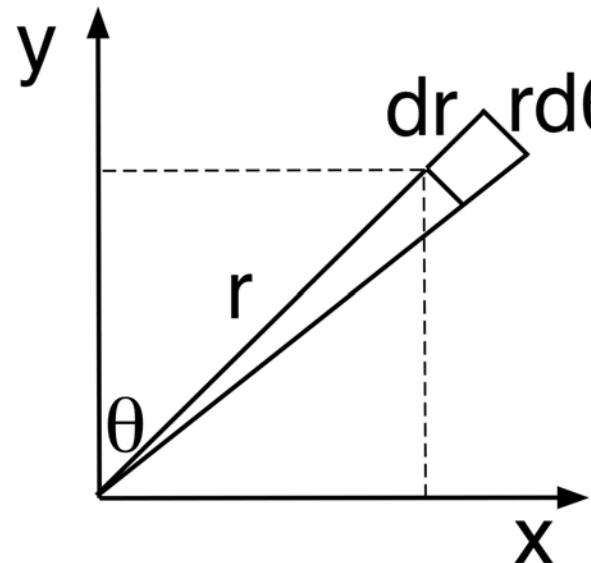
$$g(s) = g(1) + g'(1)(s-1) + \frac{1}{2} g''(1)(s-1)^2 + \dots$$

$$= -1 - \frac{1}{2} (s-1)^2 + \dots$$

Asymptotic Expansion

$$\begin{aligned}\Gamma(z+1) &= z^{z+1} \int_0^\infty ds \exp\left(z\left[-1 - \frac{1}{2}(s-1)^2 + \dots\right]\right) \\ &= z^{z+1} e^{-z} \int_0^\infty ds \exp\left(-\frac{z}{2}(s-1)^2 + \dots\right) \\ &\approx z^{z+1} e^{-z} \int_{-\infty}^\infty ds \exp\left(-\frac{z}{2}(s-1)^2\right) \\ &= z^{z+1} e^{-z} \sqrt{\frac{2}{z}} \underbrace{\int_{-\infty}^\infty du \exp(-u^2)}_{\sqrt{\pi}} \quad u = \sqrt{z/2}(s-1) \\ &= \sqrt{2\pi} z^{z+1/2} e^{-z} \sqrt{\pi}\end{aligned}$$

Gaussian Integral

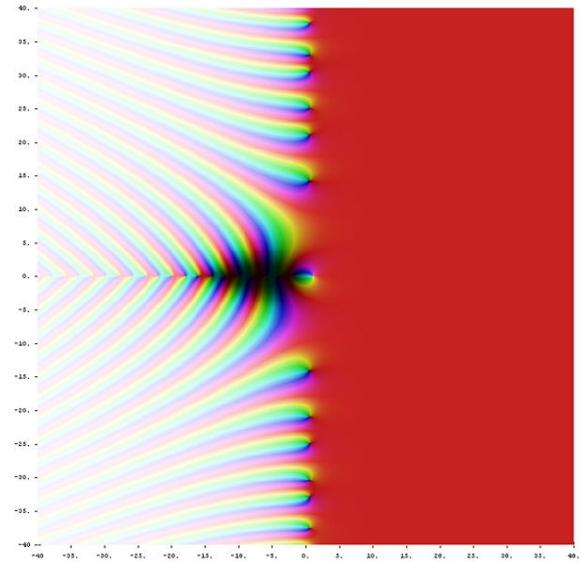
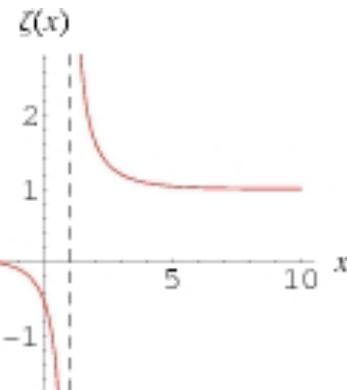
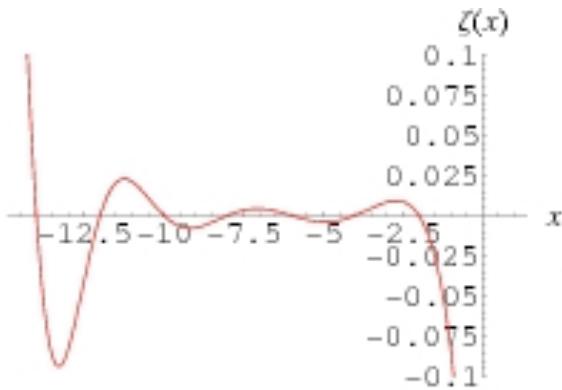


$$\begin{aligned} I^2 &\equiv \int_{-\infty}^{\infty} dx \exp(-x^2) \int_{-\infty}^{\infty} dy \exp(-y^2) \\ &= \int_0^{\infty} dr \int_0^{2\pi} r d\theta e^{-r^2} \\ &= 2\pi \int_0^{\infty} dr r e^{-r^2} \quad r^2 = x \\ &= \pi \int_0^{\infty} dx e^{-x} \quad 2rdr = dx \\ &= \pi \left[-e^{-x} \right]_0^{\infty} = \pi \end{aligned}$$

$$\therefore I \equiv \int_{-\infty}^{\infty} dx \exp(-x^2) = \sqrt{\pi}$$

Digression: Riemann Zeta Function

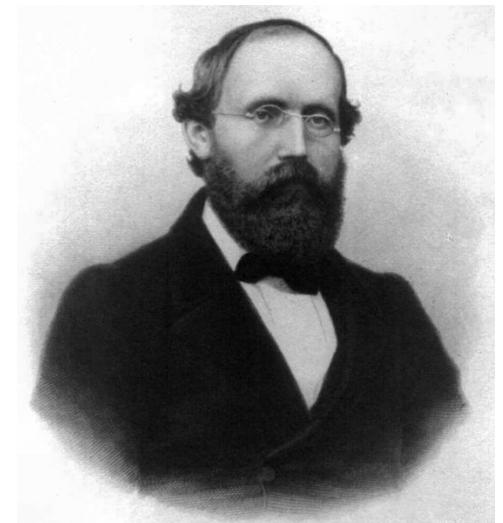
$$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}$$



- Renormalization in quantum field theory & string theory
 - > Infinite zero-point energy
 - > Regularization by analytical continuation



$$\zeta(-1) = 1 + 2 + 3 + \dots = -\frac{1}{12}$$



Bernhard Riemann
(1826-1866)

Random Walk in Finance

- Geometric Brownian motion: μ : drift; σ : volatility; ε : random variable following normal distribution with unit variance

$$dS = \mu S dt + \sigma S \varepsilon \sqrt{dt}$$

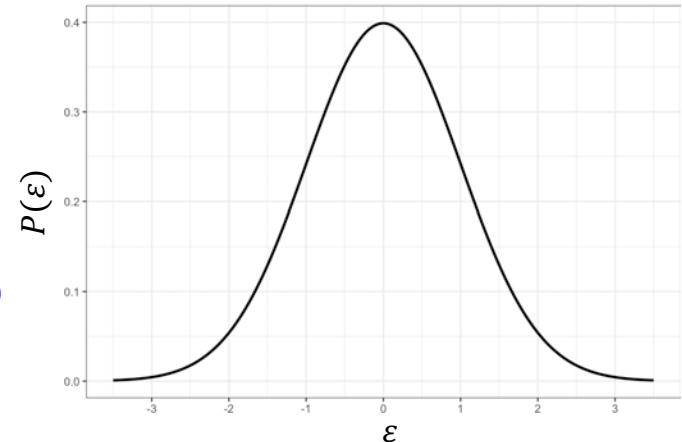
- Let the 2nd term be 0,

$$S(t) = S_0 \exp(\mu t)$$

- Let the 1st term be 0, then for $U = \ln S$ ($dU = dS/S$)

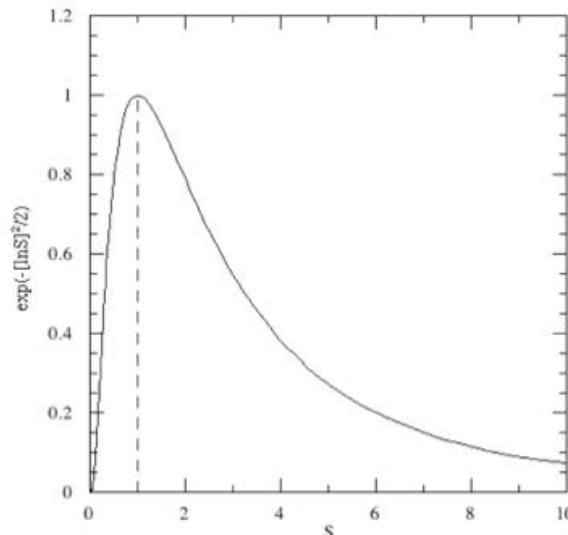
$$dU = \sigma \varepsilon \sqrt{dt}$$

$$U(t) - U(0) = \sigma \sqrt{\Delta t} \sum_{i=1}^N \varepsilon_i$$



- Central-limit theorem states that $\sum_i \varepsilon_i$ is normal distribution with variance N ; let $t = N\Delta t$

$$U(t) - U(0) = \sigma \sqrt{t} \varepsilon$$



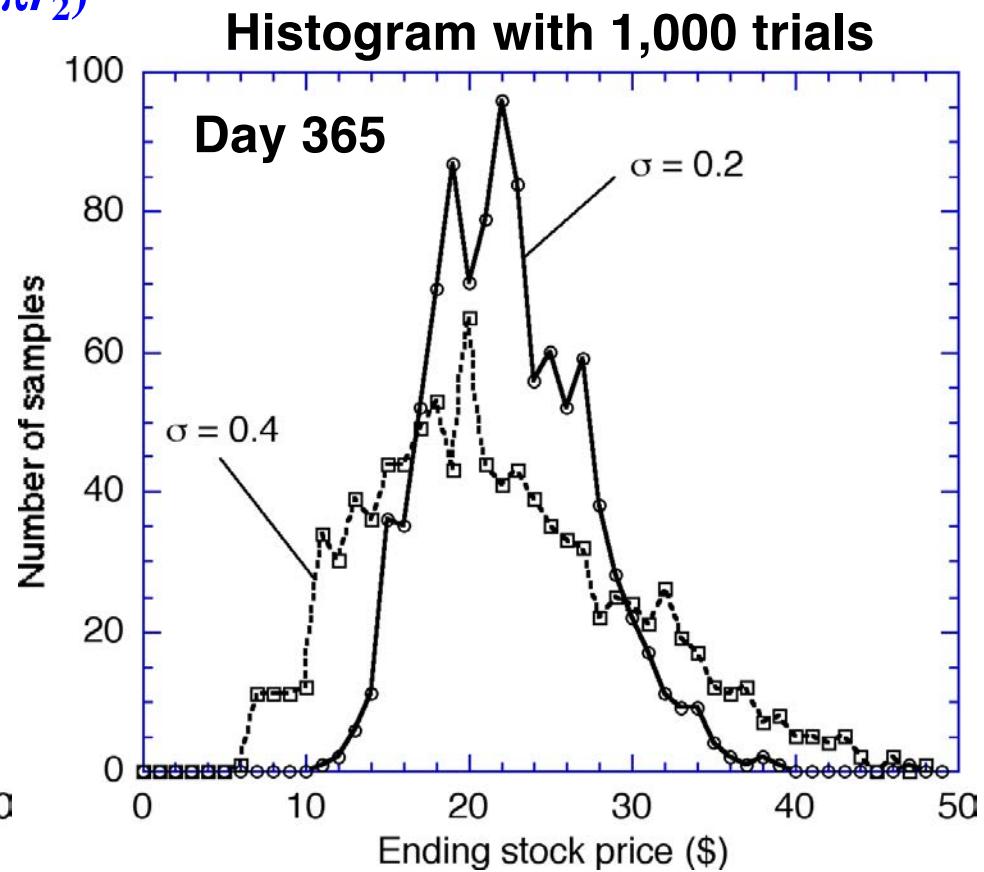
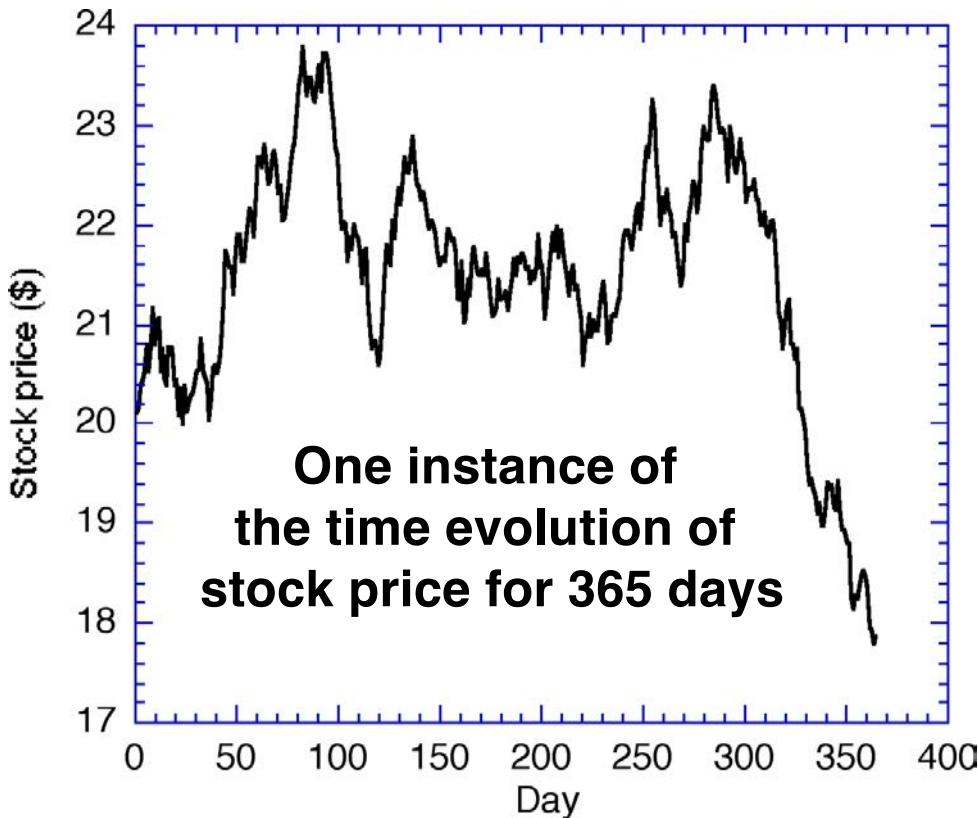
- Log-normal distribution

MC Simulation of Stock Price

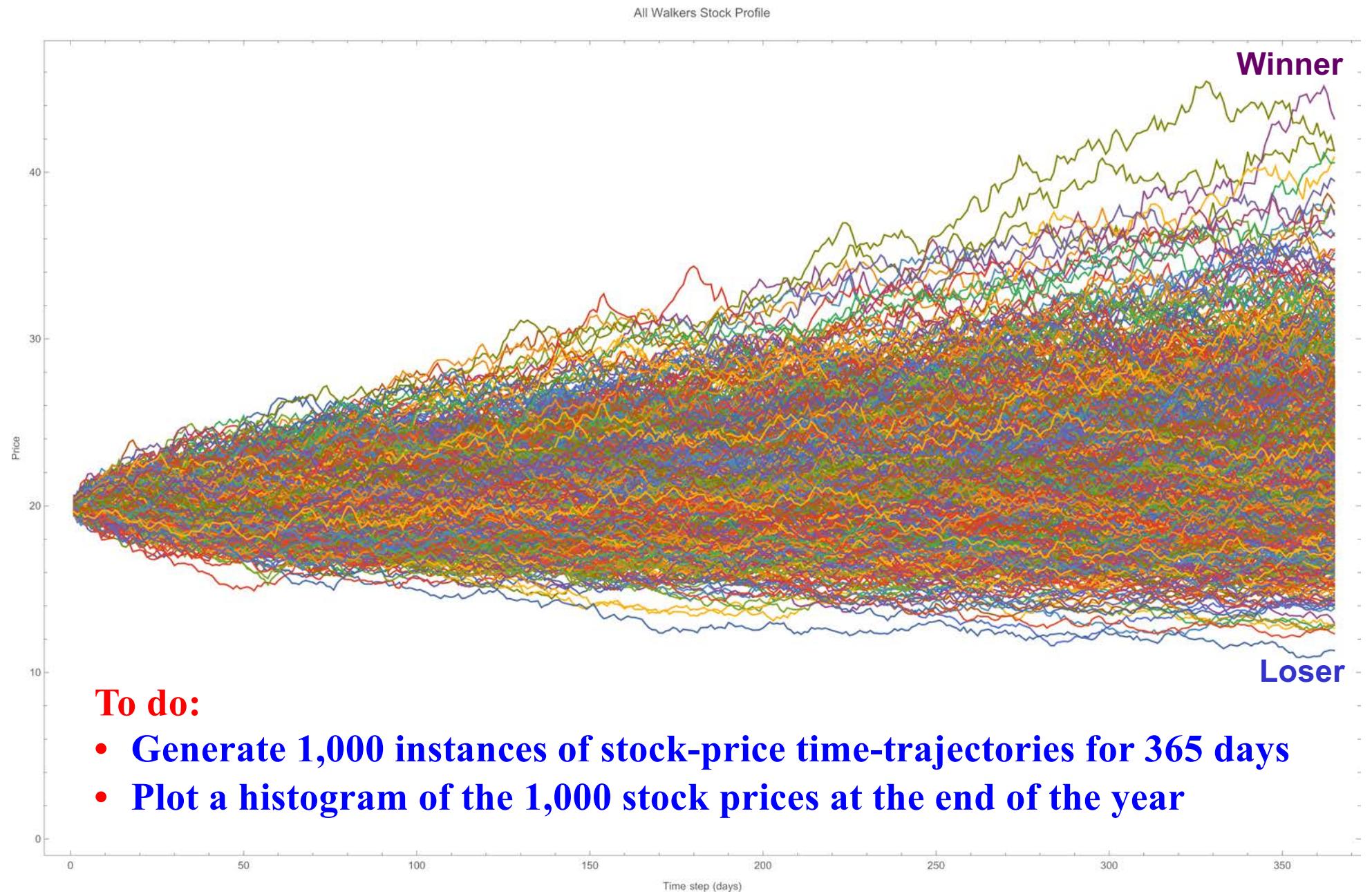
- Let: $dt = 0.00274$ year (= 1 day); the expected return from the stock be 14% per annum ($\mu = 0.14$); the standard deviation of the return be 20% per annum ($\sigma = 0.20$); & the starting stock price be \$20.0

$$\frac{dS}{S} = \mu dt + \sigma \sqrt{dt} \xi$$

- Box-Muller algorithm:** Generate uniform random numbers r_1 & r_2 in the range (0, 1), then $\xi = (-2 \ln r_1)^{1/2} \cos(2\pi r_2)$

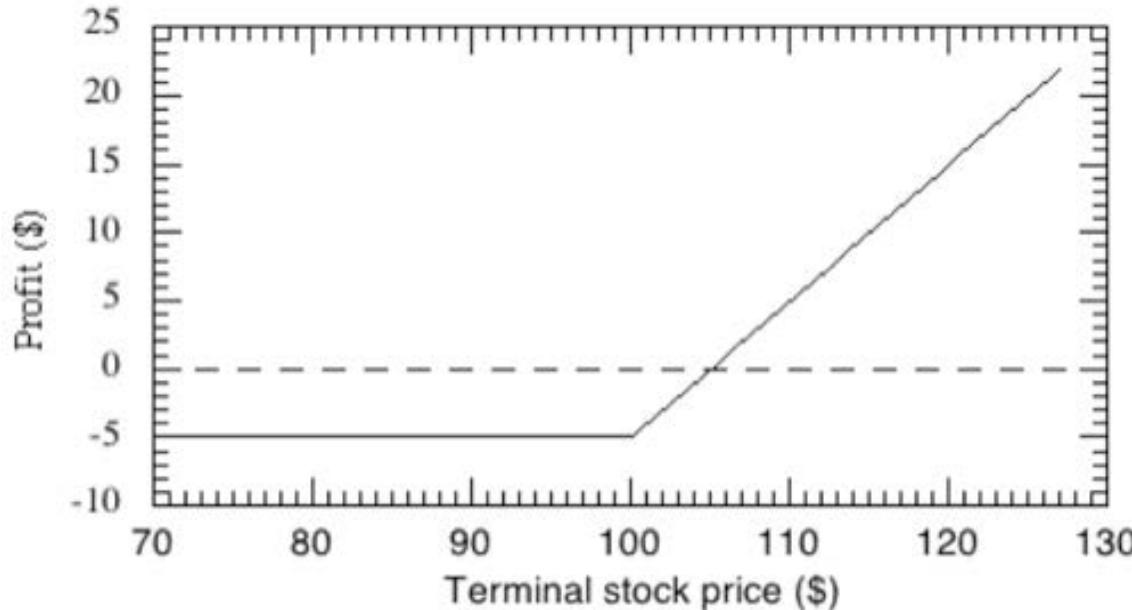


Fate of a Thousand Investors



Option Price

- A (European) **call option** gives its holder the right to buy the underlying asset at a certain date (**expiration date**) for a certain price (**strike price**)
- **Example:** European call option on IBM stock with a strike price of \$100 bought at \$5



- Assumptions in Black-Scholes analysis of the price of an option:
 - 1) The underlying stock price follows the geometric diffusive equation
 - 2) In a competitive market, there are no risk-less arbitrage opportunities (buying/selling portfolios of financial assets in such a way as to make a profit in a risk-free manner)
 - 3) The risk-free rate of interest, r , is constant & the same for all risk-free investments

Ito's Lemma

$$dS = \mu S dt + \sigma S \varepsilon \sqrt{dt}$$

- For option price f contingent on S

$$df = \left(\frac{\partial f}{\partial S} \mu S + \frac{\partial f}{\partial t} + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} \sigma^2 S^2 \right) dt + \frac{\partial f}{\partial S} \sigma S \varepsilon \sqrt{dt}$$

$$f(S + dS, t + dt) - f(S, t)$$

$$= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial S} dS + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} (dS)^2 + \dots$$

$$= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial S} (\mu S dt + \sigma S \varepsilon \sqrt{dt}) + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} (\mu S dt + \sigma S \varepsilon \sqrt{dt})^2 + \dots$$

$$= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial S} (\mu S dt + \sigma S \varepsilon \sqrt{dt}) + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} (\mu^2 S^2 dt^2 + 2\mu\sigma S^2 \varepsilon dt \sqrt{dt} + \sigma^2 S^2 \varepsilon^2 dt) + \dots$$

$$= \left(\frac{\partial f}{\partial S} \sigma S \varepsilon \right) (dt)^{1/2} + \left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial S} \mu S + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} \sigma^2 S^2 \varepsilon^2 \right) dt + O((dt)^{3/2})$$

$$= \left(\frac{\partial f}{\partial S} \sigma S \varepsilon \right) (dt)^{1/2} + \left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial S} \mu S + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} \sigma^2 S^2 \langle \varepsilon^2 \rangle \right) dt + O((dt)^{3/2})$$

$$= \left(\frac{\partial f}{\partial S} \sigma S \varepsilon \right) (dt)^{1/2} + \left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial S} \mu S + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} \sigma^2 S^2 \right) dt + O((dt)^{3/2})$$

First Gauss Prize

The International Mathematical Union (IMU) and
the Deutsche Mathematiker-Vereinigung (DMV)
jointly award the
Carl Friedrich Gauss Prize for Applications of Mathematics
to Professor Dr. Kiyoshi Itô



for laying the **foundations of the Theory of Stochastic Differential Equations and Stochastic Analysis**. Itô's work has emerged as one of the major mathematical innovations of the 20th century and has found a wide range of applications outside of mathematics. **Itô calculus** has become a key tool in areas such as **engineering** (e.g., filtering, stability, and control in the presence of noise), **physics** (e.g., turbulence and conformal field theory), and **biology** (e.g., population dynamics). It is at present of particular importance in **economics** and finance with **option pricing** as a prime example.

Madrid, August 22, 2006

Sir John Ball
President of IMU

$$dS = \mu S dt + \sigma S \varepsilon \sqrt{dt}$$

Günter M. Ziegler
President of DMV

Black-Scholes Analysis

- Construct a risk-free portfolio:

$$\Pi = -f + \frac{\partial f}{\partial S} S$$

$$d\Pi = -df + \frac{\partial f}{\partial S} dS$$

$$= -\left(\frac{\partial f}{\partial S} \mu S + \frac{\partial f}{\partial t} + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} \sigma^2 S^2 \right) dt - \frac{\partial f}{\partial S} \sigma S \varepsilon \sqrt{dt} + \frac{\partial f}{\partial S} (\mu S dt + \sigma S \varepsilon \sqrt{dt})$$

$$= -\left(\frac{\partial f}{\partial t} + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} \sigma^2 S^2 \right) dt$$

- From assumption, the growth rate of any risk-free portfolio is r

$$d\Pi = -\left(\frac{\partial f}{\partial t} + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} \sigma^2 S^2 \right) dt = r\Pi dt = r\left(f - \frac{\partial f}{\partial S} S \right) dt$$

$$\therefore \frac{\partial f}{\partial t} + r \frac{\partial f}{\partial S} S + \frac{1}{2} \frac{\partial^2 f}{\partial S^2} \sigma^2 S^2 = rf$$