STATMECH (PRACTICAL)

A) BINOMIAL DISTRO.: $$\frac{n!}{k!\,(n-k)!}\, p^k (1-p)^{n-k}$$

n = trial
k = success
p = success probability

B) χ^2 DISTRO: $$\frac{(0.5)^{k/2}}{\Gamma(k/2)}\, x^{k/2-1} e^{-x/2}$$

C) EXPONENTIAL DISTRO.: $$\frac{1}{\beta} e^{-x/\beta}$$

$\lambda = \beta^{-1}$ rate parameter

D) GAMMA DISTRO.: $$x^{k-1} \frac{e^{-x/\theta}}{\theta^k \Gamma(k)}$$

k = shape
θ = scale

\# $\mu_m = \langle x^m \rangle = \int x^m p(x)\, dx$ m^{th} moment of x

$\mu_1 = \int x\, p(x)\, dx$ = mean

\# $\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$

$= \mu_2 - \mu_1^2$ = variance / dispersion

σ is the standard deviation; $\mu_2 \geq \mu_1^2$ for $\sigma > 0$. $\sigma^2 = 0$ for Cauchy distribution

$$P(x) = \frac{\gamma}{\pi[(x-a)^2 + \gamma^2]}; \quad -\infty < x < \infty, \quad \mu_1 = a$$

\# $C(k) \overset{FT}{=} \langle e^{ikx} \rangle = \int e^{ikx} p(x)\, dx = \sum^{\infty} (ik)^m \ldots \mu$

$G(k) = \langle e^{ikx} \rangle = \int e^{ikx} p(x)\,dx = \sum_{m=0}^{\infty} \frac{(ik)^m}{m!} \mu_m$

Characteristic function / Moment generating function

$$\ln G(k) = \sum_{m=1}^{\infty} \frac{(ik)^m}{m!} \underbrace{K_m}_{\text{cumulants}}$$

$$\boxed{\begin{aligned} &K_1 = \mu_1 \,;\; K_2 = \sigma^2 ,\; K_3 = \mu_3 - 3\mu_1\mu_2 + 2\mu_1^3 \\ &K_4 = \mu_4 - 4\mu_1\mu_3 - 3\mu_2^2 + 12\mu_1^2\mu_2 - 6\mu_1^4 \end{aligned}}$$

$$\underbrace{P_s(x_1, x_2, \cdots, x_s)}_{\text{Marginal distribution}} = \int \underbrace{P_r(x_1, x_2, \cdots, x_s, x_{s+1}, \cdots, x_r)}_{\text{joint probability distribution}} \, dx_{s+1} \cdots dx_r$$

$$P_r(x_1, x_2, \cdots, x_r) = P_{r-s}(x_{s+1}, \cdots, x_r) \times P_{s|r-s}(x_1, x_2, \cdots, x_s \mid x_{s+1}, \cdots, x_r)$$

or, Joint PDF = Marginal PDF × Conditional PDF

(Baye's theorem)

If P_r factorizes, such that

$$P_r(x_1, \cdots, x_r) = P_{r-s}(x_{s+1}, \cdots, x_r)\, P_s(x_1, \cdots, x_s)$$

$\Rightarrow$ Statistically Independent

(Marginal PDF = Conditional PDF)

Moments $\mu_{m_1, \cdots, m_r} = \langle x_1^{m_1} x_2^{m_2} \cdots x_r^{m_r} \rangle$

$$= \int x_1^{m_1} x_2^{m_2} \cdots x_r^{m_r}\, p(x_1, x_2, \cdots, x_r)\, dx_1 dx_2 \cdots dx_r$$

$$G(k_1, \cdots, k_r) = \langle e^{i(k_1 x_1 + \cdots + k_r x_r)} \rangle$$

$$= \sum_{m_i=0}^{\infty} \frac{(ik_1)^{m_1} (ik_2)^{m_2} \cdots (ik_r)^{m_r}}{m_1!\, m_2! \cdots m_r!} \mu_{m_1, \cdots, m_r}$$

$$\therefore \ln G(k_1, \cdots, k_r) = \sum_{m_i=1}^{\infty} \frac{(ik_1)^{m_1} (ik_2)^{m_2} \cdots (ik_r)^{m_r}}{m_1!\, m_2! \cdots m_r!} K_{m_1, \cdots, m_r}$$

Covariance matrix : $\langle\langle x_i x_j \rangle\rangle$ 2^{nd} moment

$$= \langle (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) \rangle = \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle$$

diagonal components = variance ✓

off diagonal components = covariance ✓

Correlation Coefficient $\Rightarrow \dfrac{\langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle}{\sqrt{(\langle x_i^2 \rangle - \langle x_i \rangle^2)(\langle x_j^2 \rangle - \langle x_j \rangle^2)}}$

Statistical Independence here means

(i) All moments factorize $\langle x_1^{m_1} x_2^{m_2} \rangle = \langle x_1^{m_1} \rangle \langle x_2^{m_2} \rangle$

(ii) Characteristic function factorizes

$$G(k_1, k_2) = G(k_1)\, G(k_2)$$

(iii) Cumulants = 0 when m_1, m_2 differ from 0.

$x_1 x_2$ uncorrelated $\Rightarrow$ covariance = 0.

Joint PDF

Individual PDF

If $Y = X_1 + X_2$ then

$$P_Y(y) = \int \delta(x_1 + x_2 - y)\, P_X(x_1, x_2)\, dx_1\, dx_2$$

$$= \int P_X(x_1, y - x_1)\, dx_1 \xrightarrow{\text{independence}} \underbrace{\int P_{X_1}(x_1)\, P_{X_2}(y - x_1)\, dx_1}_{\text{convolution}}$$

\# $\langle Y \rangle = \langle X_1 \rangle + \langle X_2 \rangle$ True even if P_X is independent or not ✓

\# $\sigma_Y^2 = \sigma_{X_1}^2 + \sigma_{X_2}^2 \Leftarrow$ Uncorrelated ✓

\# $G_Y(K) = G_{X_1, X_2}(K, K) = G_{X_1}(K)\, G_{X_2}(K) \Leftarrow$ Independent ✓

characteristic function

$$\boxed{\text{PRIORY DISTRO} \longrightarrow \text{MATH. TRANSFORMATION} \longrightarrow \text{POSTERIORI DISTRO}}$$

\# Square Distribution $P(x) = 0, \ |x| > a$

$$= \frac{1}{2a}, \ |x| < a$$

\# Gauss/Normal Distro. $P(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \ -\infty < x < \infty$

\# Poisson Distro. $P_n = \frac{a^n}{n!}\, e^{-a}, \ n = 0, 1, 2, \ldots$

\# Pascal Distro./ Geometrical Distro. $P_n = (1 - \gamma)\gamma^n \, ; \ \gamma = e^{-h\nu/k_B T}$

$(Z + n - 1)!\ \gamma^n$

Negative Binomial Distribution $P_n = (1-\gamma) \cdots \frac{\cdots}{(z-1)!\, n!}$

Maxwell Distro. $P(v) = 4\pi \left(\frac{m}{2\pi k_B T}\right)^{3/2} v^2 e^{-\frac{mv^2}{2k_BT}}$

χ^2 or γ Distribution $P(E) = \frac{1}{\sqrt{2\pi (k_BT)^3}} \sqrt{E}\, e^{-E/k_BT}$

γ Distro. $P(x) = \frac{a^\gamma}{\Gamma(\gamma)} x^{\gamma-1} e^{-ax}$; $a, \gamma > 0$, $0 < x < \infty$

Lorentz Distro./ Cauchy Distro. $P(x) = \frac{\gamma}{\pi[(x-a)^2 + \gamma^2]}$; $-\infty < x < \infty$

$\Rightarrow$ For Gaussian Distro, uncorrelated implies independent.

Central limit Theorem (CLT) :

$$Y = \frac{1}{\sqrt{r}}(X_1 + X_2 + \cdots + X_r) ; \; X_i \text{ independent}$$

Y ↓ Gaussian distribution

X_1 ↓ $P_X(X_1)$ any distribution

X_r ↓ some other distribution

$$P_Y(y) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-y^2/2\sigma^2}.$$

$\boxed{\text{CLT is violated by Lorentz Distro.}}$

If $P_X(X_1) = P_X(X_2) = P_Y(y) \Rightarrow$ "Stable" Distro.

Example: Gaussian, Poisson, Lorentz, Gamma

For Poisson Distro. $\langle N^2 \rangle = \langle N \rangle^2 + \langle N \rangle$, so only mean is good enough.

STOCHASTIC PROCESS: $Y_X(t) = f(X, t)$ → Map

X = Stochastic variable ↳ Sample function ↓ time

1^{st} moment: $\langle Y(t) \rangle = \int Y_X(t) \, P_X(x) \, dx$

n^{th} moment: $\langle Y(t_1) Y(t_2) \cdots Y(t_n) \rangle$

$$= \int Y_X(t_1) Y_X(t_2) \cdots Y_X(t_n) \, P_X(x) \, dx.$$

Autocorrelation function (ACF):

$$K(t_1, t_2) = \langle Y(t_1) Y(t_2) \rangle - \langle Y(t_1) \rangle \langle Y(t_2) \rangle$$

$$= \sigma^2(t) \text{ for } t_1 = t_2.$$

When $\langle Y(t_1 + \tau) Y(t_2 + \tau) \cdots Y(t_n + \tau) \rangle$

$= \langle Y(t_1) Y(t_2) \cdots Y(t_n) \rangle \Rightarrow$ Stationary process.

$\therefore K(t_1, t_2) = f(|t_1 - t_2|)$ for stationary process.

For several components $K_{ij}(t_1, t_2) = \langle Y_i(t_1) Y_j(t_2) \rangle - \langle Y_i(t_1) \rangle \langle Y_j(t_2) \rangle$

which for zero mean stationary process is

$$K_{ij}(\tau) = K_{ji}(-\tau) = \langle Y_i(t) Y_j(t + \tau) \rangle$$

$$= \langle Y_i(0) Y_j(\tau) \rangle$$

If set is independent & Stationary ⇒

"[illegible] process" ✓

Campbell's process

Wiener Khinchin Theorem :

cosine transform

$$S(\omega) = \frac{2}{\pi}\int_0^\infty \cos(\omega\tau)\, K(\tau)\, d\tau$$

Spectral density of fluctuations

ACF

Markov Process: Brownian Motion; velocity of polen particle damps out in ACF time. Two successive positions measured in interval >> ACF time. Position is then Markov process. Velocity is non-Markovian for Brownian Motion under external field.

Position of a Brownian particle

Wiener Process (non-stationary Markov Process):

$$P_1(y,t) = \frac{1}{\sqrt{2\pi t}}\, e^{-y^2/2t} \; ; \; P_1(y_1,0) = \delta(y_1)$$

$$P_{1/1}(y_2,t_2 \mid y_1,t_1) = \frac{1}{\sqrt{2\pi(t_2-t_1)}}\, e^{-\frac{(y_2-y_1)^2}{2(t_2-t_1)}}$$

(P satisfies diffusion equation)

Ornstein-Uhlenbeck Process (stationary Markov process):

Velocity of a Brownian particle

$$P_1(y) = \frac{1}{\sqrt{2\pi}}\, e^{-y_1^2/2}$$

$(\tau = t_2 - t_1)$

$$P_{1/1}(y_2,t_2 \mid y_1,t_1) = T_\tau(y_2 \mid y_1)$$

$$= \frac{1}{\sqrt{2\pi(1-e^{-2\tau})}}\, e^{-\frac{(y_2 - y_1 e^{-\tau})^2}{2(1-e^{-2\tau})}}$$

Average $= 0$, ACF $K(\tau) = e^{-\tau}$. This is the only process which is stationary, Gaussian & Markovian $\Rightarrow$ $\boxed{\text{Doob's theorem}}$. Converse is also true, if $Y(t)$ is stationary, Gaussian & exponential ACF $K(\tau) = K(0)\, e^{-\gamma t}$ then $Y(t)$ is OU process & hence Markovian.

For Markov, $K(t_3, t_1) = K(t_3, t_2) K(t_2, t_1)$
(T satisfies forward/backward Kolmogorov equations)

✓ **Equation of Motion:** $\dot{v}(t) = -\Gamma v(t) + F(t)$

Property of Random Noise $W(t)$:-

$$F(t) = \sqrt{2 k_B T \Gamma}\, \overbrace{\mathcal{N}(0,1)}^{\text{Gaussian}}; \quad \langle F(t) \rangle = 0$$

$$\langle F(t_1) F(t_2) \rangle = 2 k_B T \Gamma \underbrace{\delta(t_1 - t_2)}_{\text{stationary}} \rightarrow \delta \text{ correlated}$$

For $|t_1 - t_2| \geq \tau_0$ (collision time)

$$\langle W(t_1) W(t_2) \rangle = \langle W(t_1) \rangle \langle W(t_2) \rangle = 0 \rightarrow \text{Markov}$$

$\Rightarrow$ **WHITE NOISE**

Variance $\langle v^2 \rangle = k_B T$,

ACF $\langle v(t)\, v(t+\tau) \rangle = k_B T\, e^{-\Gamma \tau}$

N Random Variables $x_1, x_2, \ldots, x_N$

Mean $\quad \bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$

Variance $\quad \sigma_x^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})^2$

or σ_{xx}

$$= \frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})(x_i-\bar{x})$$

Two sets of Random Variables (x, y)

$(x_1, x_2, \dots, x_N)$ & $(y_1, y_2, \dots, y_N)$

Covariance $\quad \sigma_{xy} = \frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})(y_i-\bar{y})$

Pearson Correlation coefficient $\quad \boxed{r = \frac{\sigma_{xy}}{\sigma_x \sigma_y}}$

$$= \frac{\sum(x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum(x_i-\bar{x})^2 \sum(y_i-\bar{y})^2}} \; ; \left[-1 \le r \le 1\right]$$

For ACF we take part of same set

$X^{(1)} \Rightarrow (x_1, x_2, x_3, \dots, x_{N-1}), \; (x_2, x_3, \dots, x_N) \Rightarrow X^{(2)}$

$\longleftarrow$ N-1 points $\longrightarrow \quad \longleftarrow$ N-1 points $\longrightarrow$

$$r_1 = \frac{\sum_{i=1}^{N-1}(x_i-\bar{x}^{(1)})(x_{i+1}-\bar{x}^{(2)})}{\sqrt{\sum_{i=1}^{N-1}(x_i-\bar{x}^{(1)})^2 \sum_{i=1}^{N-1}(x_{i+1}-\bar{x}^{(2)})^2}}$$

(lag 1)

Similarly $r_2, r_3, r_4, \dots$

For very large data set, $\bar{x}^{(1)} = \bar{x}^{(2)} = \bar{x} = \frac{1}{N}\sum_{i=1} x_i$

then

$$r_1 = \frac{\sum_{i=1}^{N-1}(x_i - \bar{x})(x_{i+1} - \bar{x})}{\frac{N-1}{N}\sum_{i=1}^{N}(x_i - \bar{x})^2}$$

$$\simeq \frac{\sum_{i=1}^{N-1}(x_i - \bar{x})(x_{i+1} - \bar{x})}{\sum_{i=1}^{N}(x_i - \bar{x})^2} \quad \text{(lag 1)}$$

So,

$$\text{ACF } \underline{r_K} = \frac{\sum_{i=1}^{N-K}(x_i - \bar{x})(x_{i+K} - \bar{x})}{\sum_{i=1}^{N}(x_i - \bar{x})^2} \quad \text{(lag k)}$$

$$r_K = \frac{C_K}{C_0} \text{ where } = \frac{\text{Auto Covariance}}{\text{Self Covariance}}$$

$$C_K = \frac{1}{N}\sum_{i=1}^{N-K}(x_i - \bar{x})(x_{i+K} - x) \Rightarrow$$

Auto covariance

Monte Carlo (Nuclear Decay)

$P = \alpha \Delta t$ with $\alpha \Delta t << 1$

or $\frac{dN}{N} = -\alpha \Delta t$ or $N(t) = N_0 e^{-\alpha t} = N_0 e^{-t/\tau}$

$N(t) = N_0 \left(\frac{1}{2}\right)^{t/t_{1/2}} \rightarrow$ Half life

$$\therefore \cancel{N_0} e^{-t/\tau} = \cancel{N_0}\left(\tfrac{1}{2}\right)^{t/t_{1/2}}$$

$$\text{or } \cancel{-}\frac{\cancel{t}}{\tau} = \frac{t}{t_{1/2}} \ln\left(\tfrac{1}{2}\right) = \cancel{-}\frac{0.693\,\cancel{t}}{t_{1/2}}$$

$$\alpha = \frac{1}{\tau} = \frac{0.693}{t_{1/2}} \qquad \therefore P = \alpha \Delta t = \frac{0.693}{t_{1/2}} \Delta t$$

$t_{1/2} = 1000$ (say)

choice dt so that $P = \alpha \Delta t \ll 1$

MC Integration

$\int_{\mathcal{D}} f\,dV = V\langle f\rangle \pm \sigma$ → uncertainty

→ uniform (random) sampling

Domain

n random points $\bar{x}_1, \bar{x}_2, \ldots \bar{x}_n$

standard deviation

$$\sigma = \frac{V}{\sqrt{n}}\sqrt{\langle f^2\rangle - \langle f\rangle^2} = \frac{V}{\sqrt{n}}\sigma_f$$

where $\langle f\rangle = \frac{1}{n}\sum_{i=1}^{n} f(\bar{x}_i)$, $\langle f^2\rangle = \frac{1}{n}\sum_{i=1}^{n} f^2(\bar{x}_i)$

[Trapezoidal (Quadrature) $\sigma \propto \frac{1}{n^2}$.

1D

d Dimension $\sigma \propto \frac{1}{n^{2/d}}$

MC integration any dimension $\sigma \propto \frac{1}{\sqrt{n}}$]

As $\sigma \propto \sigma_f$ its more accurate as $\langle f^2\rangle \simeq \langle f\rangle^2$ (constant function)

1D

$$I = \int_a^b f(x)dx = (b-a)\int_0^1 f[(b-a)x+a]dx$$

by change of variables $X = (b-a)x + a$.

$$\therefore I \simeq (b-a)\langle f\rangle = \frac{b-a}{n}\sum_{i=1}^{n} f[(b-a)x_i + a]$$

Importance Sampling $\Rightarrow$ variance reduction

Positive weight function $\int_0^1 \omega(x)dx = 1$.

$$\text{So } I = \int_a^b f(x)dx = (b-a)\int_0^1 f[(b-a)x+a]\,dx$$

$$= (b-a)\int_0^1 \frac{f[(b-a)x+a]}{\omega(x)}\,\omega(x)\,dx$$

$$= (b-a)\int_0^1 \frac{f[(b-a)x(\xi)+a]}{\omega[x(\xi)]}\,d\xi$$

where change of variable $\xi(x) = \int_0^x \omega(x')dx'$

$d\xi = \omega(x)dx$; $\xi(0) = 0$, $\xi(1) = 1$ $\therefore$

$\therefore d\xi = \omega(x)dx$; $\xi(0) = \ldots$

performed. So evaluating integral using MC method means averaging f/ω over uniform sample points ξ_i in $[0,1\rangle$.

↳ smooth & slowly varying

$$I \simeq \frac{b-a}{n}\sum_{i=1}^{n}\frac{f[(b-a)x(\xi_i)+a]}{\omega[x(\xi_i)]}$$

Note: $x_i = x(\xi_i)$ is nonuniform, ξ_i's are uniform, so points are weighted by $\omega(x_i)$.

Multidimensional Integrals

$\mathcal{D}$ is fairly complex domain, so

$\int_{\mathcal{D}} f\,dV = V\langle f\rangle \pm \sigma$ is intractable.

Choice an extended domain $\tilde{\mathcal{D}}$ with $\tilde{V}$

$$\tilde{f}(\bar{x}) = f(\bar{x}) \text{ if } \bar{x}\in D,\ \tilde{f}(\bar{x}) = 0 \text{ if } \bar{x}\notin D$$

$\therefore$ MC quadrature $\int_{\mathcal{D}} f\,dV \approx \tilde{V}\langle\tilde{f}\rangle \pm \tilde{\sigma}$

↳ extended volume

$$I = \iint_{x^2+y^2\le 1} dx\,dy = 4\int_0^1 dx\int_0^{\sqrt{1-x^2}} dy = \pi$$

$\mathcal{D}$ = circle in 1^{st} quadrant

$\tilde{\mathcal{D}}$ = unit square $[0,1] \times [0,1]$

$H(x) = 0$ if $x < 0$
$\quad\;\; = 1$ if $x \geq 0$

$$\therefore I = 4 \int_0^1 dx \int_0^1 dy \, H[1 - (x^2 + y^2)]$$

$$\simeq \frac{4}{n} \sum_{i=1}^{n} H[1 - (x_i^2 + y_i^2)] = 4 \frac{n_i}{n}$$

$\therefore$ n uniform sample points (x_i, y_i) in square extended domain $\tilde{\mathcal{D}}$

n_i are interior sample points in circle