Monday 6 February 221670

Recap

Law of law of numbers

$$\bar{X}_R = \frac{1}{R} \sum_r x^{(r)} \simeq \mu \qquad R \gg 1$$

Central limit theorem

$$p(s) \simeq \frac{1}{\sqrt{2\pi N\sigma^2}} \exp\left[\frac{-(s-N\mu)^2}{2N\sigma^2} \right] \qquad N \gg 1$$

single rep

gaussian prob dist.

Plan

Random walks & diffusion via CLT

Ensembles & equilibrium

Random walk

General modelling tool

Brownian motion, roulette, genetic drift, stock prices

Object takes random step

current position (state) $\rightarrow$ new position (state)

"Markov process" produces Markov chain

Simple example

1) One dimension — step right^{+} probability p
   step left$^{(-)}$ probability $q = 1 - p$

2) Fixed step length $l = 1$

3) Regular time interval Δt
   total time $t = N\Delta t$ for N steps

Representative walk

LRLRRR $N = 6$ final position $x = 2$ from starting $x = 0$

RLRLLL $x = -2$

How many walks with $N = 6$?

$$2 \cdot 2 \cdots 2 = 2^N = 2^6 = 64$$

$$P(LRLRRR) = \frac{1}{64} \text{ iff } p = \tfrac{1}{2} = q$$

$$qpqppp = p^4 q^2$$

$$P(RLRLLL) = p^2 q^4$$

Generic prob. for N-step walk with r steps to the right
$N - r$ steps to the left

$$P_r = p^r \cancel{} q^{N-r}$$

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Compute expec~~t~~ted final position $\langle x \rangle$ and $\langle x^2 \rangle - \langle x \rangle^2$ fluctuations

$$x = (+1)r + (-1)(N - r) = 2r - N \qquad -N \le x \le N$$

Checks: $2 \cdot 4 - 6 = 2$ ✓ $2 \cdot 2 - 6 = -2$ ✓

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$P(x)$ equivalent to $\underline{P_r}$ only because step size $l = 1$ fixed
not general

x unaffected ~~by~~ by order of steps

How many ways to get $x=4$ from $N=6$?

$\binom{N}{r} = \binom{6}{5} = 6$ $\qquad r = \frac{1}{2}(x+N)$

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Overall $P(x=4) = P_5 = 6p^5 q$

General $P_r = \binom{N}{r} p^r q^{N-r}$

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$$\langle x \rangle = \sum_x x P(x) = \sum_{r=0}^{N} (2r-N) P_r = 2\langle r \rangle - N$$

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$$\langle x^2 \rangle = \sum_r (2r-N)^2 P_r = 4\langle r^2 \rangle - 4N\langle r \rangle + N^2$$

Generating Function $\qquad T(\theta) = \sum_{r=0}^{N} e^{r\theta} P_r$

Set $\theta = 0$ $\qquad T(0) = 1$

$$\frac{d}{d\theta} T(\theta)\Big|_{\theta=0} = \sum_r \frac{d}{d\theta} e^{r\theta} P_r \Big|_{\theta=0} = \sum_r r e^{r\theta} P_r \Big|_{\theta=0} = \langle r \rangle$$

$$\frac{d^n}{d\theta^n} T(\theta)\Big|_{\theta=0} = \sum_r r^n e^{r\theta} P_r \Big|_{\theta=0} = \langle r^n \rangle$$

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$$T(\theta) = \sum_r e^{r\theta} \binom{N}{r} p^r q^{N-r} = \sum_r \binom{N}{r} (e^\theta p)^r q^{N-r}$$

$$= (e^\theta p + q)^N$$

(binomial formula $(a+b)^N = \sum_i \binom{N}{i} a^i b^{N-i}$

$T(0) = (p+q)^N = 1$

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

$$\frac{d^2}{d\theta^2}(e^\theta p+q)^N\Big|_{\theta=0} = \left(Ne^\theta p(e^\theta p+q)^{N-1} + N(N-1)e^\theta p(e^\theta p+q)^{N-2}e^\theta p\right)\Big|_{\theta=0}$$

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

$$= Np(Np+q) = \langle r^2\rangle$$

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

$$\langle x^2\rangle - \langle x\rangle^2 = 4\langle r^2\rangle - \cancel{4N\langle r\rangle} + \cancel{N^2} - (2\langle r\rangle - N)^2$$

$$(4\langle r\rangle^2 - \cancel{4N\langle r\rangle} + \cancel{N^2})$$

$$= 4(\langle r^2\rangle - \langle r\rangle^2)$$

$$= 4(\cancel{N^2p^2} + Npq - \cancel{N^2p^2}) = 4Npq$$

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Sanity checks

p	$\langle x\rangle$	$\langle x^2\rangle - \langle x\rangle^2$
0	$-N$	0
1	N	0
1/2	0	N

general result . . .

Diffusion

Recall $t = N\Delta t \rightarrow N = \frac{t}{\Delta t}$

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

Expected final position drifts

Drift velocity $v_{dr} = \frac{\langle x\rangle}{t}$

Similarly for Fluctuations

$$\langle x^2\rangle - \langle x\rangle^2 = 4\left(\frac{t}{\Delta t}\right) p q = \frac{4pq}{\Delta t}\, t = (\Delta x)^2$$

diffusion length

Law of diffusion

$$\Delta x \propto \sqrt{t}$$

$$\Delta x = D\sqrt{t}$$

diffusion constant governs scale of fluctations

For this simple example

$$V_{dr} = \frac{2p-1}{\Delta t} \qquad D = 2\sqrt{\frac{pq}{\Delta t}}$$

Examples

Connecting diffusion to central limit theorem

$$p(x) = \frac{1}{\sqrt{2\pi N\sigma^2}} \exp\left[\frac{-(x-N\mu)^2}{2N\sigma^2}\right] \qquad x = s = \sum_i x_i \qquad N \gg 1$$

Mean μ and variance σ^2 of single-step process

$$\boxed{\begin{aligned} \mu &= \langle x_i\rangle = \sum_i x_i P_i = (+1)p + (-1)\underbrace{q}_{1-p} = 2p-1 = V_{dr}\left(\frac{t}{N}\right) = \frac{V_{dr}\cdot t}{N} \\ \langle x_i^2\rangle &= (+1)^2 p + (-1)^2 q = 1 \\ \sigma^2 &= 1-\mu^2 = \cancel{1} - (4p^2 - 4p + \cancel{1}) = 4p(1-p) = 4pq = \frac{D^2 t}{N} \\ D^2 &= \frac{4pq}{\Delta t} = \frac{\sigma^2 N}{t} \end{aligned}}$$

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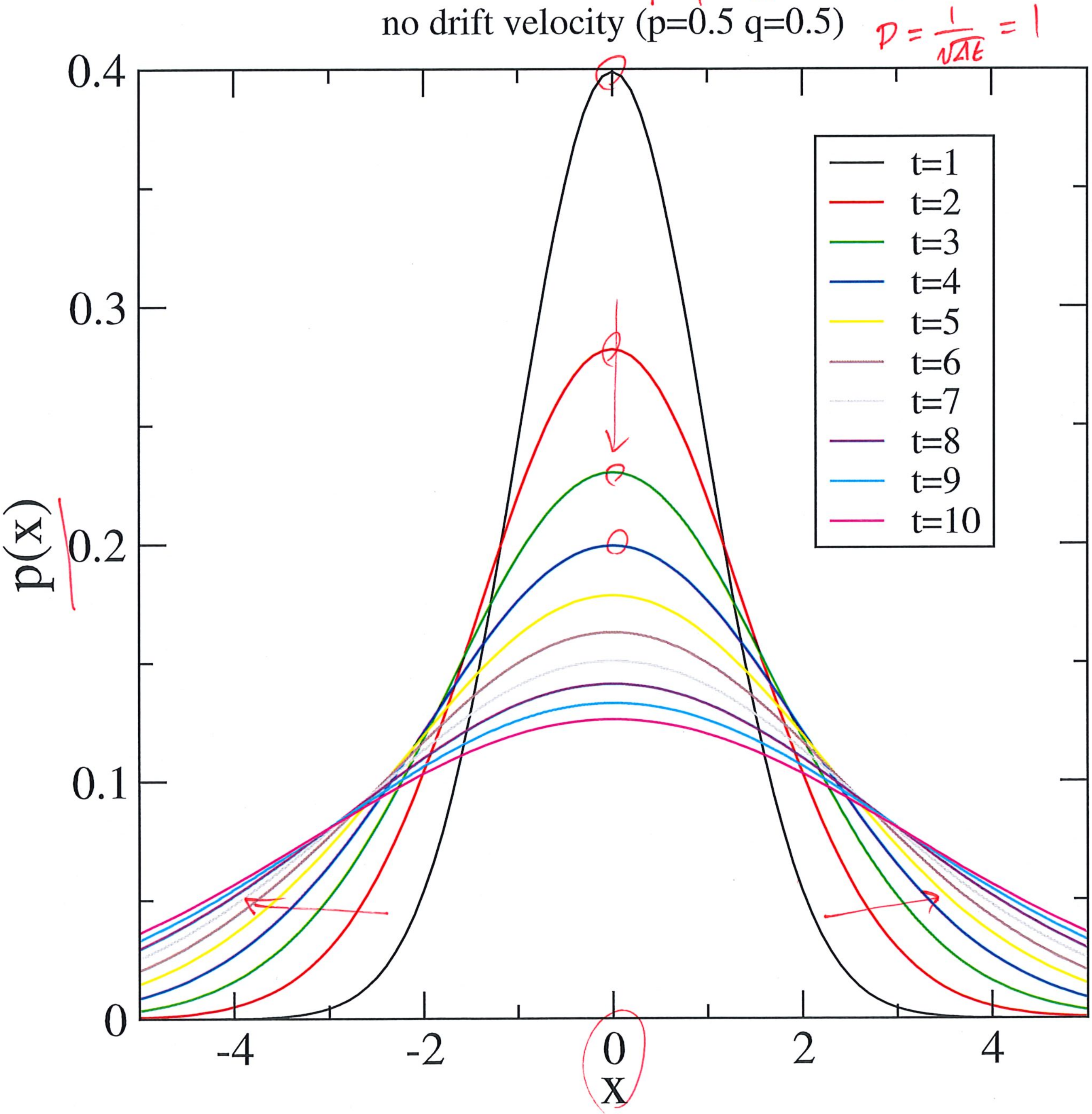
$p = q = \frac{1}{2}$

$V_{dr} = 0$

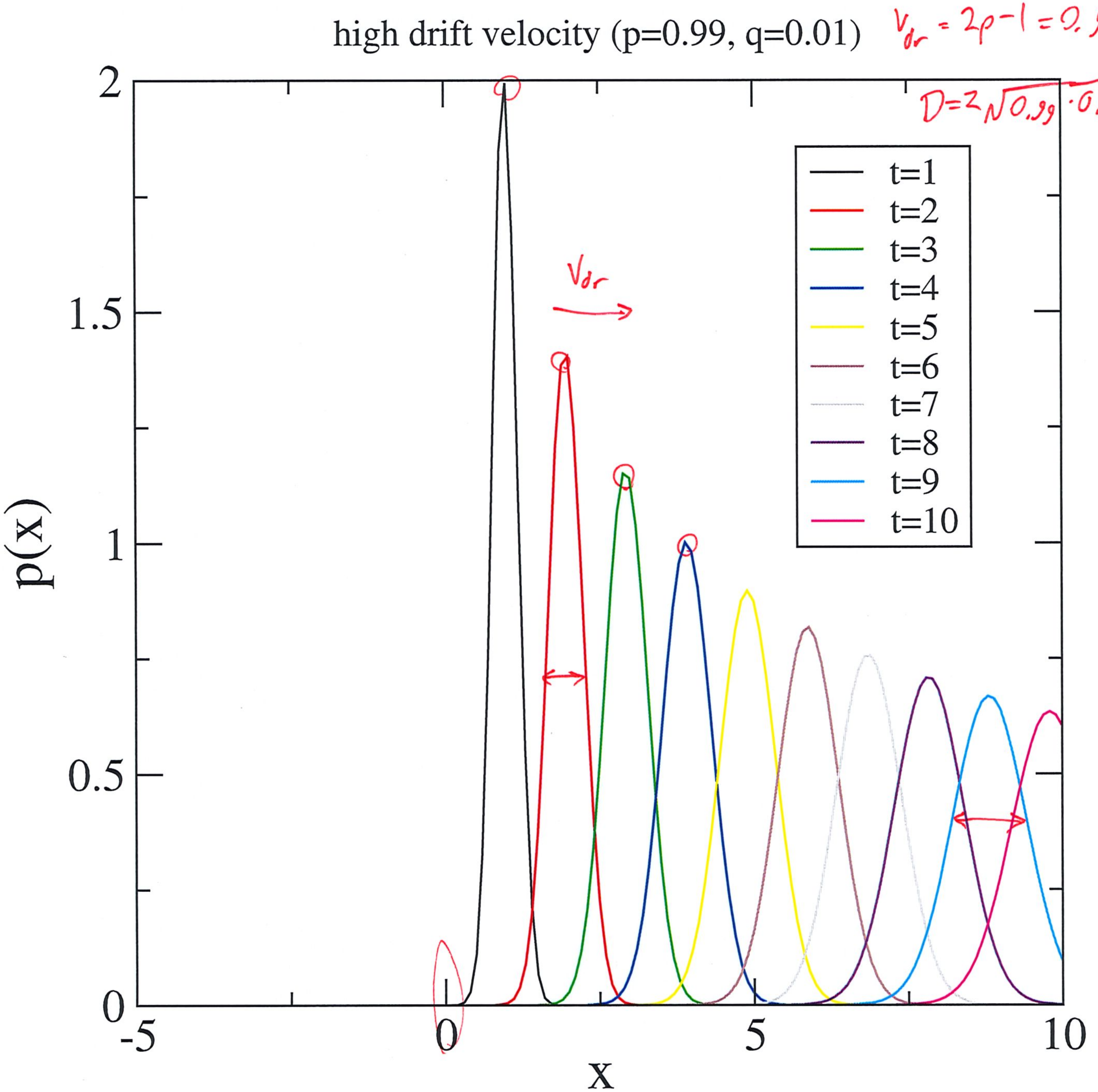
$D = \frac{1}{\sqrt{\Delta t}} = 1$



$\langle x \rangle = 0$

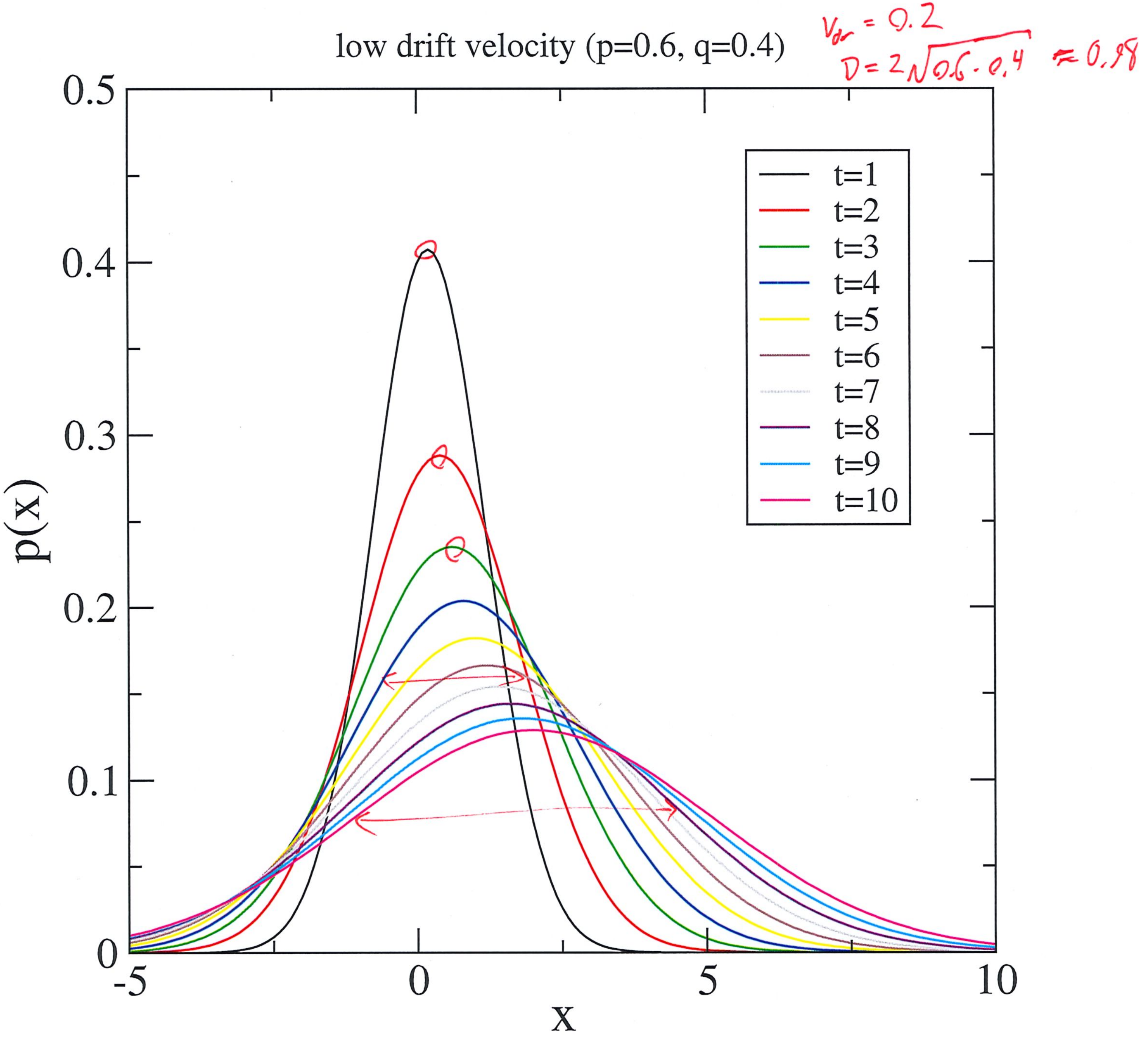
'one-sigma' interval $\sim 68\%$

$-D\sqrt{t} \leq x \leq D\sqrt{t}$



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

$D = 2\sqrt{0.99 \cdot 0.01} \approx \underline{0.199}$


low drift velocity (p=0.6, q=0.4)
p(x)
x
0
0.1
0.2
0.3
0.4
0.5
-5
0
5
10
t=1
t=2
t=3
t=4
t=5
t=6
t=7
t=8
t=9
t=10
$v_{dr} = 0.2$
$D = 2\sqrt{0.6 \cdot 0.4} \approx 0.98$

Resulting $N\mu = v_{dr} t$ and $N\sigma^2 = D^2 t$ are general

(specific expressions w/p,q not general)

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

peak at $x - v_{dr} t = 0$

width increases with $2D^2 t$

$\rightarrow$ normalization decrease $\sim D\sqrt{t}$

Drift vs. diffusion

Assuming $v_{dr} \neq 0$

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$$\boxed{\left.\begin{array}{l} \langle x\rangle \propto t \\ \Delta x \propto \sqrt{t} \end{array}\right\} \quad \frac{\Delta x}{\langle x\rangle} \propto \frac{\sqrt{t}}{t} = \frac{1}{\sqrt{t}} \rightarrow 0 \text{ as } t \rightarrow \infty}$$

Although absolute diffusion length grows $\propto \sqrt{t}$
relative uncertainty becomes negligible
when compared to non-zero drift

Law of diffusion $\longleftrightarrow$ central limit theorem

only assumes μ, σ^2 finite

(single step

~~Statistical~~

Statistical ensemble

General idea: Observe many particles evolving in time
experiment — subject to constraints

Different states w_i, w_j at different times t_i, t_j

Simple (but powerful) example: spin system

"particles" are spins that point up ↑ or down ↓

(motivation from magnetic molecules & much more)

$$\boxed{\begin{array}{l}\text{Configuration of } N=8 \text{ spins fixed in a line} \\ \uparrow\downarrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow \\ \text{Total \# of configs: } 2\cdot 2\cdots 2 = 2^N = 2^8 = 256\end{array}}$$

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Measure # of spins for all 256 configs always gives 8

→ N is <u>conserved quantity</u> same for all w_i

Another example: Total internal energy of <u>isolated</u> (closed) system

$E(w_i) = E(w_j)$ for all i, j

First ~~empirid~~ observed empirically

"First Law of Thermodynamics"

Later proven through Emmy Noether (in flat space-time)

Equivalent state: Changing internal energy of system Ω

→ equal & opposite change in energy of its surroundings