Assignment 2

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1 Kadar Ch. 2 Problem 9

Our model of random deposition essentially randomly places atoms on a set of sites. The sites are all independent. The deposition rate is d layers per second and if there are δ sites per layer then the deposition rate is δd sites filled (or atoms) per second.

1.1 Problem 9.a

What's the probability of having m atoms deposited at a given site after some time t? In that time t there have been $N = \delta dt$ deposition events *i.e.* a total of N atoms on the mirror. Since each site is independent of all the others the probability of an atom choosing our special site out of the δ sites is $p = 1/\delta$ while $q = 1 - p = 1 - 1/\delta$ is the much larger probability of choosing some toher site. The probability of having m atoms at our chosen site after N deposition events is given by the binomial distribution to be

$$\begin{aligned} p_N(m) &= \binom{N}{m} p^m q^{N-m} \\ &= \frac{N!}{m!\,(N-m)!}\left(\frac{1}{\delta}\right)^m\left(1-\frac{1}{\delta}\right)^{N-m} \\ &= \frac{(\delta dt)!}{m!\,(\delta dt - m)!}\left(\frac{1}{\delta}\right)^m\left(\frac{\delta-1}{\delta}\right)^{N-m} \end{aligned}$$

but in the limit that $N \gg !$ *i.e.* many deposition events the binomial distribution approaches the Poisson Distribution

$$\boxed{p = \frac{(\delta dt)^m\, e^{-\delta dt}}{m!}}. \tag{1}$$

We can ask, "What fraction is not covered by any gold?", in which case, we are wondering what the probability of $m = 0$ is. From Eq. (1) we know

$$\boxed{p(\delta d; 0) = \frac{(\delta dt)^0\, e^{-\delta dt}}{0!} = e^{-\delta dt}}. \tag{2}$$

Since each deposition event is independent of all others this is the fraction of sites not covered.

1.2 Problem 9.b

What's the thickness's variance?

As stated clearly in the text, every cumulant n of the Poison distribution is

$$\langle m^n \rangle_c = \delta dt \tag{3a}$$

The variance is the second cumulant

$$\left\langle m^2 \right\rangle_c = \delta dt = \sigma^2 \tag{3b}$$

2 Kadar Ch. 2 Problem 11

Consider random variables x and y with joint probability $p(x, y)$. Mutual information is defined as

$$M(x, z) \equiv \sum_{x,y} p(x, y) \ln \left(\frac{p(x, y)}{p_x(x)p_y(y)} \right) \tag{4}$$

where p_x and p_y are unconditional probabilities, i.e.

$$\begin{aligned} p_x(x) &= \int dyp(x, y) = \sum_y p(x, y) \\ p_y(y) &= \int dxp(x, y) = \sum_x p(x, y) \end{aligned} \tag{5}$$

2.1 Problem 11.a

Relate M to entropies.

$$S \quad = -\int dzp(z) \ln p(z) \quad = -\sum_{i=1}^{N} p(i) \ln p(i)$$

Then we can say that the mutual information from Eq. (4) is

$$\begin{aligned} M(x, y) &= \sum_{x,y} p(x, y) \ln \left(\frac{p(x, y)}{p_x(x)p_y(y)} \right) \\ &= \sum_{x,y} p(x, y) \{\ln p(x, y) - \ln p_x(x) - \ln p_y(y)\} \\ &= \underbrace{\sum_{x,y} p(x, y) \ln p(x, y)}_{-S(x,y)} - \sum_{x,y} p(x, y) \ln p_x(x) - \sum_{x,y} p(x, y) \ln p_y(y) \\ &= -S(x, y) - \sum_{x,y} p(x, y) \ln p_x(x) - \sum_{x,y} p(x, y) \ln p_y(y). \end{aligned}$$

If we remember the definition we gave to the unconditional probabilities in Eq. 5 (and expand the sums) we can continue:

$$\begin{aligned} M(x,y) &= -S(x,y) - \sum_x \sum_y p(x,y) \ln p_x(x) - \sum_x \sum_y p(x,y) \ln p_y(y) \\ &= -S(x,y) - \sum_x \ln p_x(x) \underbrace{\sum_y p(x,y)}_{p_x} - \sum_y \ln p_y(y) \underbrace{\sum_x p(x,y)}_{p_y} \\ &= -S(x,y) - \underbrace{\sum_x p_x(x) \ln p_x(x)}_{-S_x(x)} - \underbrace{\sum_y p_y(y) \ln p_y(y)}_{-S_y(y)} \end{aligned}$$

$$\boxed{M(x,y) = -S(x,y) + S_x(x) + S_y(y)} \tag{6}$$

2.2 Problem 11.b

Find M for

$$p(x,y) \propto \exp\left(-\frac{ax^2}{2} - \frac{by^2}{2} - cxy\right). \tag{7a}$$

We can determine the unconditional probabilities:

$$\begin{aligned} p_x(x) &= \int dy p(x,y) \\ &\propto \int_{-\infty}^{\infty} dy \exp\left(-\frac{ax^2}{2} - \frac{by^2}{2} - cxy\right) \\ &= \exp\left(-\frac{ax^2}{2}\right) \int_{-\infty}^{\infty} \exp\left(\frac{by^2}{2} - cxy\right) dy \\ &= \exp\left(-\frac{ax^2}{2}\right) \left[\sqrt{\frac{\pi}{b/2}} \exp\left(\left[\frac{cx}{2}\right]^2 /(b/2)\right)\right] \end{aligned}$$

$$\boxed{p_x(x) \propto \sqrt{\frac{2\pi}{b}} \exp\left(\frac{x^2}{2}\left[\frac{c^2}{b} - a\right]\right)} \tag{7b}$$

And in exactly the same way:

$$\boxed{p_y(y) \propto \sqrt{\frac{2\pi}{a}} \exp\left(\frac{y^2}{2}\left[\frac{c^2}{a} - b\right]\right)} \tag{7c}$$

We could substitute p_x and p_y into $M(x,y) = \sum_{x,y} p(x,y) \ln\left(\frac{p(x,y)}{p_x(x)p_y(y)}\right)$ but that leads us to a disaster that doesn't look like any fun.

Instead we try the entropy relation found in part a) *i.e.* Eq. (6) . We have to find each of the entropies. Let's start with $S_x(x)$ and let $k_x \equiv -\left(c^2/b - a\right)/2$, for convenience:

$$
\begin{aligned}
S_x(x) &= -\sum_x p_x(x) \ln p_x(x) = -\int_{-\infty}^{\infty} p_x(x) \ln p_x(x) \\
&\propto -\int_{-\infty}^{\infty} \sqrt{\frac{2\pi}{b}} \exp\left(-k_x x^2\right) \ln\left[\sqrt{\frac{2\pi}{b}} \exp\left(-k_x x^2\right)\right] \\
&= -\sqrt{\frac{2\pi}{b}} \int_{-\infty}^{\infty} \exp\left(-k_x x^2\right)\left[\ln\left(\sqrt{\frac{2\pi}{b}}\right) - k_x x^2\right] \\
&= -\sqrt{\frac{2\pi}{b}}\left[\ln\left(\sqrt{\frac{2\pi}{b}}\right) \underbrace{\int_{-\infty}^{\infty} \exp\left(-k_x x^2\right)}_{=\sqrt{\frac{\pi}{k_x}}} - k_x \underbrace{\int_{-\infty}^{\infty} x^2 \exp\left(-k_x x^2\right)}_{=\frac{1}{2}\sqrt{\frac{\pi}{k_x^3}}}\right] \\
&= -\sqrt{\frac{2\pi}{b}}\left[\ln\left(\sqrt{\frac{2\pi}{b}}\right)\sqrt{\frac{\pi}{k_x}} - k_x \frac{1}{2}\sqrt{\frac{\pi}{k_x^3}}\right] \\
&= \pi\sqrt{\frac{2}{b}}\left[-\ln\left(\sqrt{\frac{2\pi}{b}}\right)\sqrt{\frac{1}{k_x}} + \frac{1}{2}\sqrt{\frac{1}{k_x}}\right] \\
&= \pi\sqrt{\frac{2}{bk_x}}\left[\frac{1}{2} - \ln\sqrt{\frac{2\pi}{b}}\right] \\
&= \pi\sqrt{\frac{2}{b\left(a - c^2/b\right)/2}}\left[\frac{1}{2} - \ln\sqrt{\frac{2\pi}{b}}\right]
\end{aligned}
$$

$$
\boxed{S_x(x) \propto \frac{2\pi}{\sqrt{ab - c^2}}\left[\frac{1}{2} - \ln\sqrt{\frac{2\pi}{b}}\right]}. \tag{8a}
$$

Likewise we can find $S_y(y)$ by defining $k_y \equiv -\left(c^2/a - b\right)/2$ and doing the integral again or just exchanging b for a in Eq. (8a) :

$$
\boxed{S_y(y) \propto \frac{2\pi}{\sqrt{ab - c^2}}\left[\frac{1}{2} - \ln\sqrt{\frac{2\pi}{a}}\right]}. \tag{8b}
$$

$S(x, y)$ is tougher for one thing because it's a double integral.

$$
\begin{aligned}
S(x, y) &= -\sum_{x,y} p(x, y) \ln p(x, y) = -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p(x, y) \ln p(x, y) dxdy \\
&\propto -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp\left(-\frac{ax^2}{2} - \frac{by^2}{2} - cxy\right) \ln\left\{\exp\left(-\frac{ax^2}{2} - \frac{by^2}{2} - cxy\right)\right\} dxdy \\
&= -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(-\frac{ax^2}{2} - \frac{by^2}{2} - cxy\right) \exp\left(-\frac{ax^2}{2} - \frac{by^2}{2} - cxy\right) dxdy
\end{aligned}
$$

To deal with this let's try to get a handle on the x integral first. Daisy Williams handled it well and this is her idea. Consider completing the square of the terms involving x

$$
\begin{aligned}
-\frac{ax^2}{2} - cxy - \frac{by^2}{2} &= \left\{-\frac{ax^2}{2} - cxy\right\} - \frac{by^2}{2} \\
&= \left\{-\frac{a}{2}\left(x^2 + \frac{2c}{a}xy\right)\right\} - \frac{by^2}{2} \\
&= \left\{-\frac{a}{2}\left(x^2 + \frac{2c}{a}xy + \left[\frac{c}{a}\right]^2 y^2\right) + \frac{c^2}{2a}y^2\right\} - \frac{by^2}{2} \\
&= -\frac{a}{2}\left(x + \frac{c}{a}y\right)^2 - \left(\frac{b}{2} - \frac{c^2}{2a}\right)y^2 \\
&= -\frac{a}{2}u^2 - k_y y^2
\end{aligned}
$$

where $u \equiv x + cy/a$ (so $du = dx$) and we got to use k_y again. **Now** let's try the x-integral

$$
\begin{aligned}
I_x &= \int_{-\infty}^{\infty} \left(-\frac{ax^2}{2} - \frac{by^2}{2} - cxy\right) \exp\left(-\frac{ax^2}{2} - \frac{by^2}{2} - cxy\right) dx \\
&= \int_{-\infty}^{\infty} \left(-\frac{a}{2}u^2 - k_y y^2\right) \exp\left(-\frac{a}{2}u^2 - k_y y^2\right) du \\
&= \int_{-\infty}^{\infty} \left(-\frac{a}{2}u^2 - k_y y^2\right) \exp\left(-\frac{a}{2}u^2\right) \exp\left(-k_y y^2\right) du \\
&= -\exp\left(-k_y y^2\right) \left[\frac{a}{2}\underbrace{\int_{-\infty}^{\infty} u^2 \exp\left(-\frac{a}{2}u^2\right) du}_{=\frac{1}{2}\sqrt{\frac{\pi}{(a/2)^3}}} + k_y y^2 \underbrace{\int_{-\infty}^{\infty} \exp\left(-\frac{a}{2}u^2\right) du}_{=\sqrt{\frac{\pi}{a/2}}}\right] \\
&= -\exp\left(-k_y y^2\right) \left[\frac{a}{2}\frac{1}{2}\sqrt{\frac{\pi}{(a/2)^3}} + k_y y^2 \sqrt{\frac{\pi}{a/2}}\right] \\
&= -\sqrt{\frac{2\pi}{a}} \exp\left(-k_y y^2\right) \left[\frac{1}{2} + k_y y^2\right]
\end{aligned}
$$

Ok then. The entropy is

$$
\begin{aligned}
S(x, y) &\propto -\int_{-\infty}^{\infty} I_x(y) dy \\
&= \sqrt{\frac{2\pi}{a}} \int_{-\infty}^{\infty} \exp\left(-k_y y^2\right) \left[\frac{1}{2} + k_y y^2\right] dy \\
&= \sqrt{\frac{2\pi}{a}} \left[\frac{1}{2}\sqrt{\frac{\pi}{k_y}} + k_y \frac{1}{2}\sqrt{\frac{\pi}{k_y^3}}\right] \\
&= \sqrt{\frac{2\pi}{a}} \sqrt{\frac{\pi}{k_y}} \\
&= \sqrt{\frac{2\pi}{a}} \sqrt{\frac{2\pi}{(b - c^2/a)}}
\end{aligned}
$$

A	B	D
1	1	0
1	0	1
0	1	1
0	0	0

Table 1: XOR truth table.

$$\boxed{S(x,y) \propto \frac{2\pi}{\sqrt{ab-c^2}}}. \tag{8c}$$

Finally, we can use the three Eq. (8) in Eq. (6) to find the mutual information

$$\begin{aligned} M(x,y) &= -S(x,y) + S_x(x) + S_y(y) \\ &\propto -\frac{2\pi}{\sqrt{ab-c^2}} + \frac{2\pi}{\sqrt{ab-c^2}}\left[\frac{1}{2} - \ln\sqrt{\frac{2\pi}{b}}\right] + \frac{2\pi}{\sqrt{ab-c^2}}\left[\frac{1}{2} - \ln\sqrt{\frac{2\pi}{a}}\right] \\ &= \frac{2\pi}{\sqrt{ab-c^2}}\left[-\ln\sqrt{\frac{2\pi}{b}} - \ln\sqrt{\frac{2\pi}{a}}\right] \\ &= \frac{2\pi}{\sqrt{ab-c^2}}\left[\ln\sqrt{\frac{b}{2\pi}} + \ln\sqrt{\frac{a}{2\pi}}\right] \end{aligned}$$

$$\boxed{M(x,y) \propto \frac{2\pi}{\sqrt{ab-c^2}} \ln\left(\frac{\sqrt{ab}}{2\pi}\right)}. \tag{9}$$

3 Sethna Ch. 5 Problem 3

An irreversible logic gate (an XOR). We have inputs A and B with an output $D = A \bigoplus B$. Say 1 is true and 0 is false then we have the truth table

3.1 Problem 3.a

Irreversible logic gate.

3.1.1 Problem 3.a.1

How many bits of information are lost during the gate's action?

Since entropy is a measure of ignorance in bits, a comparison of initial and final Shannon entropies ($S_{SH,i}$ and $S_{SH,f}$) gives a measure of the information lost in bits. If all states are equally likely than $p = 1/W$ where W is the number of states. Table 1 shows four separate states so the entropy is

$$\begin{aligned}
S_{SH,i} &= -k_{SH}\sum_i p_i \ln p_i = -\sum_i p_i \log_2 p_i \\
&= -\sum_1^4 \frac{1}{4}\log_2\left(\frac{1}{4}\right) \\
&= -4\frac{1}{4}\log_2(1/4) \\
&= \log_2 4 = \frac{2\ln 2}{\ln 2} \\
&= 2 \text{ bits}
\end{aligned} \tag{10}$$

where we have set $k_{SH} = 1/\ln 2$ so that S_{SH} is in bits. In the same way, we can find the Shannon entropy after the operation

$$\begin{aligned}
S_{SH,f} &= -\sum_1^2 \frac{1}{2}\log_2\left(\frac{1}{2}\right) \\
&= -2\frac{1}{2}\left(-\frac{\ln 2}{\ln 2}\right) \\
&= 1 \text{ bit}
\end{aligned} \tag{11}$$

So the lose is

$$\boxed{\Delta S_{SH} = S_{SH,i} - S_{SH,f} = 1 \text{ bit}} \tag{12}$$

3.1.2 Problem 3.a.2

What is the minimum work needed to perform the operation at some temperature T?

From $\Delta E = T\Delta S - \Delta W$ we can see that since the operation does not require or emit energy

$$\boxed{\Delta W = T\Delta S = T \times 1 \text{ bit}} \tag{13}$$

3.2 Problem 3.a

Reversible logic gate.

3.2.1 Problem 3.b.1

Make a truth table for a CNOT gate which has two outputs a $D = A \bigoplus B$ as before and a $C = A$ as seen in Table 2.

3.2.2 Problem 3.b.2

Run the outputs C and D as inputs for a second CNOT. The net operation of two CNOTs in series is transmission. The set of outcomes is equivalent to the inputs meaning that this operation is reversible. This can be seen in Table 3.

A	B	C	D
1	1	1	0
1	0	1	1
0	1	0	1
0	0	0	0

Table 2: CNOT truth table.

A	B	C A'	D B'	C'	D'
1	1	1	0	1	1
1	0	1	1	1	0
0	1	0	1	0	1
0	0	0	0	0	0

Table 3: Series of 2 CNOTs.

4 Sethna Ch. 5 Problem 10

The probability of finding a particle at some position $\vec{x}$ at a time t is $p(\vec{x}, t)$. Now this is directectly related to the density $\rho(\vec{x}, t)$: The probability density and the actual concentration profile must be the same shape, right? So that means we can write the diffusion equation of concentrations

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2}$$

as an equation for probability

$$\frac{\partial p}{\partial t} = D\frac{\partial^2 p}{\partial x^2}. \tag{14}$$

There are a few things we must keep in mind and that Sethna tells us:

1. p is positive.
2. "all gradients die away rapidly at $x = \pm\infty$." This means all deriviatives of ρ (and therefore p) are zero when evaluated at $\pm\infty$.
3. there is no advection so the complete time derivative becomes the partial time derivative

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \rho\frac{\partial \vec{x}}{\partial t} = \frac{\partial \rho}{\partial t} + 0 = \frac{\partial \rho}{\partial t}$$

We are now ready to show that entropy increases with time

$$
\begin{aligned}
\frac{dS}{dt} &= \frac{\partial S}{\partial t} \\
&= -k_\mathrm{B} \frac{\partial}{\partial t} \left[\int_{-\infty}^{\infty} p \ln p \, dx \right] \\
&= -k_\mathrm{B} \int_{-\infty}^{\infty} \left[p \frac{\partial \ln p}{\partial t} + \ln p \frac{\partial p}{\partial t} \right] dx \\
&= -k_\mathrm{B} \int_{-\infty}^{\infty} \left[p \left(\frac{\partial \ln p}{\partial p} \frac{\partial p}{\partial t} \right) + \ln p \frac{\partial p}{\partial t} \right] dx \\
&= -k_\mathrm{B} \int_{-\infty}^{\infty} \left[\frac{\partial p}{\partial t} + \ln p \frac{\partial p}{\partial t} \right] dx \\
&= -k_\mathrm{B} \int_{-\infty}^{\infty} \left[1 + \ln p \right] \frac{\partial p}{\partial t} dx
\end{aligned}
$$

At this point we substitute the time derivative for the diffusion equation Eq. (14) to get

$$
\begin{aligned}
\frac{dS}{dt} &= -k_\mathrm{B} \int_{-\infty}^{\infty} \left[1 + \ln p \right] \left(D \frac{\partial^2 p}{\partial x^2} \right) dx \\
&= -k_\mathrm{B} D \left\{ \int_{-\infty}^{\infty} \frac{\partial^2 p}{\partial x^2} dx + \int_{-\infty}^{\infty} \ln p \frac{\partial^2 p}{\partial x^2} dx \right\} \\
&= -k_\mathrm{B} D \left\{ \left[\frac{\partial p}{\partial x} \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \ln p \frac{\partial^2 p}{\partial x^2} dx \right\} \\
&= -k_\mathrm{B} D \left\{ [0 - 0] + \int_{-\infty}^{\infty} \ln p \frac{\partial^2 p}{\partial x^2} dx \right\} \\
&= -k_\mathrm{B} D \int_{-\infty}^{\infty} \ln p \frac{\partial^2 p}{\partial x^2} dx
\end{aligned}
$$

which we integrate by parts:

$$
\begin{aligned}
u &= \ln p \\
du &= \frac{1}{p} \frac{\partial p}{\partial x} dx \\
v &= \frac{\partial p}{\partial x} \\
dv &= \frac{\partial^2 p}{\partial x^2} dx
\end{aligned}
$$

So

$$
\begin{aligned}
\frac{dS}{dt} &= -k_\mathrm{B} D \int_{-\infty}^{\infty} \ln p \frac{\partial^2 p}{\partial x^2} dx \\
&= -k_\mathrm{B} D \int_{-\infty}^{\infty} u \, dv = [uv]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} v \, du \\
&= -k_\mathrm{B} D \left\{ \left[\ln p \frac{\partial p}{\partial x} \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{1}{p} \frac{\partial p}{\partial x} \frac{\partial p}{\partial x} dx \right\}
\end{aligned}
$$

$$\boxed{\frac{dS}{dt} = k_{\mathrm{B}} D \int_{-\infty}^{\infty} \frac{1}{p} \left(\frac{\partial p}{\partial x} \right)^2 dx > 0} \tag{15}$$

since $p \geq 0$ and the derivative is squared.