Tue 3 Feb

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Recap

Law of large numbers $\bar{X}_R \approx \mu \quad R \gg 1$

Central limit theorem $p(x)$ gaussian

single-step μ, σ^2

Simple random walk

Today

Random walks $\rightarrow$ law of diffusion

$$\langle x \rangle = 2\langle r \rangle - N \qquad \Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$\langle x^2 \rangle = 4\langle r^2 \rangle - 4N\langle r \rangle + N^2$$

$\langle r \rangle, \langle r^2 \rangle$ From $G(\theta) = \sum_{r=0}^{N} e^{r\theta} \underline{P_r}$

$$\boxed{\begin{aligned} \frac{d}{d\theta} G(\theta)\Big|_{\theta=0} &= \sum_r \frac{d}{d\theta} e^{r\theta} P_r \Big|_{\theta=0} = \sum_r r \underbrace{e^{r\theta}}_{1} P_r \Big|_{\theta=0} = \langle r \rangle \\ \frac{d^n}{d\theta^n} G(\theta)\Big|_{\theta=0} &= \sum_r r^n \underbrace{e^{r\theta}}_{1} P_r \Big|_{\theta=0} = \langle r^n \rangle \end{aligned}}$$

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In this case $G(\theta) = \sum_r e^{r\theta} \binom{N}{r} p^r q^{N-r} = \sum_r \binom{N}{r} (e^{\theta} p)^r q^{N-r}$

$$(a+b)^N = \sum_{i=0}^{N} \binom{N}{i} a^i b^{N-i}$$

$$\therefore G(\theta) = (e^{\theta} p + q)^N$$

$$G(0) = (p+q)^N = 1 \checkmark$$

$$\langle r\rangle = \frac{d}{d\theta}\left(e^\theta p+q\right)^N\Big|_{\theta=0} = N\left(\underbrace{e^\theta}_{1} p+q\right)^{N-1} \underbrace{e^\theta}_{1} p\Big|_{\theta=0} = Np \quad ✓$$

$$\langle r^2\rangle = \frac{d}{d\theta}\left(N e^\theta p \left(e^\theta p+q\right)^{N-1}\right)_{\theta=0}$$

$$= \left[N e^\theta p \left(e^\theta p+q\right)^{N-1} + N(N-1)\left(e^\theta p+q\right)^{N-2} e^\theta p\, e^\theta p\right]_{\theta=0}$$

$$= Np + N(N-1)p^2 = Np\left(Np - p + 1\right)$$

$$= Np\left(Np+q\right) = N^2p^2 + Npq$$

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Final result:

$$\langle x\rangle = 2\langle r\rangle - N = 2Np - N = N(2p-1)$$

$$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2$$

$$= 4\langle r^2\rangle - \cancel{4N\langle r\rangle} + \cancel{N^2} - \underbrace{\left(2\langle r\rangle - N\right)^2}_{4\langle r\rangle^2 - \cancel{4N\langle r\rangle} + \cancel{N^2}}$$

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$$\Delta x = \sqrt{4\left(\langle r^2\rangle - \langle r\rangle^2\right)}$$

$$= 2\sqrt{\cancel{N^2p^2} + Npq - \cancel{N^2p^2}} = 2\sqrt{Npq}$$

Sanity checks:

p	$\langle x\rangle$	Δx	
0	$-N$	0	✓
1	N	0	✓
1/2	0 ✓	$\sqrt{N}$	

$\Delta x \propto \sqrt{N}$ generic...

Diffusion

Recall $t = N\,\delta t$ $\qquad N = \dfrac{t}{\delta t}$

$$\langle x \rangle = \frac{t}{\delta t}(2p-1) \simeq \left(\frac{2p-1}{\delta t}\right) t = v_{dr}\, t$$

$v_{dr} = \frac{\langle x \rangle}{t}$ is <u>drift velocity</u> of expected final position

Fluctuations $\Delta x = 2\sqrt{Npq} = \left(2\sqrt{\frac{pq}{\delta t}}\right)\sqrt{t} = D\sqrt{t}$

diffusion length

diffusion constant

$\Delta x \propto \sqrt{t}$ is <u>law of diffusion</u>

very general

Diffusion – "spreading out" as time passes

Repeat random walk many times → t-dependents prob. dist.

Connect diffusion to CLT ($N \gg 1$)

$$p(x) \approx \frac{1}{\sqrt{2\pi N \sigma^2}} \exp\left[-\frac{(x-N\mu)^2}{2N\sigma^2}\right]$$

Need single-step μ, σ^2 (finite)

$$\boxed{\begin{aligned} \mu &= \langle x_i \rangle = \sum_i x_i P_i = (+1)p + (-1)\overset{1-p}{q} = 2p - 1 = v_{dr} \\ \langle x_i^2 \rangle &= (+1)^2 p + (-1)^2 q = p + q = 1 \\ \sigma^2 &= \cancel{1} - (4p^2 - 4p \cancel{+1}) = 4p(1-p) = 4pq = D^2 \end{aligned}}$$

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General results: $\mu = v_{dr}\,\delta t = \frac{v_{dr}\cdot t}{N} = \frac{\langle x \rangle}{N}$

$$\sigma^2 = D^2\,\delta t = \frac{D^2 \cdot t}{N} = \frac{(\Delta x)^2}{N}$$

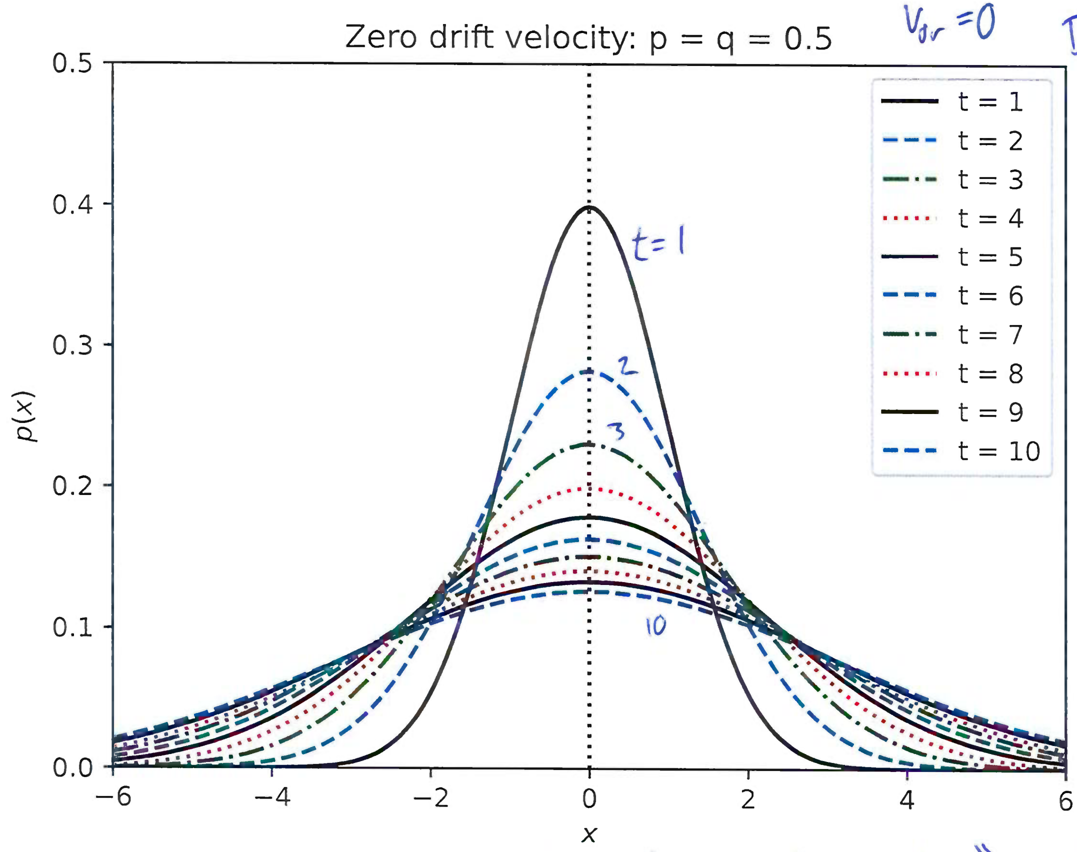
$$p(x) \approx \frac{1}{\sqrt{2\pi D^2 t}} \exp\left[-\frac{(x - v_{dr}\cdot t)^2}{2D^2 t}\right]$$

peak at $x = v_{dr}\cdot t = \langle x \rangle$

width increases $\propto D\sqrt{t}$

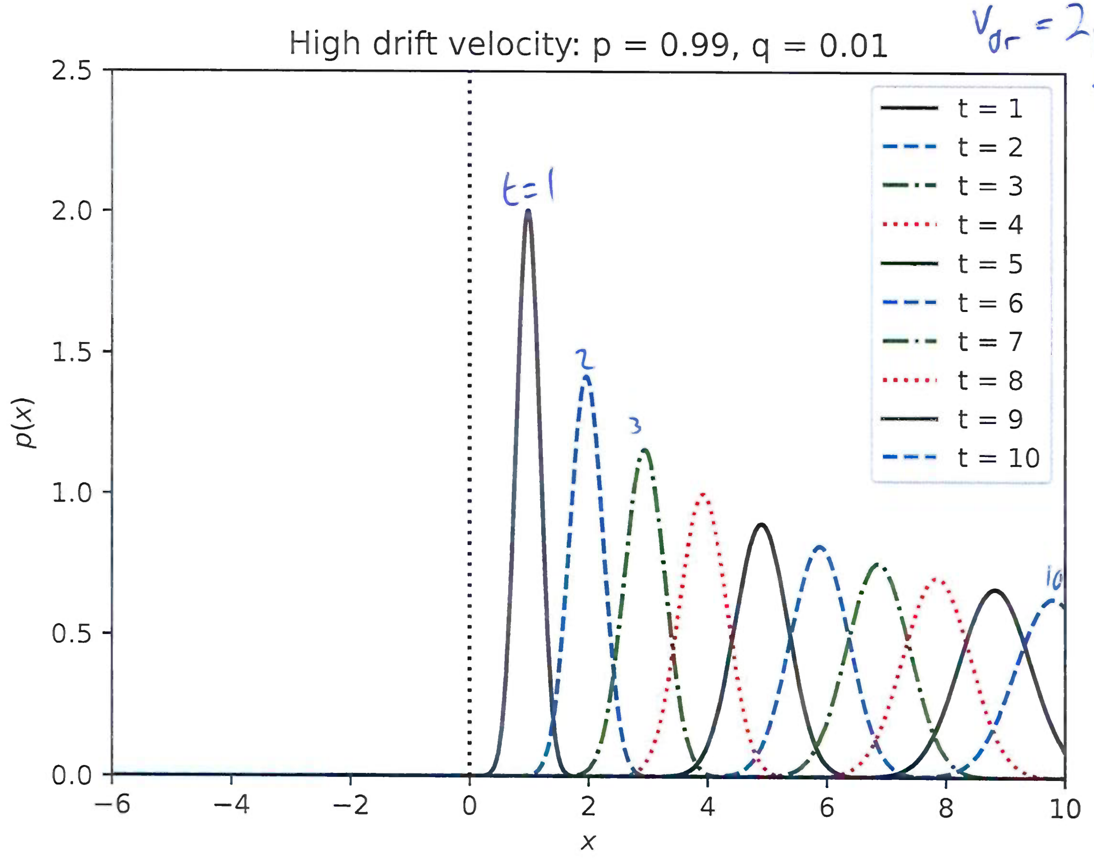
height decreases $\propto 1/D\sqrt{t}$

$V_{dr} = 0$ $D = 2\Delta\sqrt{pq/\delta t} = 1$



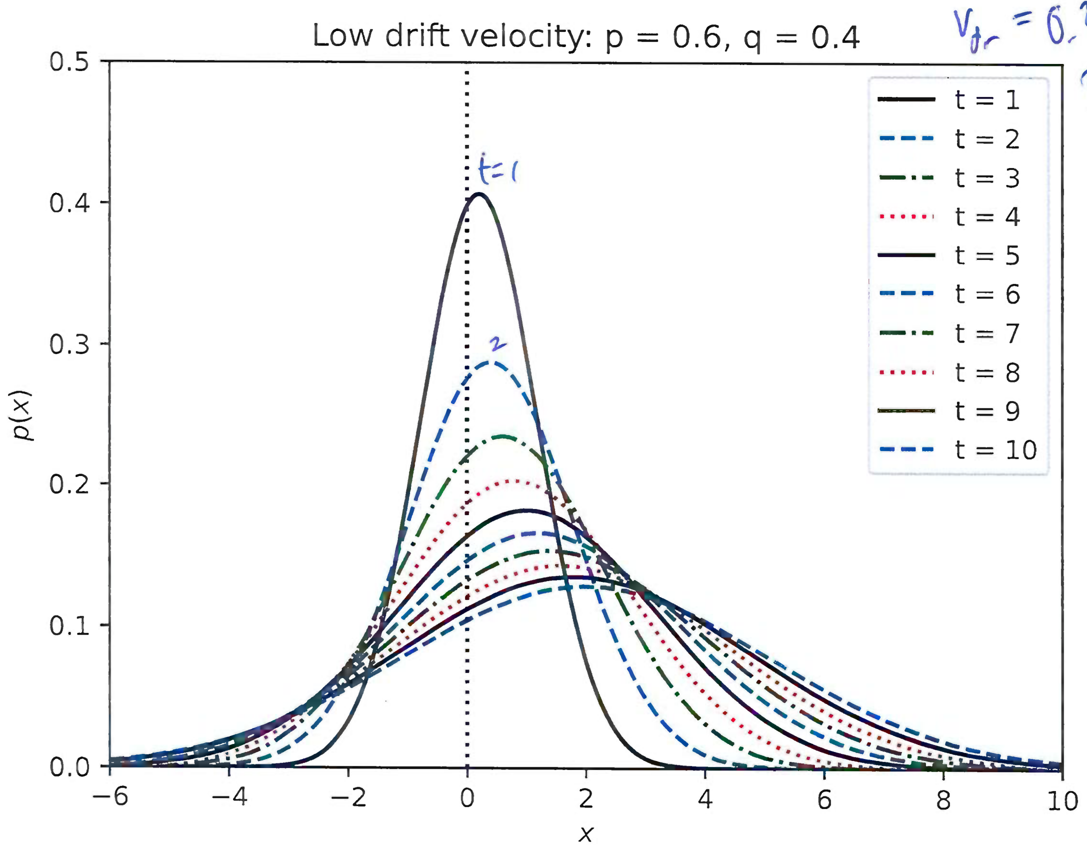
$\langle x \rangle = 0$

"one-sigma" ~ 68%
steadily grows $-D\sqrt{t} \le x \le D\sqrt{t}$



$V_{dr} = 2p-1 = 0.98$

$D = 2\sqrt{pq} = 0.199$



$v_{dr} = 0.2$

$D = 2\sqrt{0.24} = 0.98$