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INTERNATIONAL ATOMIC ENERGY AGENCY
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

H4.SMR/916 -19

SEVENTH COLLEGE ON BIOPHYSICS:

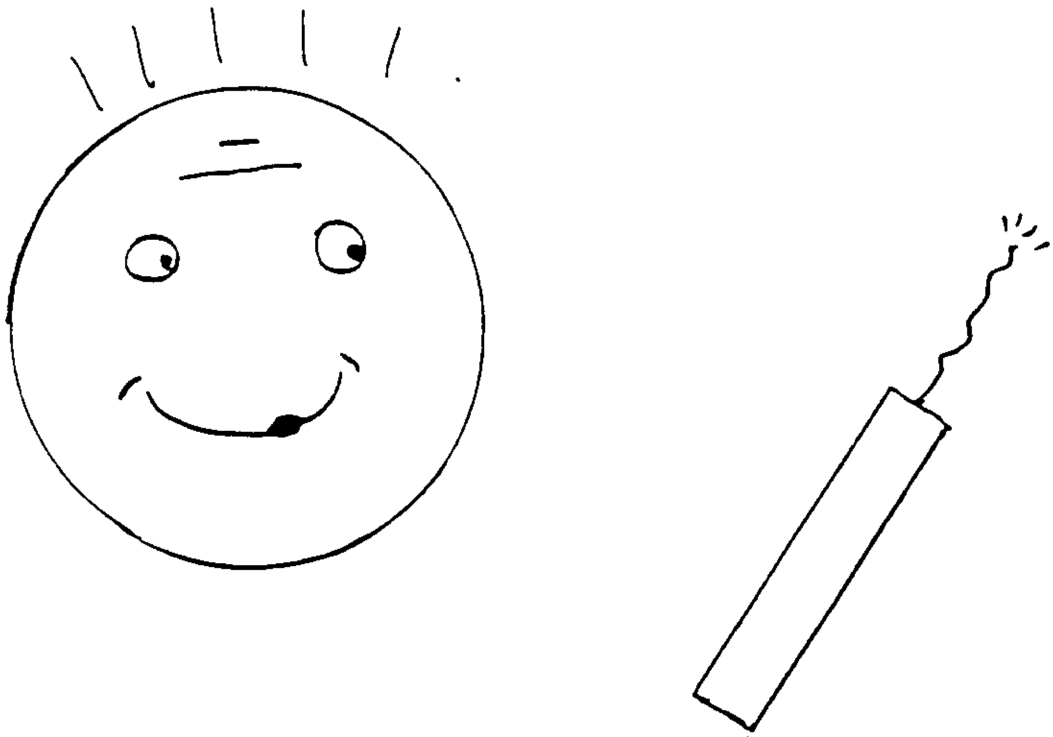
Structure and Function of Biopolymers: Experimental and Theoretical Techniques.

4 - 29 March 1996

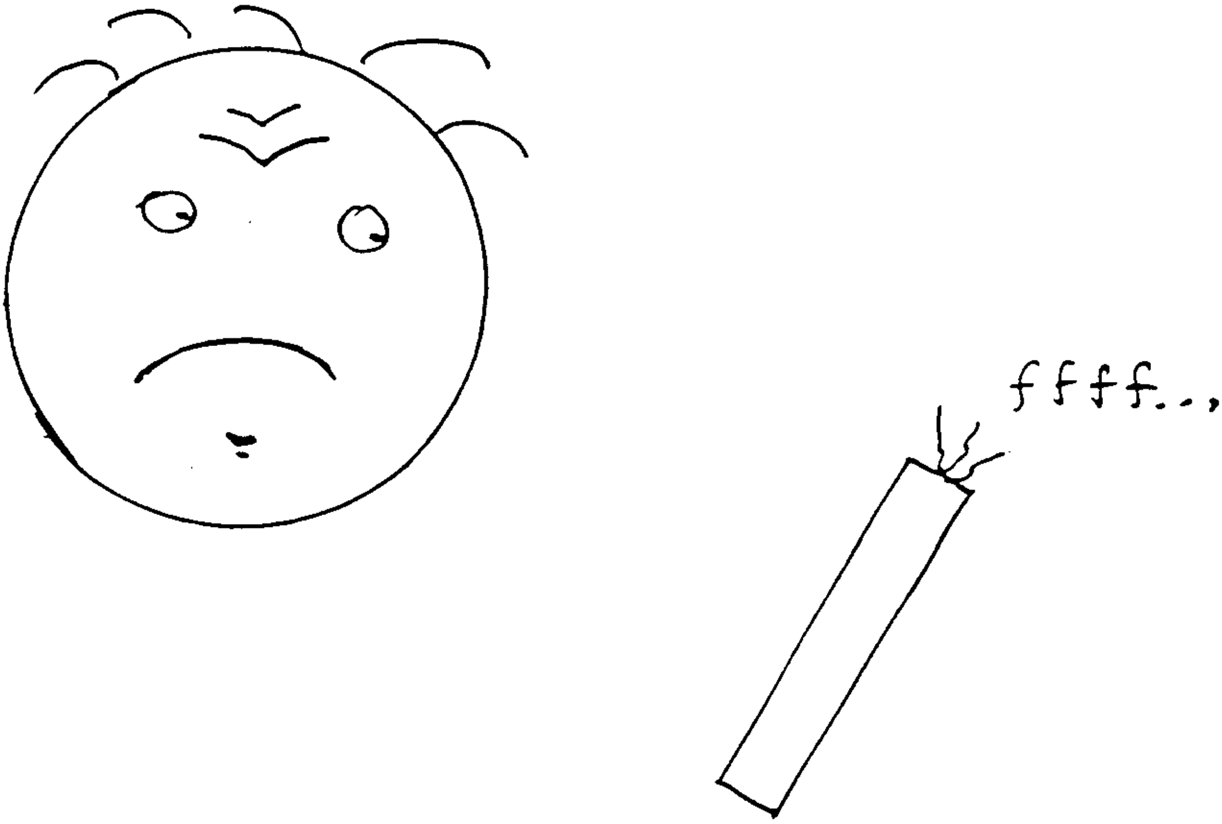
Monte Carlo

H.A. Farach
University of Pennsylvania
Lab. for Research on the Structure of Matter
Philadelphia
U.S.A.

Expected



Reality



MONTE CARLO

TRANSFORM

DETERMINISTIC PROBLEMS

INTO

PROBABILISTIC PROBLEMS

COMPUTER PROGRAMMING

2 C's   C = 2

5 B's   B = 3

8 A's   A = 4

Average grade $\langle G \rangle$

$$\langle G \rangle = (2 \times 2 + 5 \times 3 + 8 \times 4)/15$$

$$= \frac{56}{15}$$

$$\langle G \rangle = 3.73$$

$$p(C) = \frac{2}{15} \qquad p(B) = \frac{5}{15}$$

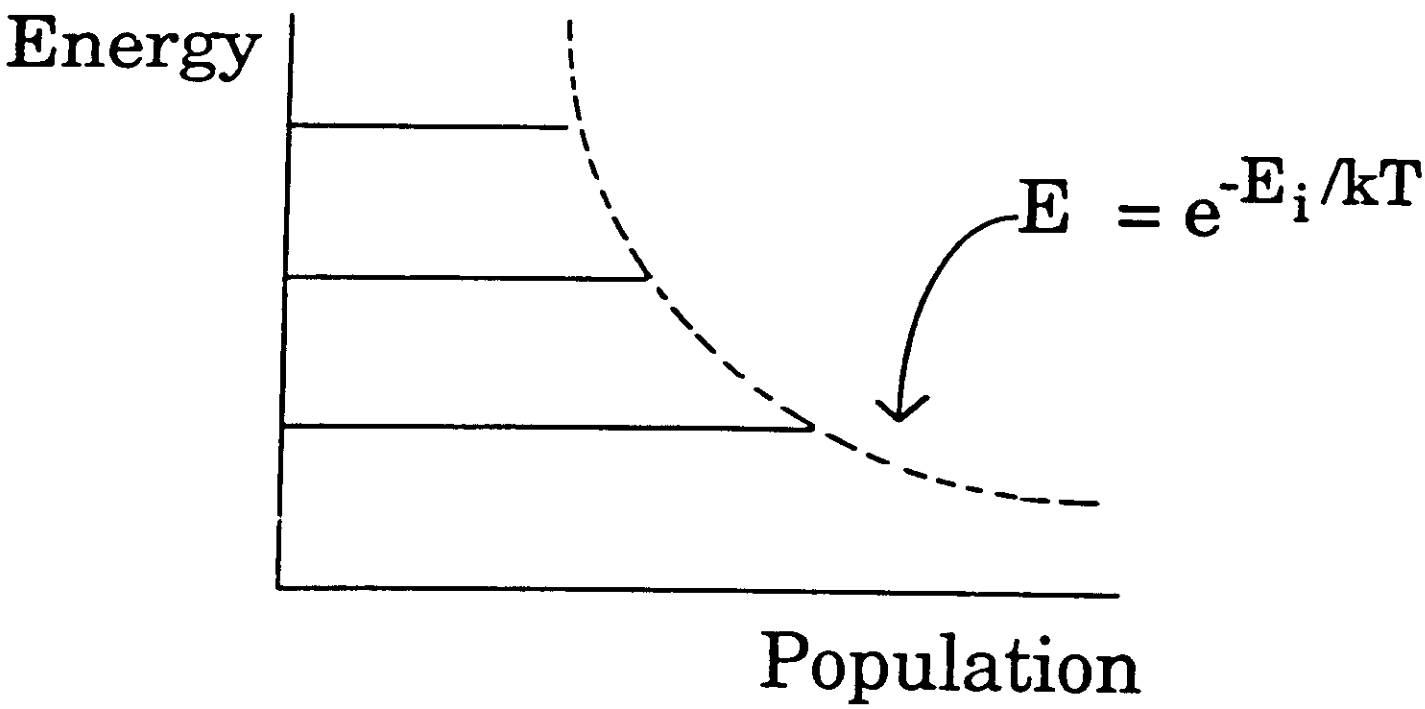
$$p(A) = \frac{8}{15}$$

$$\langle G \rangle = \sum_{i=1}^{3} G_i p_i$$

$$p_i = \frac{n_i}{\sum n_i}$$

$$= \frac{n_i}{N}$$

E population $\propto$ Boltzman factor

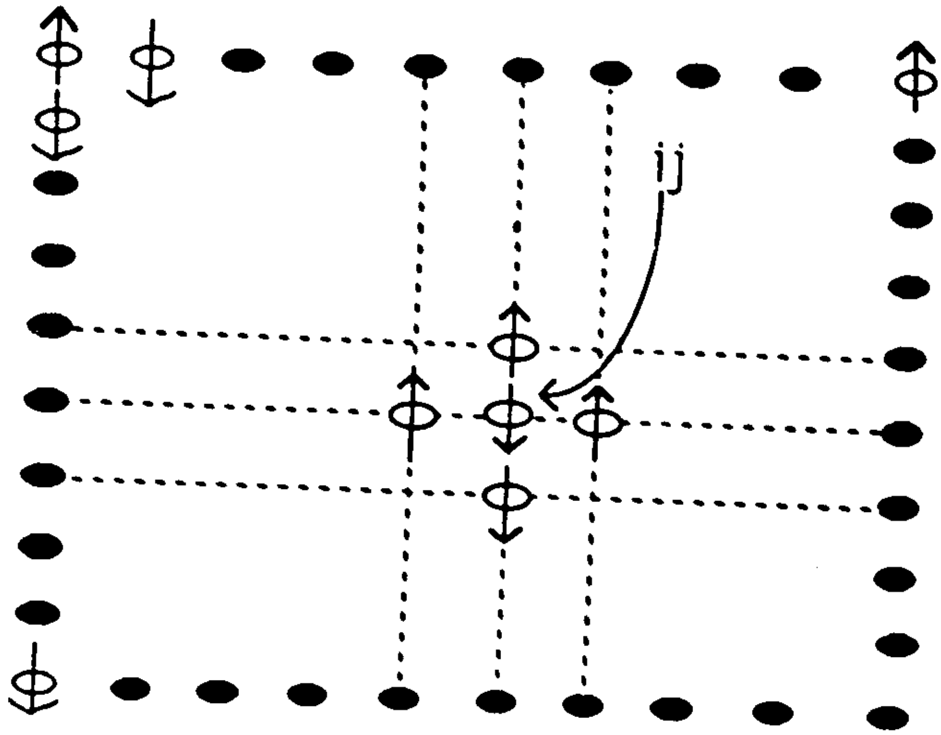


$$\langle E \rangle = \sum_{i=1}^{n} E_i \cdot P_i$$

$$P_i = \frac{e^{-E_i/kT}}{\Sigma e^{-E_i/kT}}$$

$$= \frac{e^{-E_i/kT}}{Z}$$

$Z = \Sigma e^{-E_i/kT}$ partition function



$$10 \times 10 = 100$$

$$E_{ij} = J\left(S_{ij}\left[S_{i,j+1} + S_{i+1,j} + S_{i,j-1} + S_{i-1}, S_j\right]\right)$$

Since $S_{ij} = \pm 1$

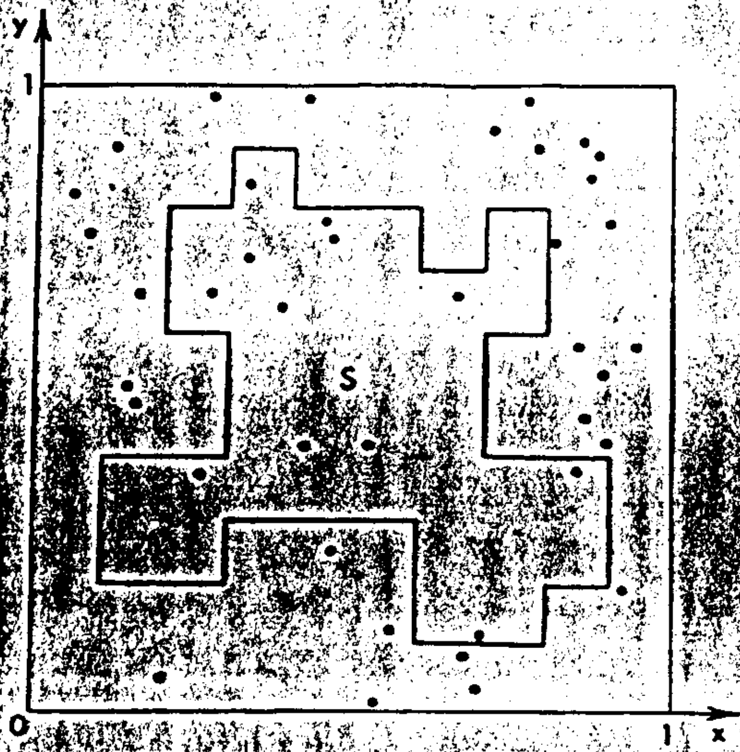
$$E_{ij} = J[-1 - 1 - 1 + 1] = -2J$$

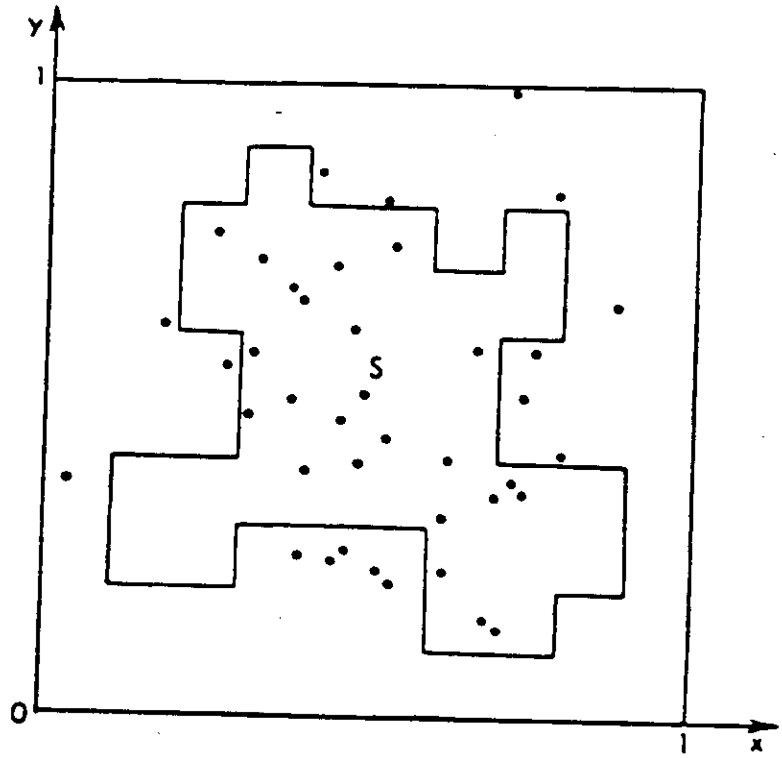
N° of states $2^{100} \sim 10^{30}$

$$\langle E \rangle = \frac{\sum E_i e^{-E_i / kT}}{Z} \rightarrow 1\mu s$$

$$t = 10^{30} \times 10^{-6}\ s = 10^{24}\ s$$

$= 10^8$ times $\times$ life of Univ!!


y
1
S
0
1
x


y
1
S
0
1
x

Monte Carlo

$$N = 40$$

$$n = 12$$

$$\frac{n}{N} = \frac{12}{40} = 0.30$$

$$S_c = 0.30$$

$$Se = 0.35$$

Shotgun

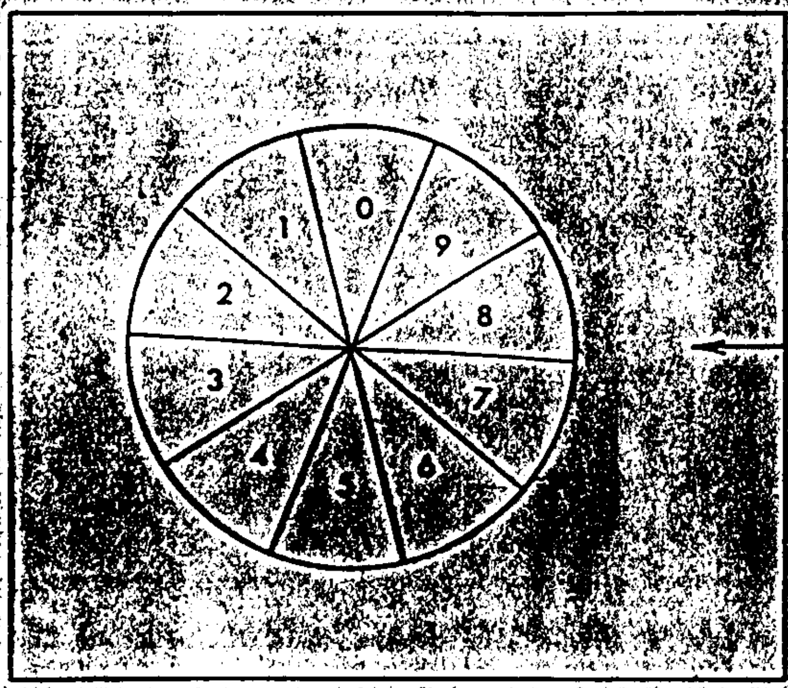
$$N = 40$$

$$n = 24$$

$$\frac{n}{N} = \frac{24}{40} = 0.60$$

$$S_c = 0.60$$

$$Se = 0.35$$


0
1
2
3
4
5
6
7
8
9

Discrete Distributions

Bernoulli

$$f(x) = p^x(1-p)^{1-x},\ x = 0,\ 1$$

$$M(t) = 1 - p + pe^t$$

$$\mu = p,\ \sigma^2 = p(1-p)$$

Binomial

$$f(x) = \frac{n!}{x!(n-x)!}\, p^x(1-p)^{n-x},\ x = 0,\ 1,\ 2,\ \ldots,\ n$$

$$M(t) = (1 - p + pe^t)^n$$

$$\mu = np,\ \sigma^2 = np(1-p)$$

Geometric

$$f(x) = (1-p)^{x-1}p,\ x = 1,\ 2,\ \ldots$$

$$M(t) = \frac{pe^t}{1-(1-p)e^t},\ t < -\ln(1-p)$$

$$\mu = \frac{1}{p},\ \sigma^2 = \frac{1-p}{p^2}$$

Negative Binomial

$$f(x) = \binom{x-1}{r-1} p^r (1-p)^{x-r},\ x = r, r+1, r+2, \ldots$$

$$M(t) = \frac{(pe^t)^r}{[1-(1-p)e^t]^r},\ t < -\ln(1-p)$$

$$\mu = r\left(\frac{1}{p}\right),\ \sigma^2 = \frac{r(1-p)}{p^2}$$

Poisson

$$f(x) = \frac{\lambda^x e^{-\lambda}}{x!},\ x = 0, 1, 2, \ldots$$

$$M(t) = e^{\lambda(e^t - 1)}$$

$$\mu = \lambda,\ \sigma^2 = \lambda$$

Hypergeometric

$$f(x) = \frac{\binom{n_1}{x}\binom{n_2}{r-x}}{\binom{n}{r}},\ x \le r,\ x \le n_1,\ r - x \le n_2$$

$$\mu = r\left(\frac{n_1}{n}\right)$$

$$\sigma^2 = r\left(\frac{n_1}{n}\right)\left(\frac{n_2}{n}\right)\left(\frac{n-r}{n-1}\right)$$

Distributions of the Continuous Type

Gamma

$$f(x) = \frac{1}{\Gamma(\alpha)\theta^{\alpha}} x^{\alpha - 1} e^{-x/\theta}, \; 0 \leq x < \infty$$

$$M(t) = \frac{1}{(1 - \theta t)^{\alpha}}, \; t < 1/\theta$$

$$\mu = \alpha\theta, \; \sigma^2 = \alpha\theta^2$$

Chi-Square

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-[(x-\mu)^2/2\sigma^2]}, \; -\infty < x < \infty$$

$$M(t) = e^{\mu t + \sigma^2 t^2/2}$$

$$E(X) = \mu, \; \mathrm{Var}(X) = \sigma^2$$

Normal

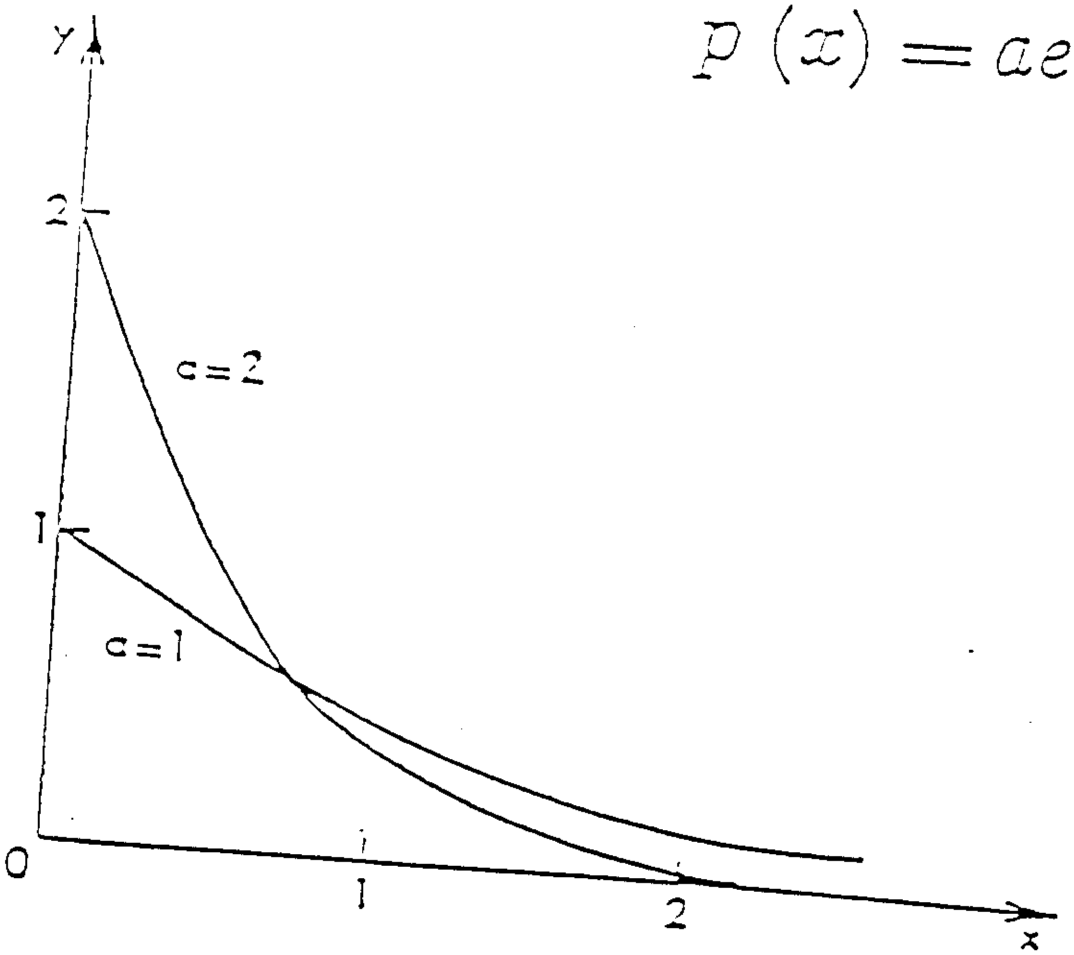
$$f(x) = \frac{1}{\Gamma(r/2)2^{r/2}} x^{r/2 - 1} e^{-x/2}, \; 0 \leq x < \infty$$

$$M(t) = \frac{1}{(1 - 2t)^{r/2}}, \; t < \frac{1}{2}$$

$$\mu = r, \; \sigma^2 = 2r$$

Poisson

$$p(x) = ae^{-ax}$$



For $x = 1$ $\quad 0 < R < 1/6$

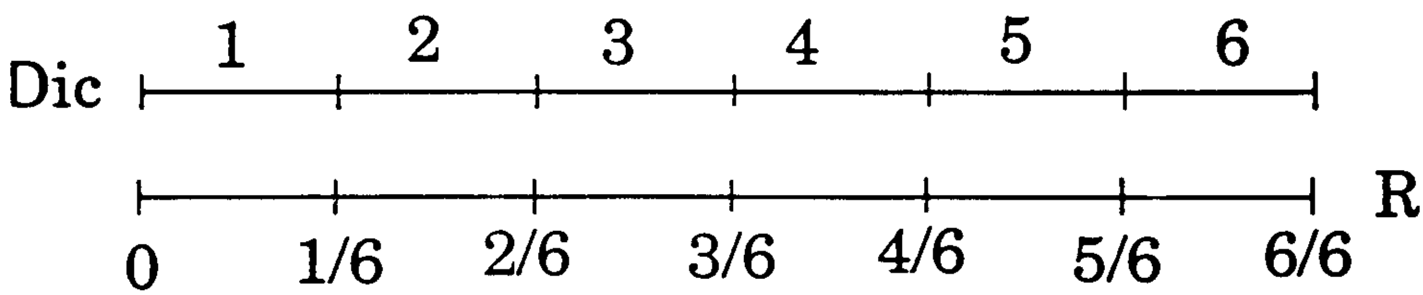
For $x = 2$ $\quad 1/6 < R < 2/6$

For $x = 3$ $\quad 2/6 < R < 3/6$

For $x = 4$ $\quad 3/6 < R < 4/6$

For $x = 5$ $\quad 4/6 < R < 5/6$

For $x = 6$ $\quad 5/6 < R < 6/6$



$$R = \int_a^{\xi} p\left(x \right) dx$$

for a dice p(x) = 1/6 and

$$\int \rightarrow \sum$$

$$R = \sum_1^6 p\left(x \right)$$

$$\int_{a}^{\xi} p(x)\,dx = \gamma$$

$$p(x) = \frac{1}{b-a} \qquad a < x < b$$

$$\int_{a}^{\eta} \frac{dx}{b-a} = \gamma$$

$$\frac{\eta - a}{b - a} = \gamma$$

$$\eta = a + \gamma(b - a)$$

(i) $f(x) > 0,\ x \in R.$

(ii) $\int_R f(x)dx = 1.$

(iii) The probability of the event $x \in A$ is

$$P(X \in A) = \int_A f(x)dx.$$

Example Let the random variable X be the distance in feet between bad records on a used computer tape. Suppose that a reasonable probability model for X is given by the p. d. f.

$$f(x) = \frac{1}{40}e^{-x/40}, \qquad 0 \le x < \infty.$$

Note that $R = \{x : 0 \le x < \infty\}$ and $f(x) > 0$ for $x \in R$. Also,

$$\int_R f(x)dx = \int_0^\infty \frac{1}{40} e^{-x/40} dx$$

$$= \lim_{b \to \infty} \left[-e^{-x/40} \right]_0^b$$

$$= 1 - \lim_{b \to \infty} e^{-b/40} = 1.$$

The probability that the distance between bad records is greater than 40 feet is given by

$$P(X > 40) = \int_{-0}^{\infty} \frac{1}{40} e^{-x/40} dx$$

$$= e^{-1} = 0.368.$$

APPLICATIONS

MACHINE THAT PERFORM INTEGRALS

N	R1	R2
1	0.38	0.26
2	0.18	0.73
3	0.73	0.82
4	0.38	0.88
5	0.83	0.06
6	0.89	0.81
7	0.86	0.88
8	0.58	0.55
9	0.07	0.44
10	0.02	0.14
11	0.65	0.67
12	0.12	0.70

N	R1	R2
13	0.14	0.52
14	0.87	0.60
15	0.72	0.99
16	0.42	0.63
17	0.96	0.09
18	0.88	0.50
19	0.04	0.77
20	0.24	0.56
21	0.19	0.08
22	0.82	0.14
23	0.48	0.64
24	0.53	0.37

N	R1	R2
25	0.46	0.42
26	0.44	0.80
27	0.90	0.16
28	0.89	0.87
29	0.20	0.41
30	0.67	0.27
31	0.64	0.38
32	0.49	0.57
33	0.96	0.65
34	0.28	0.85
35	0.62	0.01
36	0.50	0.94

MONTE CARLO INTEGRATION

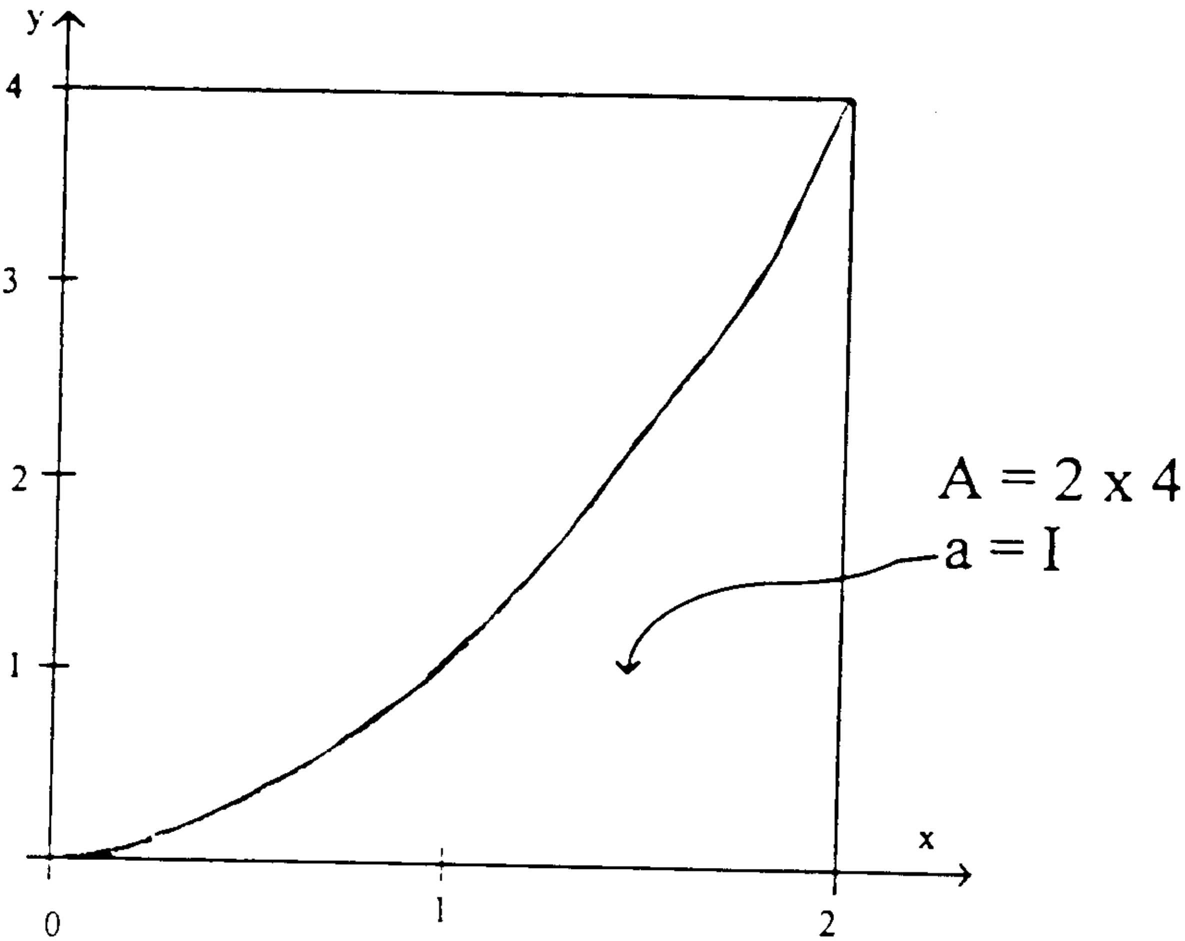
INT (X**2) /0-2=2.67

N	X=2*R1	Y=X**2	R=4*R2	M	S
1	0.75	0.57	1.05	0	0.00
2	0.36	0.13	2.91	0	0.00
3	1.46	2.13	3.30	0	0.00
4	0.77	0.59	3.52	0	0.00
5	1.66	2.75	0.23	1	1.60
6	1.77	3.15	3.23	1	1.33
7	1.71	2.94	3.53	1	1.14
8	1.17	1.36	2.21	1	1.00
9	0.14	0.02	1.77	1	0.89
10	0.04	0.00	0.56	1	0.80
11	1.31	1.71	2.67	1	0.73
12	0.24	0.06	2.80	1	0.67

N	X=2*R1	Y=X**2	R=4*R2	M	S
13	0.27	0.07	2.06	1	0.62
14	1.74	3.04	2.38	2	1.14
15	1.45	2.10	3.96	2	1.07
16	0.85	0.72	2.52	2	1.00
17	1.92	3.69	0.35	3	1.41
18	1.76	3.11	1.99	4	1.78
19	0.08	0.01	3.06	4	1.68
20	0.48	0.23	2.24	4	1.60
21	0.38	0.14	0.34	4	0.52
22	1.63	2.67	0.55	5	1.82
23	0.96	0.93	2.58	5	1.74
24	1.06	1.12	1.47	5	1.67

N	X=2*R1	Y=X**2	R=4*R2	M	S
25	0.91	0.83	1.69	5	1.60
26	0.87	0.76	3.21	5	1.54
27	1.80	3.23	0.65	6	1.78
28	1.78	3.16	3.47	6	1.71
29	0.40	0.16	1.66	6	1.66
30	1.33	1.78	1.10	7	1.87
31	1.28	1.64	1.51	8	2.06
32	0.99	0.97	2.26	8	2.00
33	1.91	3.65	2.59	9	2.18
34	0.56	0.31	3.42	9	2.12
35	1.23	1.51	0.02	10	2.29
36	1.00	1.00	3.75	10	2.22

$$I = \int_0^2 x^2 dx$$
$$= 2.33$$



$$\frac{M}{N} = \frac{a}{A} \quad \text{or} \quad \frac{M}{N} = \frac{I}{A} : \quad I = \frac{MA}{N}$$

$N = 36$
$M = 10$
$A = 8$

$\boxed{I = 2.22}$

MONTE CARLO INTEGRATION

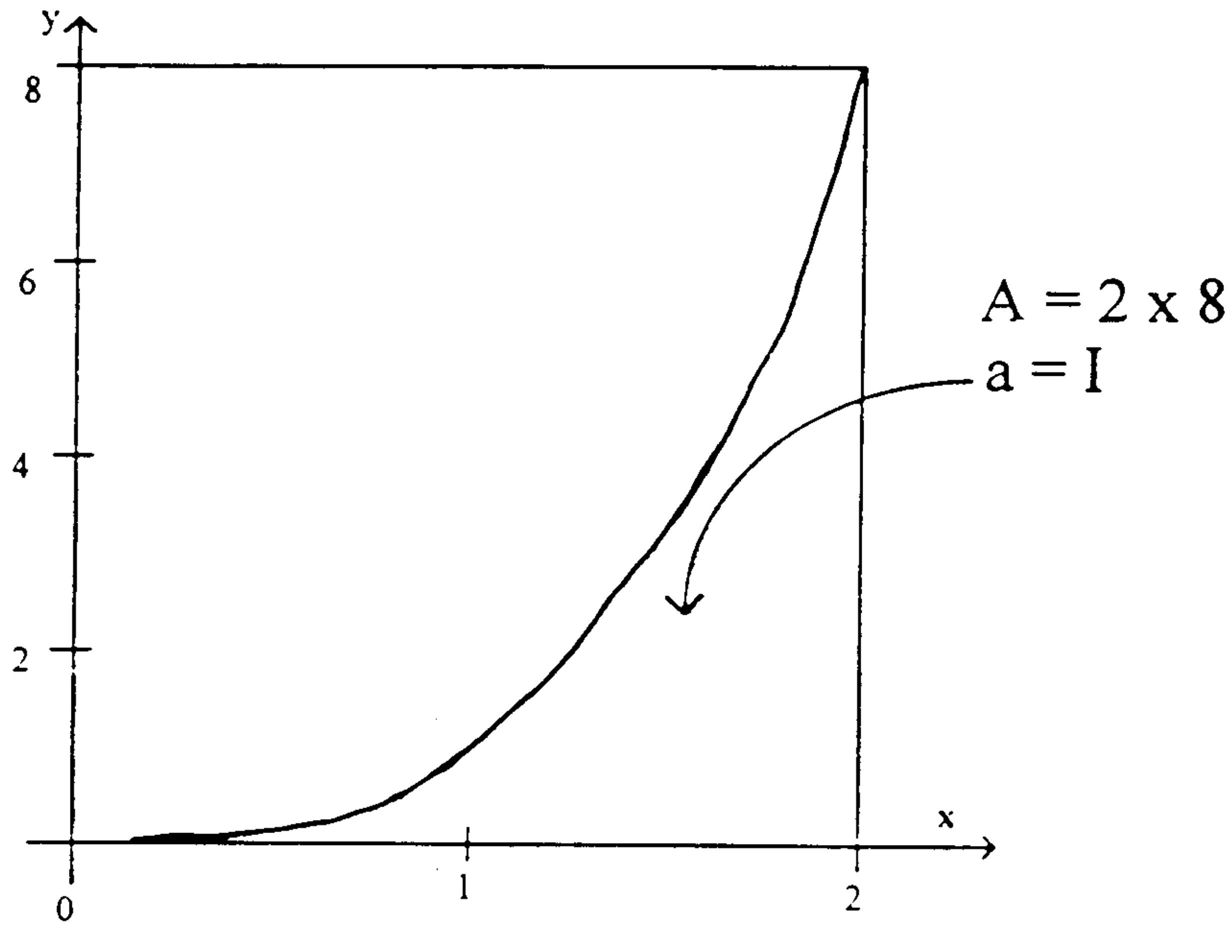
INT (X**3) /0-2=4.0

N	X=2*R1	Y=X**3	R=8*R2	M	S
1	0.75	0.43	2.10	0	0.00
2	0.36	0.05	5.82	0	0.00
3	1.46	3.10	6.59	0	0.00
4	0.77	0.45	7.03	0	0.00
5	1.66	4.55	0.46	1	3.20
6	1.77	5.58	6.45	1	2.67
7	1.71	5.04	7.06	1	2.29
8	1.17	1.59	4.43	1	2.00
9	0.14	0.00	3.54	1	1.78
10	0.04	0.00	1.12	1	1.60
11	1.31	2.24	5.34	1	1.45
12	0.24	0.01	5.60	1	1.33

N	X=2*R1	Y=X**3	R=8*R2	M	S
13	0.27	0.02	4.12	1	1.23
14	1.74	5.30	4.76	2	2.29
15	1.45	3.04	7.93	2	2.13
16	0.85	0.61	5.05	2	2.00
17	1.92	7.10	0.71	3	2.82
18	1.76	5.49	3.97	4	3.56
19	0.08	0.00	6.12	4	3.37
20	0.48	0.11	4.48	4	3.20
21	0.38	0.05	0.68	4	3.05
22	1.63	4.36	1.11	5	3.64
23	0.96	0.90	5.16	5	3.48
24	1.06	1.18	2.94	5	3.33

N	X=2*R1	Y=X**3	R=8*R2	M	S
25	0.91	0.76	3.39	5	3.20
26	0.87	0.66	6.43	5	3.08
27	1.80	5.81	1.30	6	3.56
28	1.78	5.61	6.93	6	3.43
29	0.40	0.07	3.31	6	3.31
30	1.33	2.38	2.19	7	3.73
31	1.28	2.11	3.02	7	3.61
32	0.99	0.96	4.52	7	3.50
33	1.91	6.98	5.17	8	3.88
34	0.56	0.17	6.82	8	3.76
35	1.23	1.86	0.05	9	4.11
36	1.00	0.99	7.50	9	4.0

$$I = \int_0^2 x^3 dx$$
$$= 4.0$$



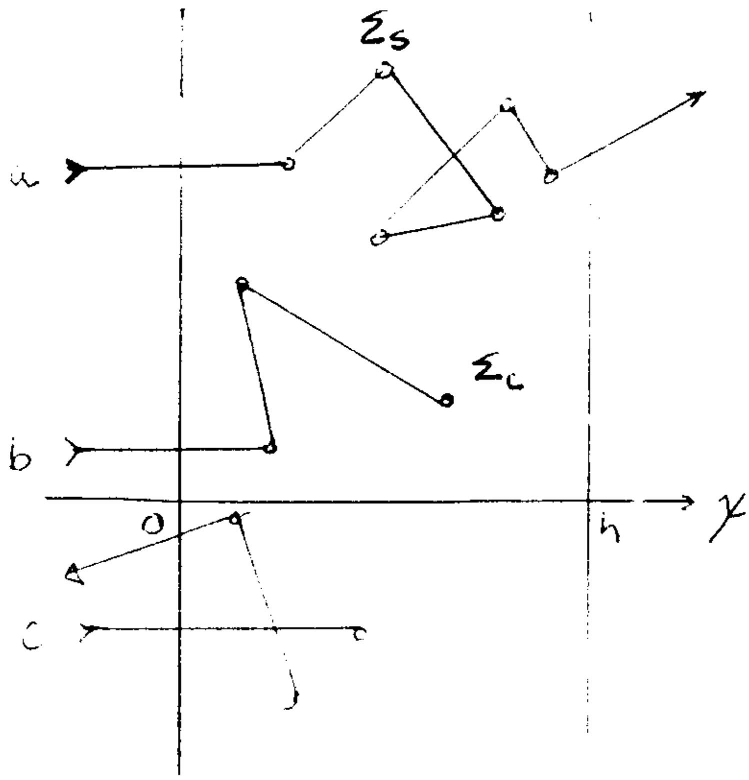
$$\frac{M}{N} = \frac{a}{A} \quad \text{or} \quad \frac{M}{N} = \frac{I}{A} : \quad I = \frac{MA}{N}$$

$$\frac{9}{36} = \frac{a}{A}$$
$$= \frac{I}{16}$$

N = 36
M = 9
A = 16

$\boxed{I = 4.0}$

Neutrons Across a Wall of width h



Σ_s
Σ_c
a
b
c
0
h
y

$$\Sigma = \Sigma_c + \Sigma_s$$

$$\Sigma_c / \Sigma$$

$$p(x) = \Sigma\, e^{-\Sigma x}$$

$$R = \int_0^{\lambda} p(x')\, dx'$$

$$\lambda = -\frac{1}{\Sigma} \ln \gamma.$$

$$\mu = 2\gamma - 1.$$

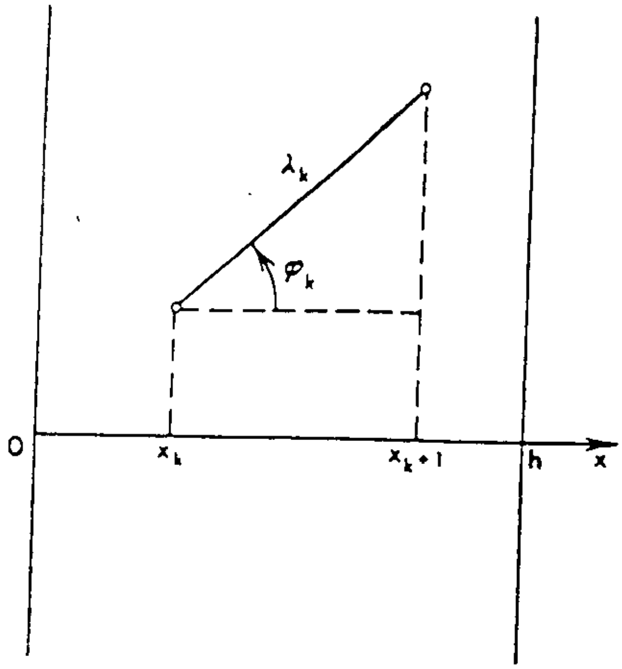
$$\lambda_k = -(1/\Sigma) \ln \gamma$$

$$x_{k+1} = x_k + \lambda_k \mu_k.$$

$$x_{k+1} > h.$$

$$x_{k+1} < 0.$$

4



$$\gamma < \Sigma_c / \Sigma .$$

$$\mu_{k+1} = 2\gamma - 1$$

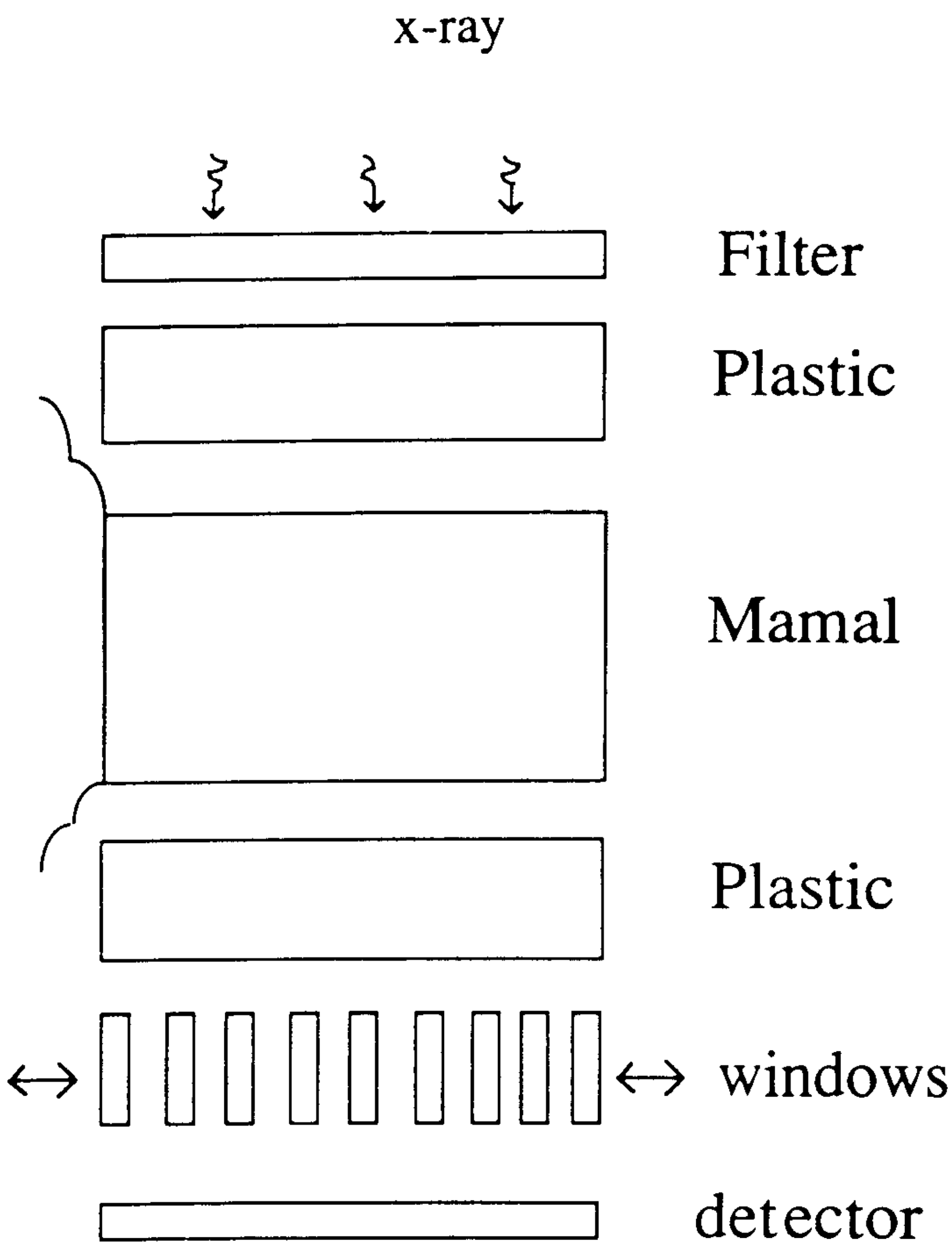
$$x_0 = 0 \text{ y } \mu_0 = 1 .$$

$$p^+ \approx \frac{N^+}{N} ,$$

$$p^0 \approx \frac{N^0}{N} ,$$

$$p^- \approx \frac{N^-}{N}$$

Mamography


x-ray
Filter
Plastic
Mamal
Plastic
windows
detector

The distance x travel before collision have a probability

$$p(x) = \lambda\, e^{-\lambda x}$$

So

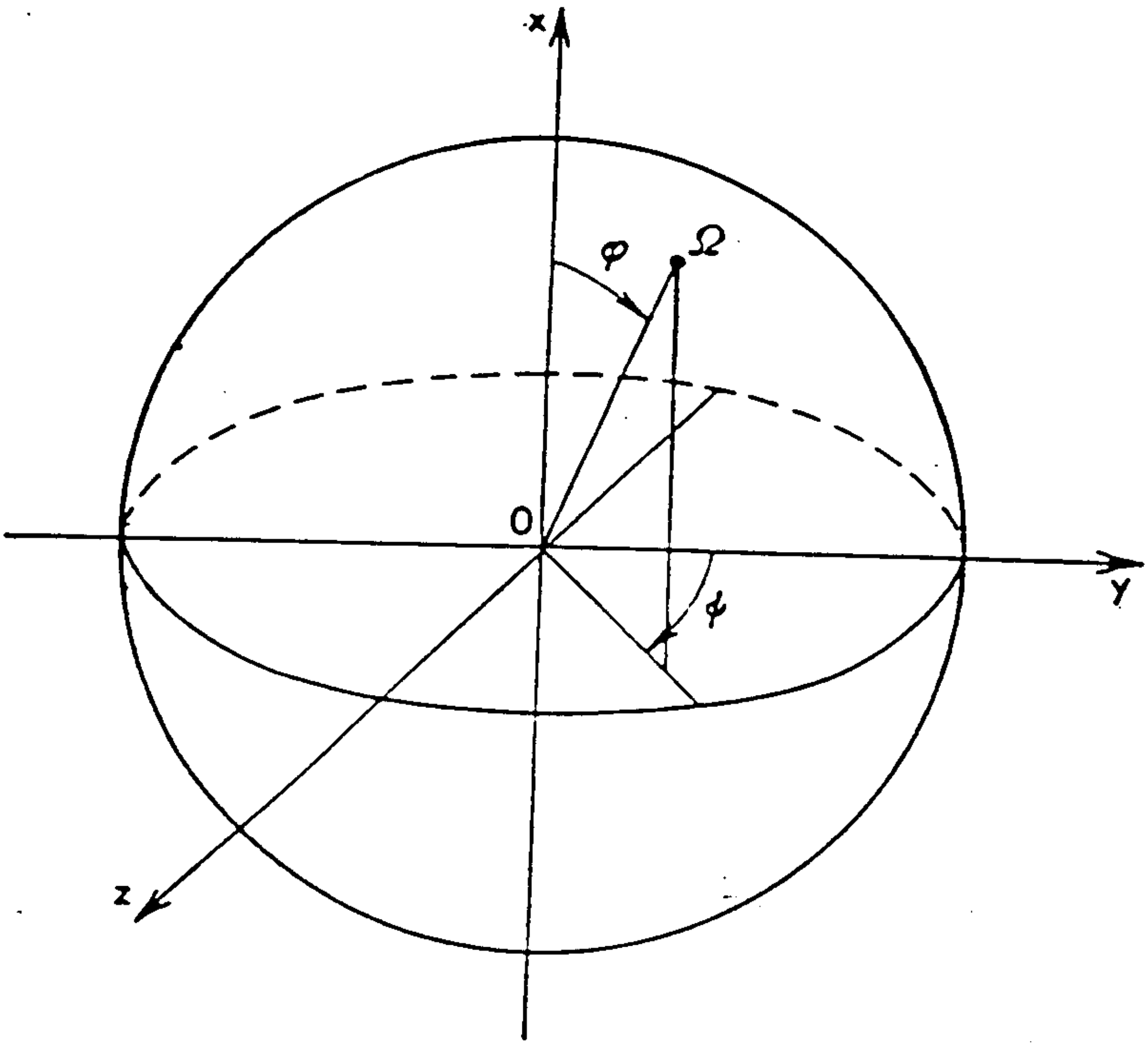
$$R = \int_0^x \lambda e^{-\lambda x'} dx'$$

$$= 1 - e^{-\lambda x}$$

$$\text{or } x = -\frac{1}{\lambda} \ln(1-R)$$

1 - R has the same distribution as R so

$$x = -\frac{1}{\lambda} \ln R$$



x
φ
Ω
O
Y
ψ
z

$$dS = \text{sen}\ \varphi\ d\varphi\ d\psi$$

$$0 \leqslant \varphi \leqslant \pi,\ \ 0 \leqslant \psi < 2\pi.$$

$$p\ (\varphi,\ \psi)\ d\varphi\ d\psi = dS/4\pi$$

$$p\ (\varphi,\ \psi) = \frac{\text{sen}\ \varphi}{4\pi}$$

$$p_{\varphi}(\varphi) = \int_0^{2\pi} p(\varphi,\ \psi)\, d\psi = \frac{\text{sen}\ \varphi}{2}$$

$$p_{\psi}(\psi) = \int_0^{\pi} p(\varphi,\ \psi)\, d\varphi = \frac{1}{2\pi}$$

$$p(\varphi,\ \psi) = p_{\varphi}(\varphi)\, p_{\psi}(\psi)$$

$$\psi = 2\pi\gamma$$

$$\frac{1}{2}\int_0^{\varphi} \text{sen}\ x\, dx = \gamma$$

$$\cos\varphi = 1 - 2\gamma$$

Total Compton Cross Section

$$\sigma_C = 2\pi r_0^2 \left\{ \frac{1+\alpha_0}{\alpha_0^2} \left[\frac{2(1+\alpha_0)}{1+2\alpha_0} - \frac{\ln(1+2\alpha_0)}{\alpha_0} \right] + \frac{\ln(1+2\alpha_0)}{2\alpha_0} - \frac{1+3\alpha_0}{(1+2\alpha_0)^2} \right. .$$

The expression for α as a function of α_0 and of the angle of photon scattering θ is given by

$$\alpha = \alpha_0 / [1 + \alpha_0 (1 - \cos\theta)].$$

The cross section for photoelectric effect in K shell of an atom with atomic number Z for a photon of energy hν is

$$\sigma_P = \phi_0 4\sqrt{2}\left(\frac{1}{\alpha}\right)^{7/2} \frac{Z^5}{137^4}; \phi_0 = \frac{8}{3}\pi r_0^2.$$

where $r_0^2 = \left(e^2/mc^2\right)^2 = 7.94 \times 10^{26} \mathrm{cm}^2$,

$\alpha = h\nu/mc^2$ is the energy in units of mc^2

$$\sigma = \sigma_c + \sigma_p$$

Probability that it will be a compton process $P(c) = \frac{\sigma_c}{\sigma}$

Probability that it will be a Photo Eletric Process

$$P(p) = \frac{\sigma_p}{\sigma} \quad \text{or} \quad P(p) = 1 - P(c)$$

The mean free path is

$$\lambda = \frac{1}{\sigma\rho}$$