Discretização

$$\frac{dv}{dt} = -\gamma v + \sqrt{\frac{2\gamma k_B T}{m}}\, \xi(t)$$

$$\frac{v_{n+1} - v_n}{\tau} = -\gamma v_n + \sqrt{\frac{2\gamma k_B T}{m}}\, \frac{1}{\sqrt{\tau}}\, N(0,1)$$

$$v_{n+1} = v_n - \gamma \tau v_n + \sqrt{\frac{2\gamma k_B T}{m}}\, \sqrt{\tau}\, N(0,1)$$

$$v_{n+1} = \overbrace{(1-\gamma\tau)}^{a} v_n + \sqrt{\Gamma \tau}\, N(0,1)$$

não é estritamente necessário ser gaussian

$$\boxed{v_{n+1} = a v_n + \sqrt{\Gamma\tau}\, \xi_n}$$

$$\xi_n = \xi(t_n) = \xi(n\tau)$$

$$\langle \xi_j \xi_k \rangle = \langle \xi(j\tau)\, \xi(k\tau) \rangle = \delta((j-k)\tau)$$

$$= \delta_{jk} = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases}$$

$$v_1 = a v_0 + \sqrt{\Gamma\tau}\, \xi_0$$

$$v_2 = a v_1 + \sqrt{\Gamma\tau}\, \xi_1 = a(v_0 + \sqrt{\Gamma\tau}\, \xi_0) + \sqrt{\Gamma\tau}\, \xi_1$$

$$= a v_0 + \sqrt{\Gamma\tau}\, (a\xi_0 + \xi_1)$$

$$v_{n+1} = a v_n + \sqrt{\Gamma\tau}\,\xi_n$$

$$v_2 = a v_0 + \sqrt{\Gamma\tau}\,(a\xi_0 + \xi_1)$$

$$v_3 = a\left[a v_0 + \sqrt{\Gamma\tau}\,(a\xi_0 + \xi_1)\right] + \sqrt{\Gamma\tau}\,\xi_3$$

$$= a^2 v_0 + \sqrt{\Gamma\tau}\,(a^2\xi_0 + a\xi_1 + \xi_3)$$

$$\vdots$$

$$v_{n+1} = a^n v_0 + \sqrt{\Gamma\tau}\,(a^n\xi_0 + a^{n-1}\xi_1 + \cdots + \xi_n)$$

$$= a^n v_0 + \sqrt{\Gamma\tau}\sum_{j=0}^{n} a^j \xi_{n-j}$$

$$v_n = a^{n-1} v_0 + \sqrt{\Gamma\tau}\sum_{l=0}^{n-1} a^l \xi_{n-1-l}$$

- Se $v_0 = 0$ (*)

$$\boxed{v_n = \sqrt{\Gamma\tau}\sum_{l=0}^{n-1} a^l \xi_{n-1-l}}$$

Soma de variáveis aleatórias independentes

OBS:

(*) $$a^{n-1} v_0 = (\underbrace{1-\tau\gamma}_{a<1})^{n-1} v_0 \xrightarrow{n\to\infty} 0$$

$$U_n = \sum_{l=0}^{n-1} w_l \, ;$$

$$w_l = a^l \sqrt{\tau \Gamma} \, \underbrace{\xi_{n-1-l}}_{\text{independentes e identicamente distribuídos}}$$

<u>Função característica</u>

$$g_n(k) = \langle e^{ikU_n} \rangle = \langle e^{ik\sum_{l=0}^{n-1} w_l} \rangle$$

$$= \prod_{l=0}^{n-1} \langle e^{ikw_n} \rangle$$

Novamente, se ξ_n é variável aleatória gaussiana de média 0 e variância 1 então

. w_l é gaussiana de média 0

e variância $a^{2l}\tau\Gamma$, portanto

$$\langle e^{ikw_n} \rangle = e^{-k^2 a^{2l} \tau \Gamma / 2}$$

(característica da gaussiana: $\frac{e^{-(y-\mu)^2/2\sigma^2}}{\sqrt{2\pi\sigma^2}}$

$$g(k) = e^{ik\mu - k^2\sigma^2/2} \quad (1.49)$$
)

$$g_n = \prod_{l=0}^{n-1} e^{-k^2 a^{2l} \tau \Gamma / 2} = \exp\left\{ -\frac{k^2 \tau \Gamma}{2} \sum_{l=0}^{n-1} a^{2l} \right\}$$

$$g_n = \prod_{\ell=0}^{n-1} e^{-k^2 a^{2\ell} \tau \Gamma/2} = \exp\left\{-\frac{k^2 \tau \Gamma}{2} \sum_{\ell=0}^{n-1} a^{2\ell}\right\}$$

$$\boxed{g_n(k) = e^{-b_n k^2/2}}$$ onde $b_n = \tau\Gamma \sum_{\ell=0}^{n-1} a^{2\ell}$

Transformada inversa

$$P_n(v_n) = \frac{1}{\sqrt{2\pi b_n}} e^{-v_n^2/2b_n}$$; b_n é a variância de v_n

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$$b_n = \tau\Gamma(1 + a^2 + \cdots + a^{2n-2})$$

$$- \quad a^2 b_n = \tau\Gamma(a^2 + a^4 + \cdots + a^{2n})$$

$$(1-a^2) b_n = \tau\Gamma(1-a^{2n})$$

$$b_n = \tau\Gamma \frac{1-a^{2n}}{1-a^2}$$

Fazendo $\tau \to 0$ com $n\tau = t$ fixo, temos

$$\rho(v,t) = \frac{1}{\sqrt{2\pi b(t)}} e^{-v^2/2b(t)} ;$$

onde $b(t) = \lim_{\substack{\tau \to 0 \\ n\tau \to t}} b_n$

$$b_n = \tau\Gamma\left(\frac{1-a^{2n}}{1-a^2}\right) \qquad n\tau = t, \quad \tau = \frac{t}{n}$$

$$= \tau\Gamma\left[\frac{1-(1-\gamma\tau)^{2n}}{1-(1-\gamma\tau)^2}\right]$$

$$= \frac{t}{n}\Gamma\left[\frac{1-(1-\gamma t/n)^{2n}}{1-(1-\gamma t/n)^2}\right]$$

$$b(t) = \lim b_n = \lim t\Gamma\left\{1-\left[\left(1-\frac{\gamma t}{n}\right)^n\right]^2\right\}\frac{1}{n}\frac{1}{1-(1-\gamma t/n)^2}$$

$$= t\Gamma\left(1-e^{-2\gamma t}\right)\lim\left\{n\left[\cancel{1}-(\cancel{1}-2\gamma t/n+\gamma^2t^2/n^2)\right]\right\}^{-1}$$

$$= t\Gamma(1-e^{-2\gamma t})\lim\left[\cancel{n}\left(\frac{2\gamma t}{\cancel{n}}+\frac{\gamma^2t^2}{n^{\cancel{2}}}\right)\right]^{-1}$$

$$= t\Gamma(1-e^{-2\gamma t})\left[2\gamma t+\lim \cancel{\frac{\gamma^2t^2}{n}}^{\,0}\right]^{-1}$$

$$= \frac{t\Gamma}{2\gamma t}(1-e^{-2\gamma t})$$

$$b(t) = \frac{\Gamma}{2\gamma}(1-e^{-2\gamma t}) \xrightarrow{t\to\infty} \frac{\Gamma}{2\gamma}$$

regime estacionário

$$\rho(v,t) \longrightarrow \rho(v) = \frac{1}{\sqrt{2\pi\,\Gamma/2\gamma}}\,e^{-v^2/(2\Gamma/2\gamma)}$$

$$\rho(v) = \frac{1}{\sqrt{2\pi \, \Gamma/2\gamma}} \, e^{-v^2/(2\Gamma/2\gamma)}$$

$$\rho(v) = \frac{1}{\sqrt{\pi \, \Gamma/\gamma}} \, e^{-v^2/(\Gamma/\gamma)}$$

$$\Gamma = \frac{2\gamma k_B T}{m} \rightarrow \frac{\Gamma}{\gamma} = \frac{2 k_B T}{m}$$

$$\boxed{\rho(v) = \sqrt{\frac{m}{2\pi k_B T}} \, e^{-m v^2/2 k_B T}}$$

energia cinética

$$= \sqrt{\frac{m}{2\pi k_B T}} \, e^{-E_c/k_B T}$$

Distribuição de velocidades de Maxwell em 1D

Note que $k_B T$ é energia, de modo que o argumento da exponencial é adimensional.