CHAPTER 3. BASIC MATHEMATICAL MODELLING

Mathematical Modelling is the art of using mathematics to analyse SIMPLE situations which are supposed to approximate VERY COMPLICATED realistic situations.

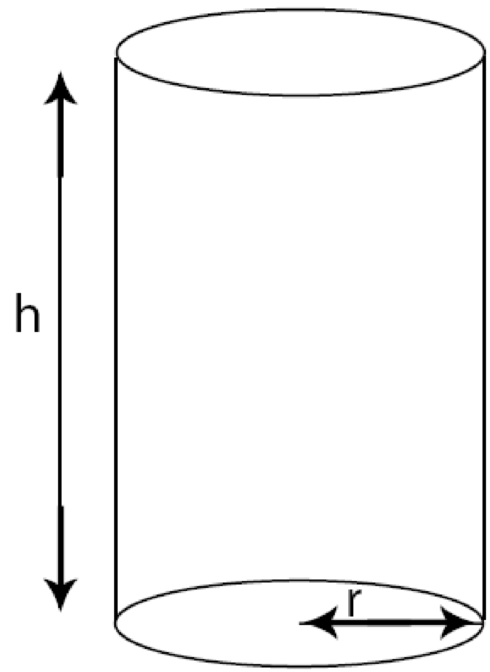
How should CANS be made?

Suppose you are an engineer helping to turn a factory making "tin" cans. Your objective is to MINIMIZE the cost of this process.

Now IN REALITY the function $C()$, which gives you the cost of making one can, depends on a large number of things: the price of "tin", the shape of the can, cost of sticking its parts together, etc... Very complicated. So let's start with the SIMPLEST POSSIBLE MODEL:

Model 1

In THIS [very simple] model, we only care about the amount of "tin" actually in the CAN.



If the height of the can is h and its radius is r, you can easily see that the area is:

$$A = 2\pi r^2 + 2\pi rh$$

This is minimized by setting $r = 0$... the cheapest way to make cans IS NOT TO MAKE THEM AT ALL! TRUE!

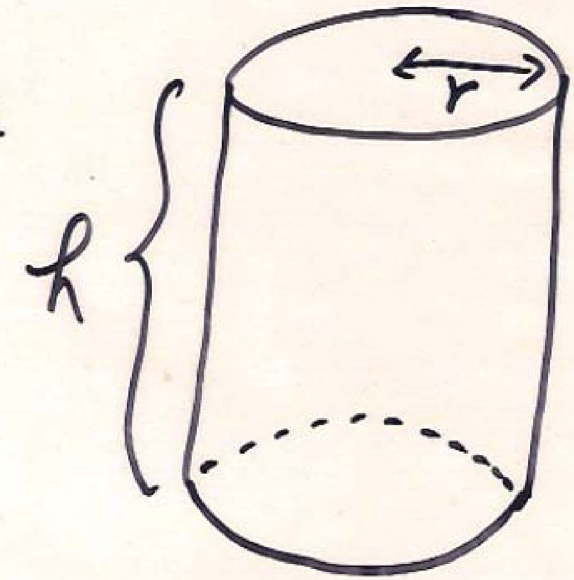
oh, OK, you want to put something inside those cans!

Job: To make a can of fixed volume V with minimum cost!

$\because$ material cost $\sim$ surface area

$\therefore$ we want surface area

$A = \min!$



$$A = \pi r^2 + 2\pi r h + \pi r^2 = 2\pi r^2 + 2\pi r h$$

$$\because \pi r^2 h = V$$

$$\therefore A = 2\pi r^2 + \frac{2V}{r}$$

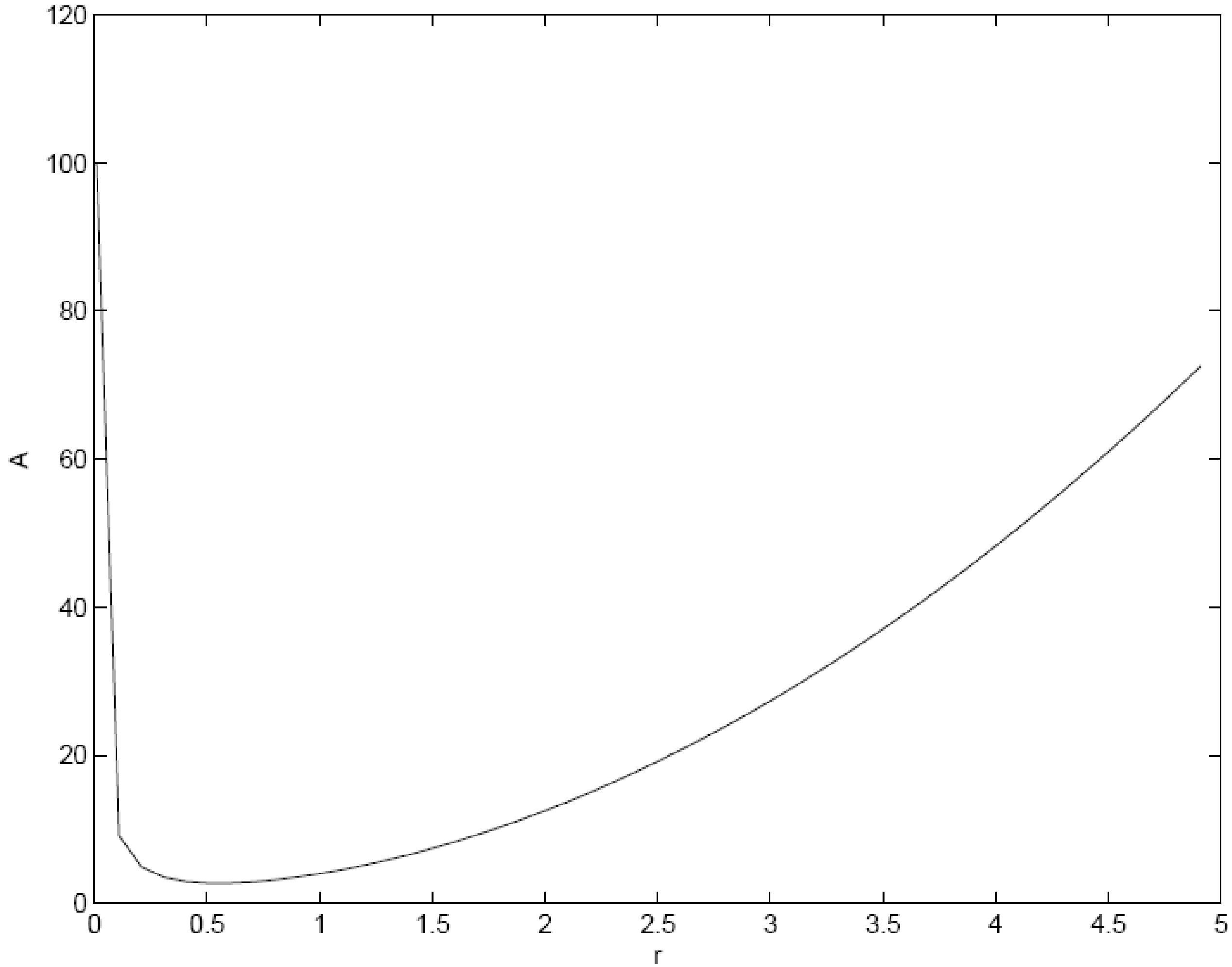
$$\frac{dA}{dr} = 0 \Rightarrow 4\pi r - \frac{2V}{r^2} = 0$$

$$\Rightarrow 4\pi r - \frac{2\pi r^2 h}{r^2} = 0$$

$$\Rightarrow \underline{\underline{h = 2r}}$$

We see that, when we impose the condition that the volume should be constant, the area becomes a function of r, as shown in the graph.

In the graph, we chose $h = 1$, and you can see that the minimum is indeed, as calculus shows, at $r = 1/2$: the radius should be half the height,



that is, the diameter should EQUAL the height.

SO CANS SHOULD EITHER NOT BE MADE **OR** THEY SHOULD ALWAYS BE EXACTLY AS HIGH AS THEY ARE WIDE

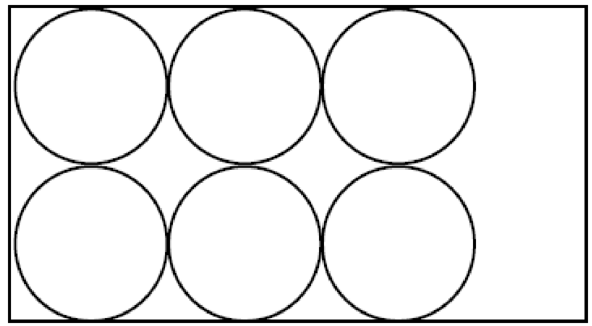
But can-manufacturers don't usually do this, except for LARGE cans, like cans of paint! So our model is predicting something wrong →


NIPPON
PAINT


COCA
COLA

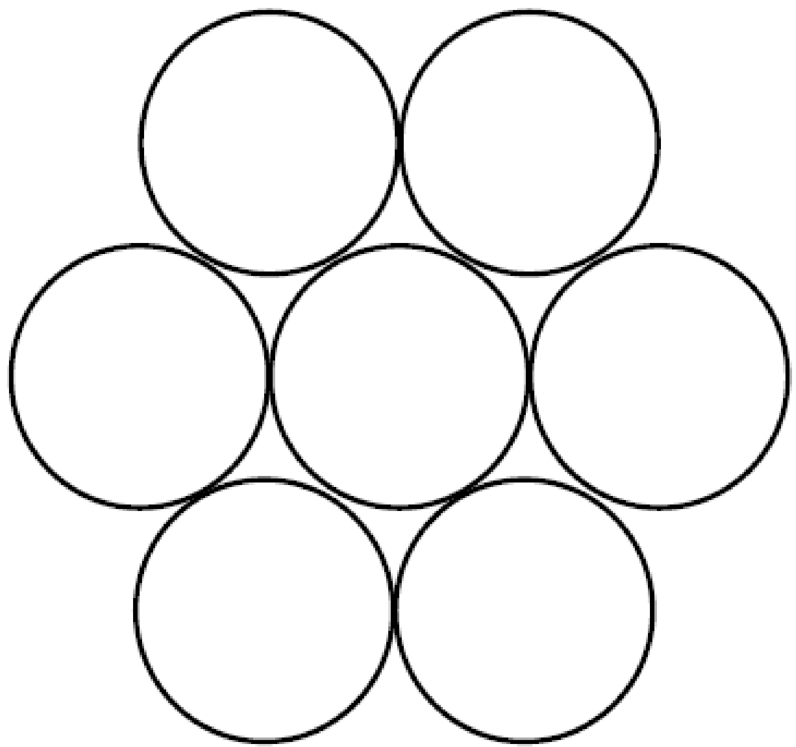
WE NEED A MORE COMPLEX MODEL

Model 2 As with model 1, BUT also we care



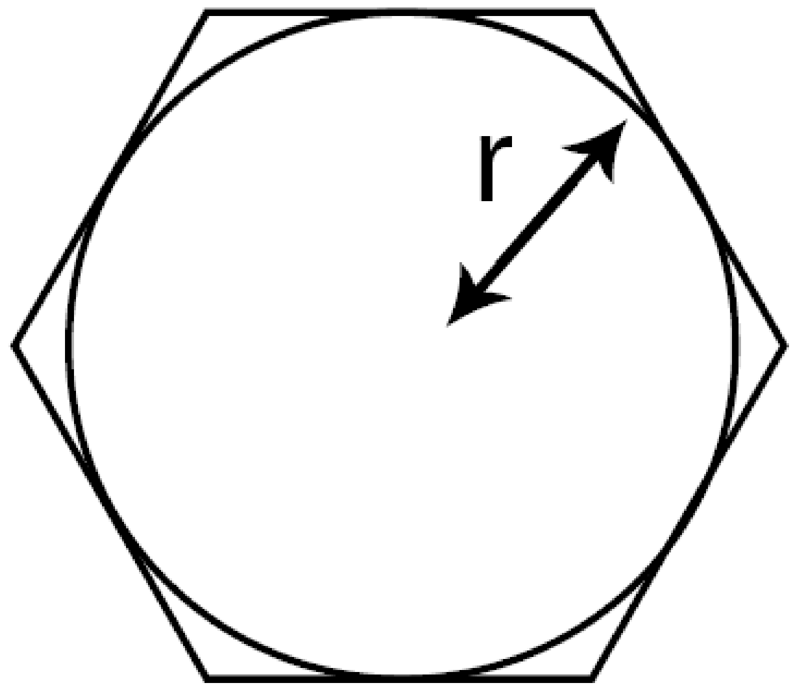
about WASTAGE. The top and bottom of the can are punched out of flat metal, perhaps in the way shown. YOU HAVE TO PAY for the whole sheet!

Well actually you should not punch the holes in this way, but rather in this way instead:

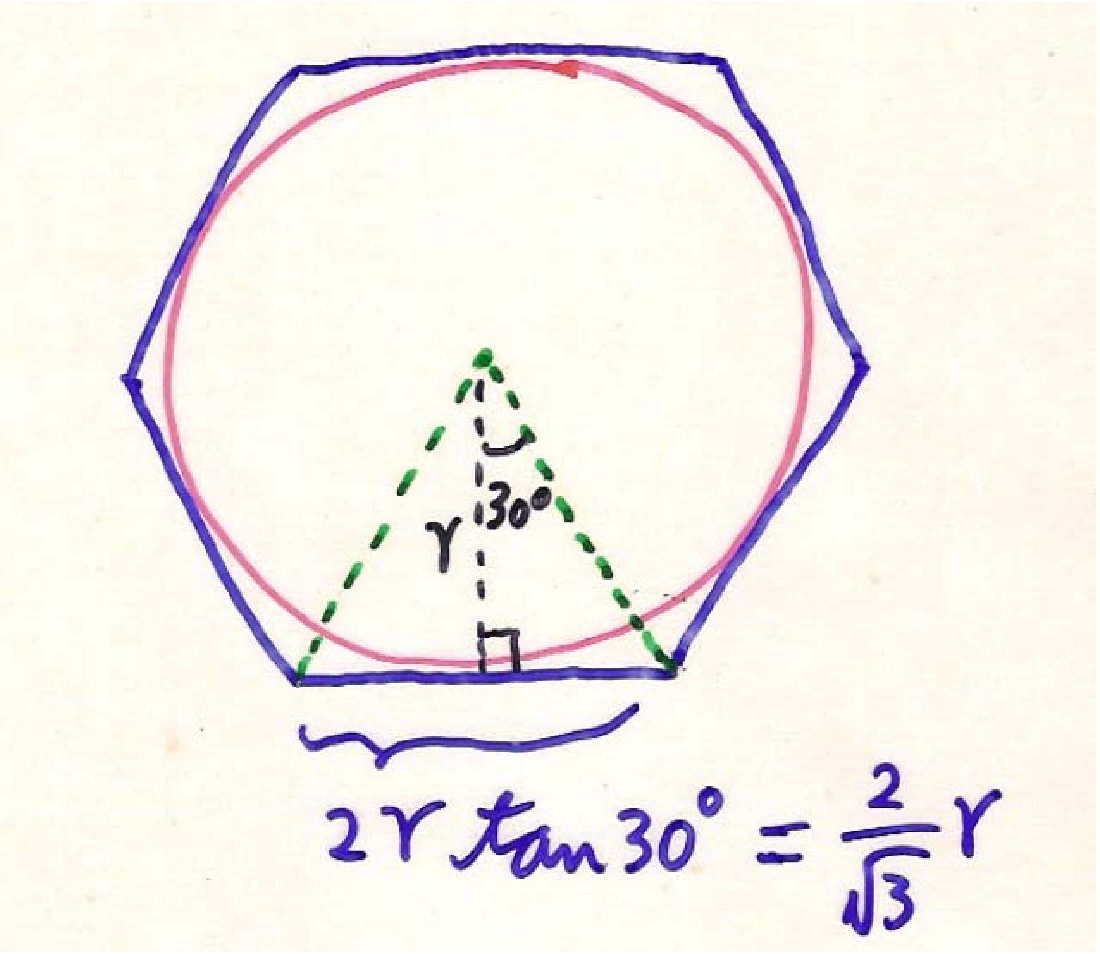


But still you have to pay for a whole HEXAGON,

as shown:



An exercise in trigonometry



Area of hexagon $= 6 \times \frac{2}{\sqrt{3}} r \times \frac{1}{2} r$

$= 4\sqrt{3}\, r \times \frac{1}{2} r$

$= 2\sqrt{3}\, r^2$

$V = \pi r^2 h \Rightarrow h = \frac{V}{\pi r^2}$

$$A = 2 \times 2\sqrt{3}\, r^2 + 2\pi r h$$

$$= 4\sqrt{3}\, r^2 + \frac{2V}{r}$$

$$\frac{dA}{dr} = 8\sqrt{3}\, r - \frac{2V}{r^2} = \frac{2}{r^2}\left(4\sqrt{3}\, r^3 - V\right)$$

$$\frac{dA}{dr} = 0 \Rightarrow 4\sqrt{3}\, r^3 = V = \pi r^2 h$$

$$\Rightarrow \underline{\underline{h = 4\sqrt{3}\, r / \pi}}$$

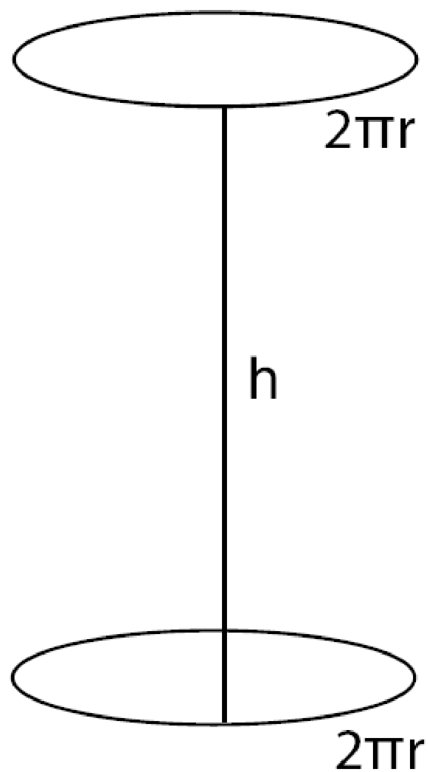
$$h = \frac{4\sqrt{3}}{\pi} r \text{ instead of } 2r$$

BUT $\frac{4\sqrt{3}}{\pi} \approx 2.21 > 2$. So our NEW MODEL SAYS THAT CANS SHOULD BE ABOUT 10 % HIGHER THAN WIDE... BETTER!

Well this can't be the whole story, since it does not explain the difference of shapes of LARGE cans and SMALL ones! We need a STILL MORE COMPLEX MODEL:

Model 3

As in model 2, but now we care about the PROCESS OF MANUFACTURE, *ie* the cost of actually sticking the can together! The top and bottom have to be welded onto the wall, which itself has a seam. Let's **ASSUME** that the cost of this welding is proportional to its length with constant K (units: \$ / cm)



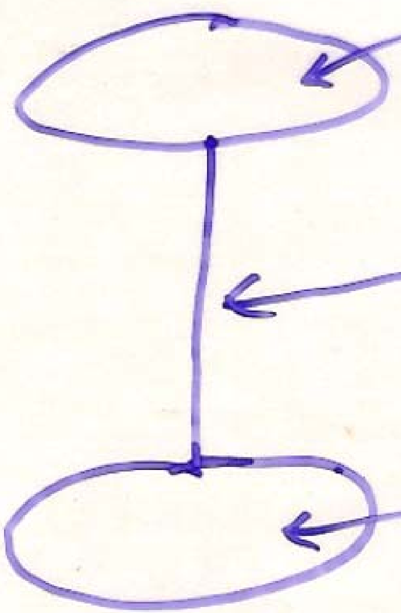
Model 3 calculations

From Model 2:

$$\text{cost of material} = \left(4\sqrt{3}r^2 + \frac{2V}{r}\right)\underset{\uparrow}{J} \quad \$/\text{cm}^2$$

where J = cost of "tin"/cm^2.

Labour cost of welding : $K \leftarrow \$/\text{cm}$



for top : $2\pi r K$

for the seam : hK

for bottom : $2\pi r K$

$\because$ vol $= V = \pi r^2 h$

$$\therefore h = \frac{V}{\pi r^2}$$

$\therefore$ total labour cost $= 2\pi r K + hK + 2\pi r K$

$$= 4\pi r K + \frac{V}{\pi r^2} K$$

$\therefore$ Total cost:

$$C = J\left(4\sqrt{3}\,r^2 + \frac{2V}{r}\right) + K\left(4\pi r + \frac{V}{\pi r^2}\right)$$

$$\frac{dC}{dr} = J\left(8\sqrt{3}\,r - \frac{2V}{r^2}\right) + K\left(4\pi - \frac{2V}{\pi r^3}\right)$$

$$= J\left(8\sqrt{3}\,r - 2\pi h\right) + K\left(4\pi - \frac{2h}{r}\right)$$

$$= Jr\left(8\sqrt{3} - 2\pi\frac{h}{r}\right) + K\left(4\pi - \frac{2h}{r}\right)$$

$$\therefore \frac{dC}{dr} = 0 \Rightarrow \left(8\sqrt{3}\,Jr + 4\pi K\right) - \frac{h}{r}\left(2\pi r J + 2K\right) = 0$$

$$\Rightarrow \frac{h}{r} = \frac{8\sqrt{3}\,Jr + 4\pi K}{2\pi r J + 2K}$$

$$\Rightarrow \frac{h}{r} = \frac{4\sqrt{3}\,J + 2\pi \frac{K}{r}}{\pi J + \frac{K}{r}}$$

$$\Rightarrow \frac{h}{r} = \frac{4\sqrt{3} + 2\pi \frac{K/J}{r}}{\pi + \frac{K/J}{r}}$$

[Notice by the way that the units of K/J are centimetres:

$$\frac{K}{J} = \frac{\$/cm}{\$/cm^2} = cm$$

.

We say that K/J SETS THE SCALE of this problem: when we say that a can is "large", we mean that its diameter or height is large COM-

PARED TO K/J. In engineering problems, one of the most important things to do is to IDENTIFY THE SCALES of the problem, so you know what the words “large” and “small” actually MEAN!]

Case 1: r "large"

$$\frac{h}{r} = \frac{4\sqrt{3} + 2\pi \frac{K/J}{r}}{\pi + \frac{K/J}{r}}$$

$$r \to \infty \Rightarrow \frac{h}{r} \longrightarrow \frac{4\sqrt{3}}{\pi}$$

i.e. r "large" $\Rightarrow h \simeq \frac{4\sqrt{3}}{\pi} r$

$$\Rightarrow \frac{h}{2r} \simeq \frac{2\sqrt{3}}{\pi} \simeq 1.1$$

So for "large" r, the height h

is approximately the same

as the width $2r$.

Note: Here "large" r means that

r is large compare to K/J.

Case 2: r "small"

We can also write

$$\frac{h}{r} = \frac{4\sqrt{3}\,r + 2\pi K/J}{\pi r + K/J}$$

$$\therefore\ r \longrightarrow 0 \implies \frac{h}{r} \longrightarrow 2\pi \approx 6.28$$

$$\implies \frac{h}{2r} \longrightarrow \pi \approx 3.14$$

$\therefore$ r "small" $\Longrightarrow \frac{h}{2r} \approx 3.14$

So for "small" r, the height is approximately 3 times larger than the width.

Here "small" r means that r is small compare to K/J.

So LARGE CANS SHOULD BE ALMOST "SQUARE", $h/2r \approx \frac{2\sqrt{3}}{\pi} \approx 1.1$. But SMALL CANS SHOULD BE MADE ABOUT π TIMES AS HIGH AS WIDE, ie they should be tall and thin!

Still not satisfied?

Model 4

And so on...

SUMMARY:

We have been constructing MODELS, that is, very simple versions of a real problem. The real problem is very very complicated, the model is just an APPROXIMATION, but it is easier to understand. BASIC PRINCIPLE: BE-

GIN WITH SIMPLE MODELS, UNDERSTAND THEIR WEAKNESSES, and only then MAKE THEM MORE COMPLICATED!

3.2. MALTHUS MODEL OF POPULATION

The total population of a country is clearly a function of time. Given the population now, can we predict what it will be in the future?

Suppose that B is a function giving the PER CAPITA BIRTH-RATE in a given society, *ie* B is the number of babies born per second, divided by the total population of the country at that moment. Note that B could be small in a big country and large in a small country - it depends on whether there is a strong social pressure on people to get married and have kids. Now B could depend on time (people might gradually come to realise that large families are no fun, etc...) and it could depend on N

But SUPPOSE YOU DON'T BELIEVE THESE THINGS: suppose you think that people will always have as many kids as they can, no matter what. Then B is constant. Now just as

$$\textsc{Distance} = \textsc{Speed} \times \textsc{Time}$$

when SPEED IS CONSTANT, so also we have

$$\#\text{babies born in time } \delta t = BN\delta t$$

Similarly let D be the death rate per capita; again, it could be a function of t (better medicine, fewer smokers) or N (overcrowding leads to famine/disease) but if we assume that it is constant, then

$$\#\text{deaths in time } \delta t = DN\delta t$$

So the change in N, δN, during δt is

$$\delta N = \#birth - \#deaths$$

PROVIDED there is no emigration or immigration. Thus,

$$\delta N = (B - D)N\delta t$$

and so $\frac{\delta N}{\delta t} = (B - D)N$ or in the limit as $\delta t \to$

0,

$$\frac{dN}{dt} = (B - D)N = kN \tag{1}$$

if $k = B - D$.

This model of society was put forward by THOMAS MALTHUS in 1798. Clearly Malthus was assuming a socially STATIC society in which human reproductive behaviour never changes with time or overcrowding, poverty etc... What does Malthus' model predict? Suppose that the population NOW is $\hat{N}$, and let $t = 0$ NOW.

From $\frac{dN}{dt} = kN$ we have $\int \frac{dN}{N} = \int kdt = k \int dt = kt + c$

so $ln(N) = kt + c$ and thus $N(t) = Ae^{kt}$.

Since $\hat{N} = N(0) = A$, we get:

$$N(t) = \hat{N}e^{kt} \tag{2}$$

with graphs as shown on figure 1.

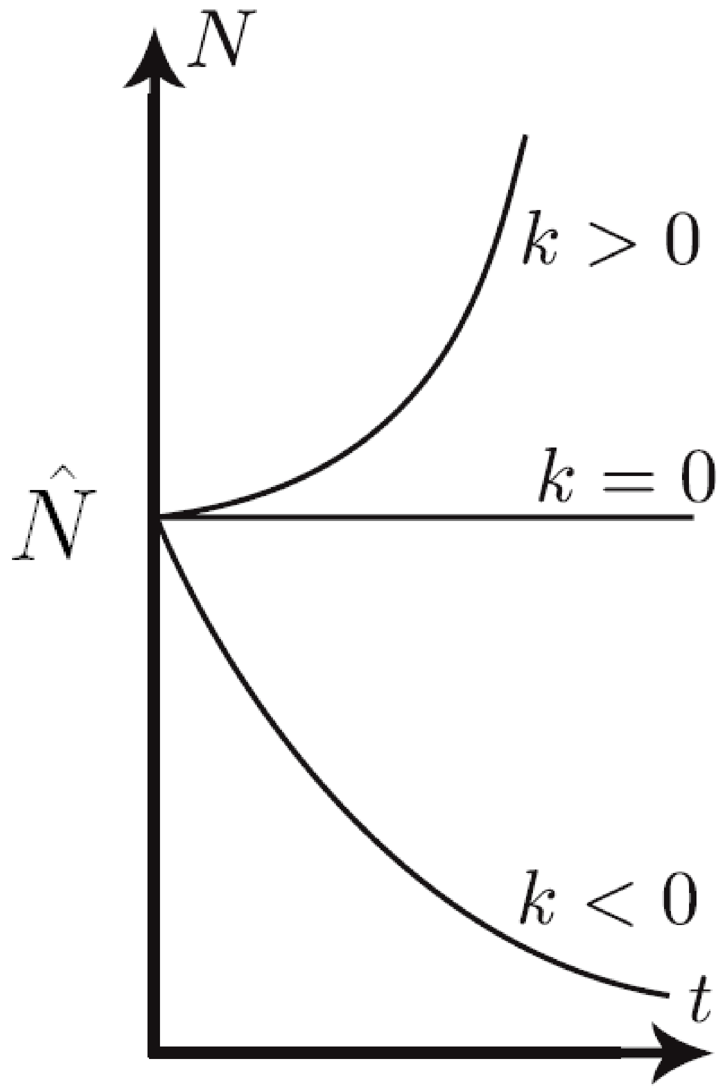


Figure 1: Graphs of $N(t)$, for different values of k

The population collapses if $k < 0$ (more deaths than births per capita), remains stable if (and only if) $k = 0$, and it EXPLODES if $k > 0$ (more births than deaths). Malthus observed that the population of Europe was increasing, so he predicted a catastrophic POPULATION EXPLOSION; since the food supply could not be expanded so fast, this would be disastrous.

In fact, this didn't happen (in Europe). So Malthus' model is wrong: many millions went to the US, many millions died in wars.

Second, the “static society” assumption has turned out to be wrong in many societies, with B and D both declining as time passed after WW2.

SUMMARY: The Malthus model of population is based on the idea that per capita birth and death rated are independent of time and N. It leads to EXPONENTIAL growth or decay of N.

3.3. IMPROVING ON MALTHUS

Malthus' model is interesting because it shows that static behaviour patterns can lead to disaster. But precisely because e^{kt} grows so quickly, Malthus' assumptions must eventually go wrong

- obviously there is a limit to the possible population. Eventually, if we don't control B, then D will have to increase. So we have to assume that D is a function of N.

Clearly, D must be an increasing function of N... but WHICH function? Well, surely the SIMPLEST POSSIBLE CHOICE (Remember: always go for the SIMPLE model before trying a complicated one!) is

$$\boxed{D = sN, \quad \begin{array}{c} \text{(LOGISTIC)} \\ \text{ASSUMPTION} \\ s = \text{constant} \end{array}} \tag{3}$$

This represents the idea that, in a world with FINITE RESOURCES, large N will eventually cause starvation and disease and so increase D.

Remark: In modelling, it is often useful to take note of $\boxed{\text{units}}$. Units of D are (#dead people) / second / (total # people) = $(\text{sec})^{-1}$.

Units of N are # (ie no units). So if $D = sN$, units of s must be $(\text{sec})^{-1}$.

As before, let $\hat{N}$ be the value of N at $t = 0$.

We have to solve

$$\frac{dN}{dt} = BN - DN = BN - sN^2$$

with the condition $N(0) = \hat{N}$

We can and will solve this, but let's try to GUESS what the solution will look like (a useful skill - in many other cases you won't be able to solve exactly!).

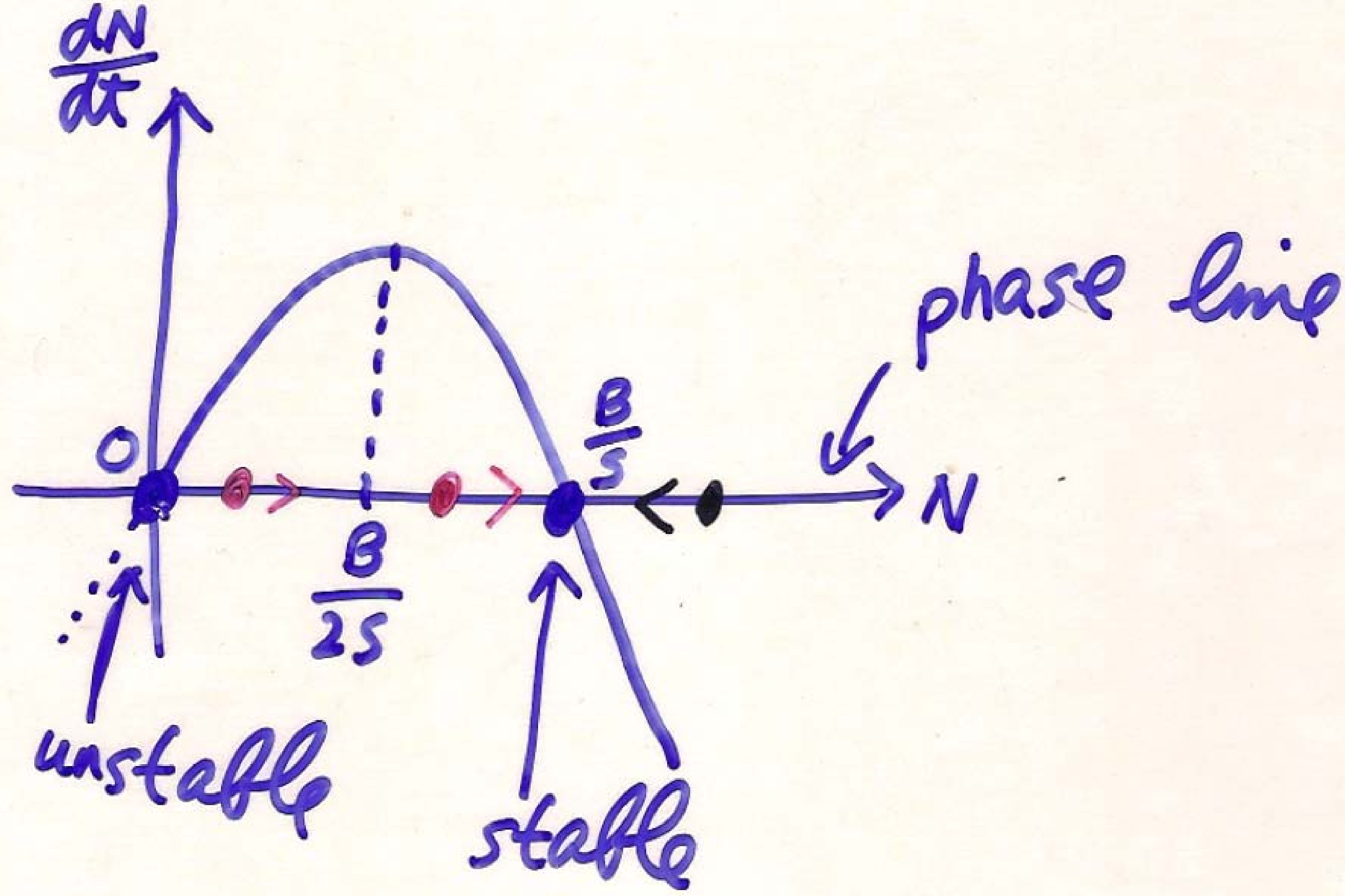
$$\frac{dN}{dt} = BN - SN^2$$ Logistic equation

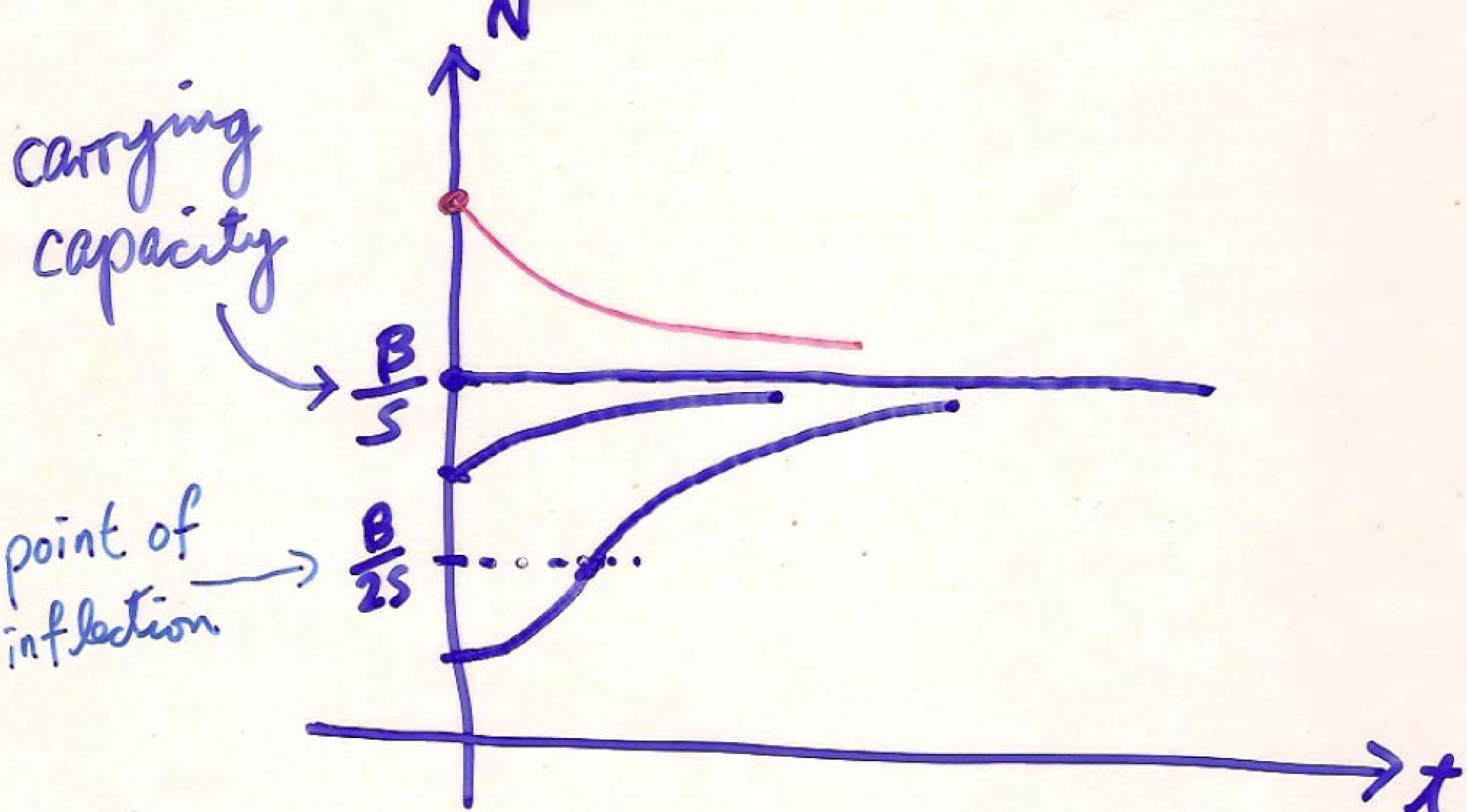
$$= N(B - SN)$$

$$= 0 \implies N = 0, \; N = \frac{B}{S}$$

equilibrium solutions

$$\frac{dN}{dt} = BN - SN^2 = N(B - SN)$$





see next page for concavity and inflection points

$$\frac{dN}{dt} = BN - SN^2$$

$$\frac{d^2N}{dt^2} = \left(\frac{d}{dN}\left(\frac{dN}{dt}\right)\right)\frac{dN}{dt}$$

$$= (B - 2SN)(BN - SN^2)$$

$$= (B - 2SN)\,N\,(B - SN)$$

	0		$\frac{B}{2S}$		$\frac{B}{S}$	
$\frac{d^2N}{dt^2}$		$+$		$-$		$+$
Concavity		concave up		concave down		concave up
			point of inflection			

Note: The two points 0 and $\frac{B}{S}$ are not considered to be points of inflection because any non-equilibrium solution curves cannot cross these two values by the "no crossing rule".

The NO CROSSING RULE

Consider the equation

$$\frac{dy}{dt} = f(y).$$

autonomous i.e. R.H.S. is independent of time t.

If $f'(y)$ is continuous, then the solution curves corresponding to different initial values do not cross each other.

Now we want to solve

$$\frac{dN}{dt} = BN - SN^2, \quad N(0) = \hat{N}.$$

Rewrite the equation as

$$\frac{dN}{dt} - BN = -SN^2$$

We can think of it as a Bernoulli Equation.

Let $z = N^{1-2} = \frac{1}{N}$

$\therefore \; dz = -\frac{1}{N^2} dN$

$\therefore \; \frac{-N^2 dz}{dt} - BN = -SN^2$

$$\frac{dz}{dt} + \beta\frac{1}{N} = S$$

$$\frac{dz}{dt} + \beta z = S$$

A linear equation in z.

Integrating factor

$$r = e^{\int B\,dt} = e^{Bt}$$

$$\therefore \; z = e^{-Bt} \int s e^{Bt}\,dt$$

$$= e^{-Bt} \left\{ \frac{s}{B} e^{Bt} + c \right\}$$

$$\therefore \; \frac{1}{N} = \frac{s}{B} + c e^{-Bt}$$

Let $N_\infty = \frac{B}{S}$ = carrying capacity

$$\therefore \frac{1}{N} = \frac{1}{N_\infty} + Ce^{-Bt}$$

$$N(0) = \hat{N} \Rightarrow \frac{1}{\hat{N}} = \frac{1}{N_\infty} + C$$

$$\Rightarrow C = \frac{1}{\hat{N}} - \frac{1}{N_\infty}$$

$$\frac{1}{N} = \frac{1}{N_\infty} + \left(\frac{1}{\hat{N}} - \frac{1}{N_\infty}\right) e^{-Bt}$$

$$= \frac{1}{\hat{N} N_\infty} \left\{ \hat{N} + N_\infty e^{-Bt} - \hat{N} e^{-Bt} \right\}$$

$$\therefore \quad N = \frac{\hat{N} N_\infty}{\hat{N} + (N_\infty - \hat{N}) e^{-Bt}}$$

i.e. $$\boxed{N = \frac{N_\infty}{1 + \left(\frac{N_\infty}{\hat{N}} - 1\right) e^{-Bt}}}$$

Observe: $\lim_{t \to \infty} N = N_\infty$ $\quad (\because B > 0)$

This shows that the asymptotic behaviour of N as shown by the graphs we had before by using the phase line is correct.

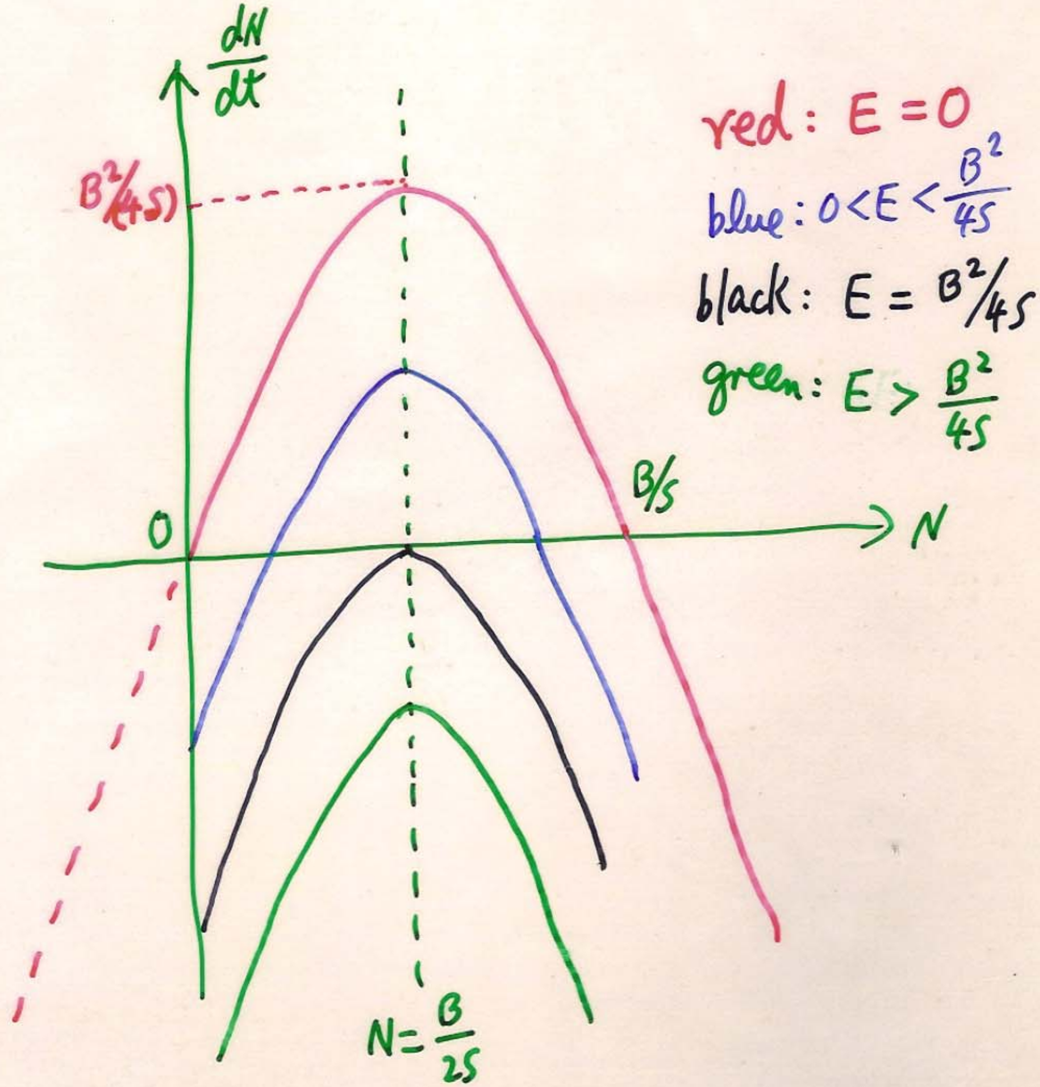
3.5. HARVESTING

A major application of modelling is in dealing with populations of animals e.g. fish. We want to know how many we can eat without wiping them out. Let's build on our logistic model, *ie* $\boxed{\text{assume}}$ that the fish population WOULD follow that model if we didn't catch any. Next, $\boxed{\text{assume}}$ that we catch E (constant) fish per year. Then we have:

$$\frac{dN}{dt} = (B - sN)N - E \quad \boxed{\begin{array}{c}\text{Basic}\\ \text{Harvesting}\\ \text{Model}\end{array}}$$

We'll now try to guess what the solutions should look like. We are particularly interested in the long term - will the harvesting eventually exterminate the fish? Consider the function:

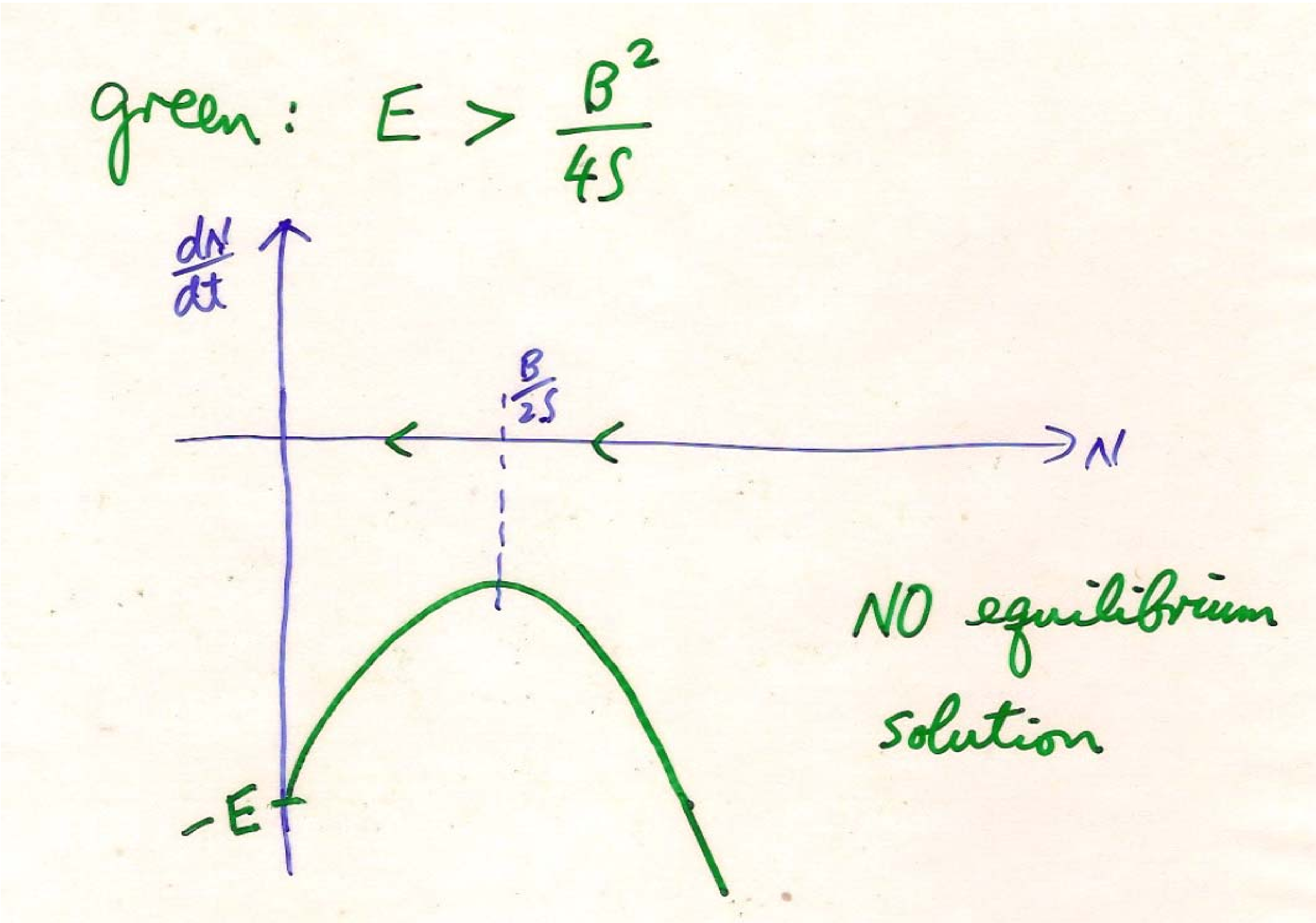
$$\frac{dN}{dt} = BN - SN^2 - E$$

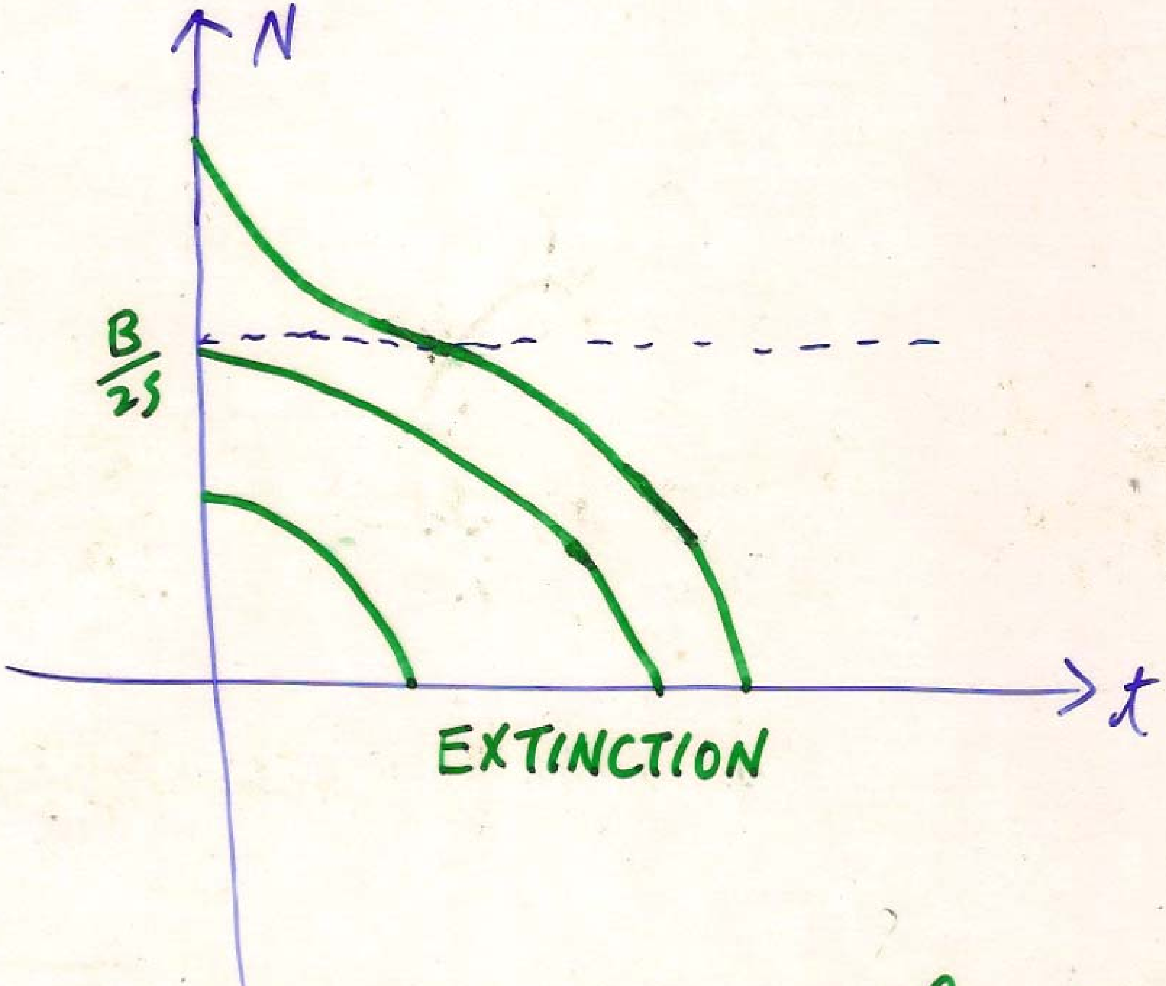


- The E=0 case is just the logistic case and we have already studied that.

- In the following we shall consider the remaining three cases.

Case 1:


green: $E > \frac{B^2}{4S}$
$\frac{dN}{dt}$
$\frac{B}{2S}$
N
-E
NO equilibrium solution



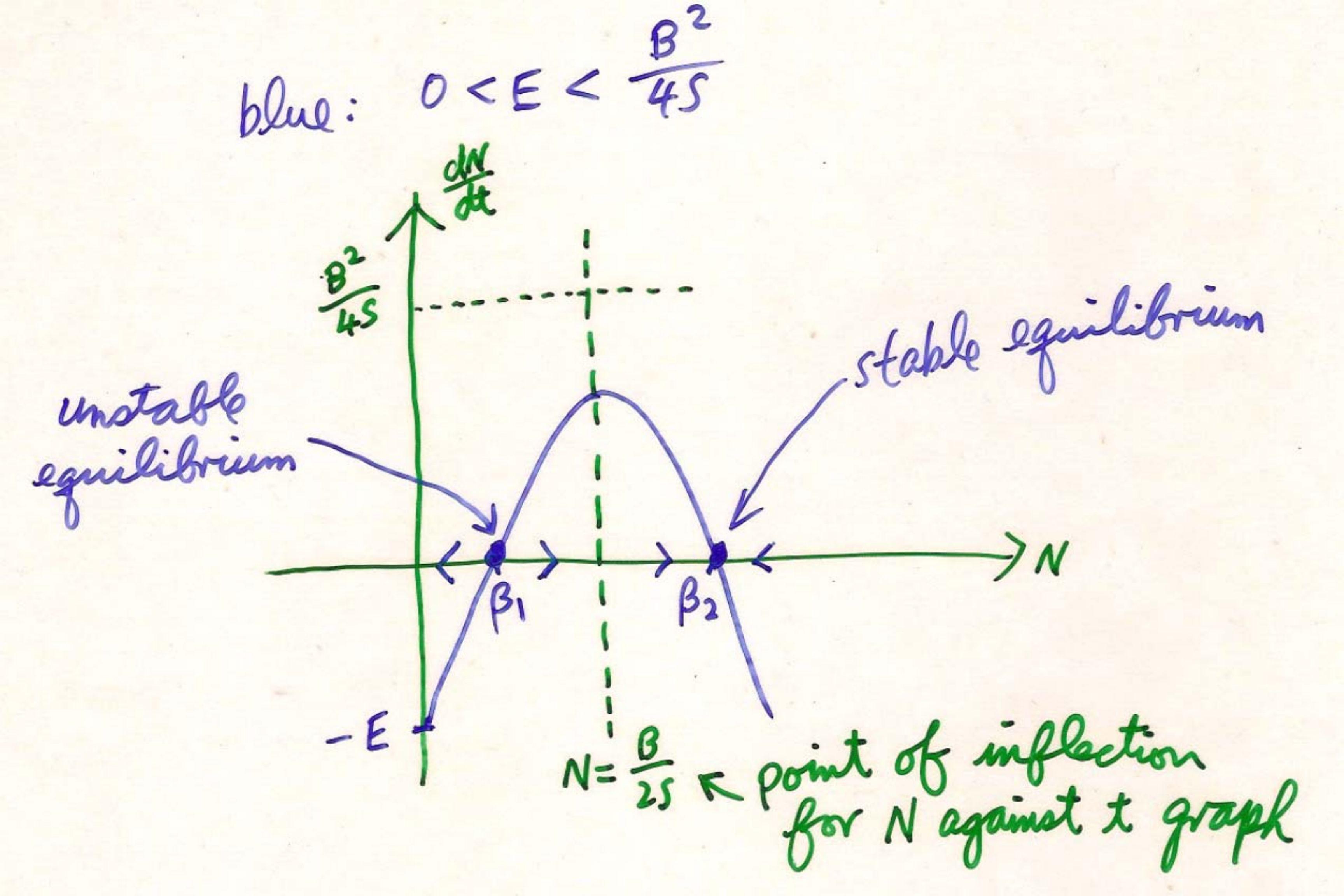
see next page for an explanation of concavity and inflection points.

$$\frac{d^2N}{dt^2} = (B - 2SN)(BN - SN^2 - E)$$

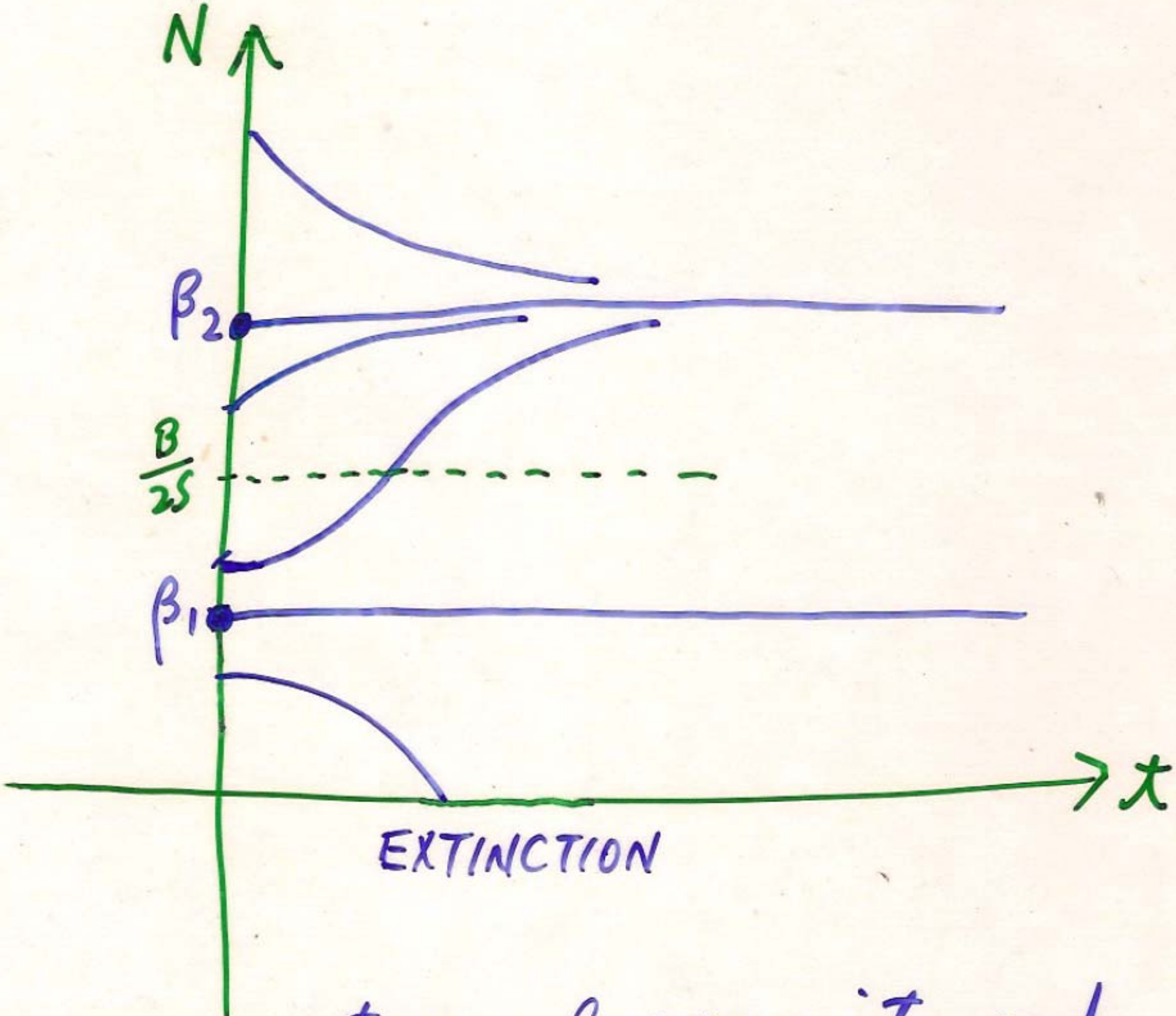
Note that $BN - SN^2 - E$ is always negative when $E > \frac{B^2}{4S}$ as the graph of $\frac{dN}{dt}$ against N is below the horizontal axis.

$\frac{d^2N}{dt^2}$	$-$		$+$
N against t graph	concave down	$\frac{B}{2S}$	concave up
		point of inflection	

Case 2:



blue: $0 < E < \frac{B^2}{4S}$
$\frac{dN}{dt}$
$\frac{B^2}{4S}$
stable equilibrium
unstable equilibrium
N
β_1
β_2
$-E$
$N = \frac{B}{2S}$
point of inflection for N against t graph



see next page for concavity and inflection points.

$$\frac{dN}{dt} = BN - SN^2 - E$$

$$\frac{d^2N}{dt^2} = \left[\frac{d}{dN}\left(\frac{dN}{dt}\right)\right]\frac{dN}{dt}$$

$$= (B - 2SN)(BN - SN^2 - E)$$

$$= -S(B - 2SN)(N - \beta_1)(N - \beta_2)$$

		β_1		$\frac{B}{2S}$		β_2	
$\frac{d^2N}{dt^2}$	$-$		$+$		$-$		$+$
N against t	concave down		concave up		concave down		concave up

point of inflection

NOT considered as points of inflection because any non-equilibrium solution curves cannot cross here

Suppose we start with $\hat{N} < \beta_1$

Then $N \to 0$ in finite time T.

We want to find T.

We use $$\frac{dN}{dt} = BN - SN^2 - E$$

$$\therefore \frac{dN}{BN - SN^2 - E} = dt$$

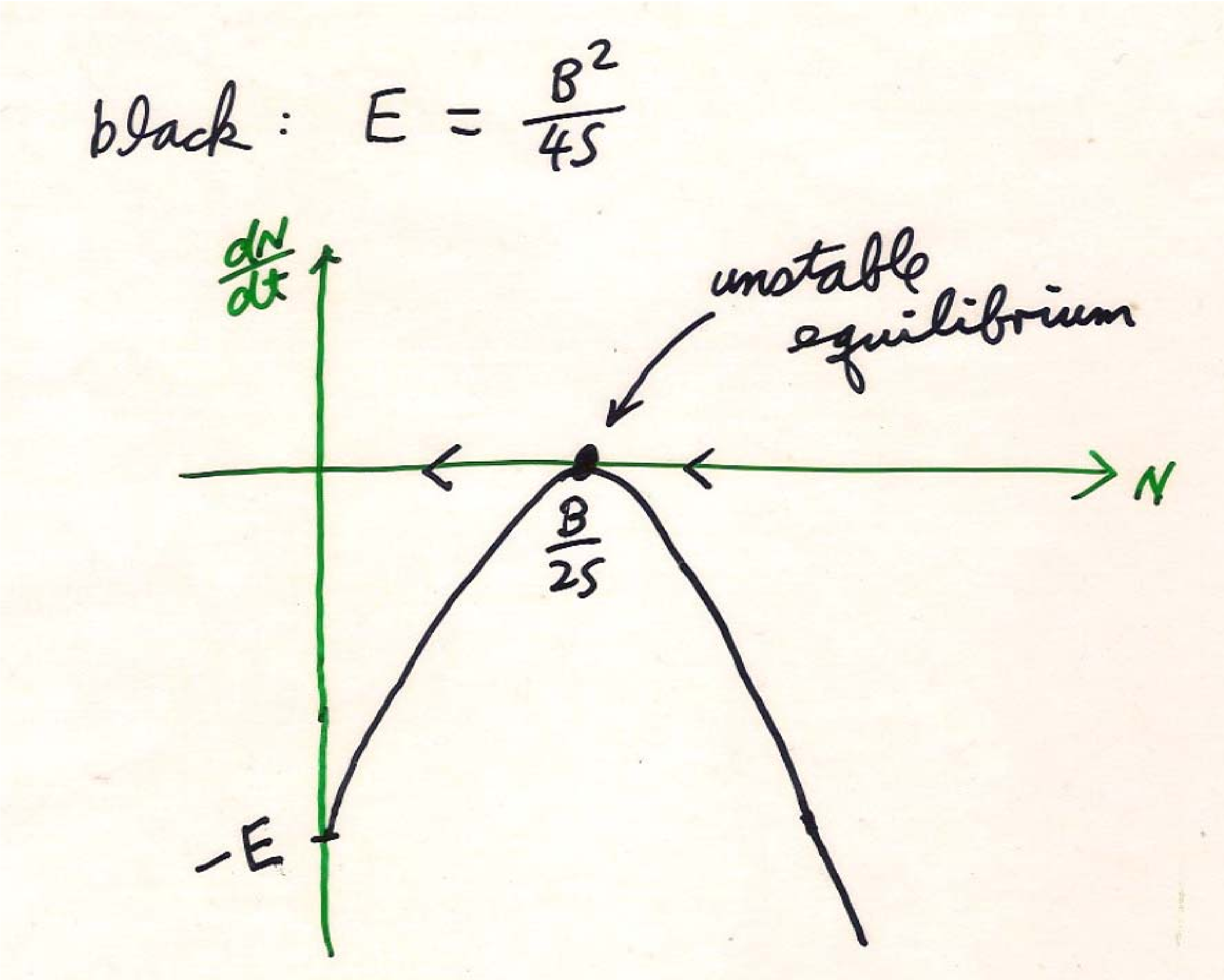
When $t = 0$, we have $N = \hat{N}$

and when $t = T$, we have $N = 0$

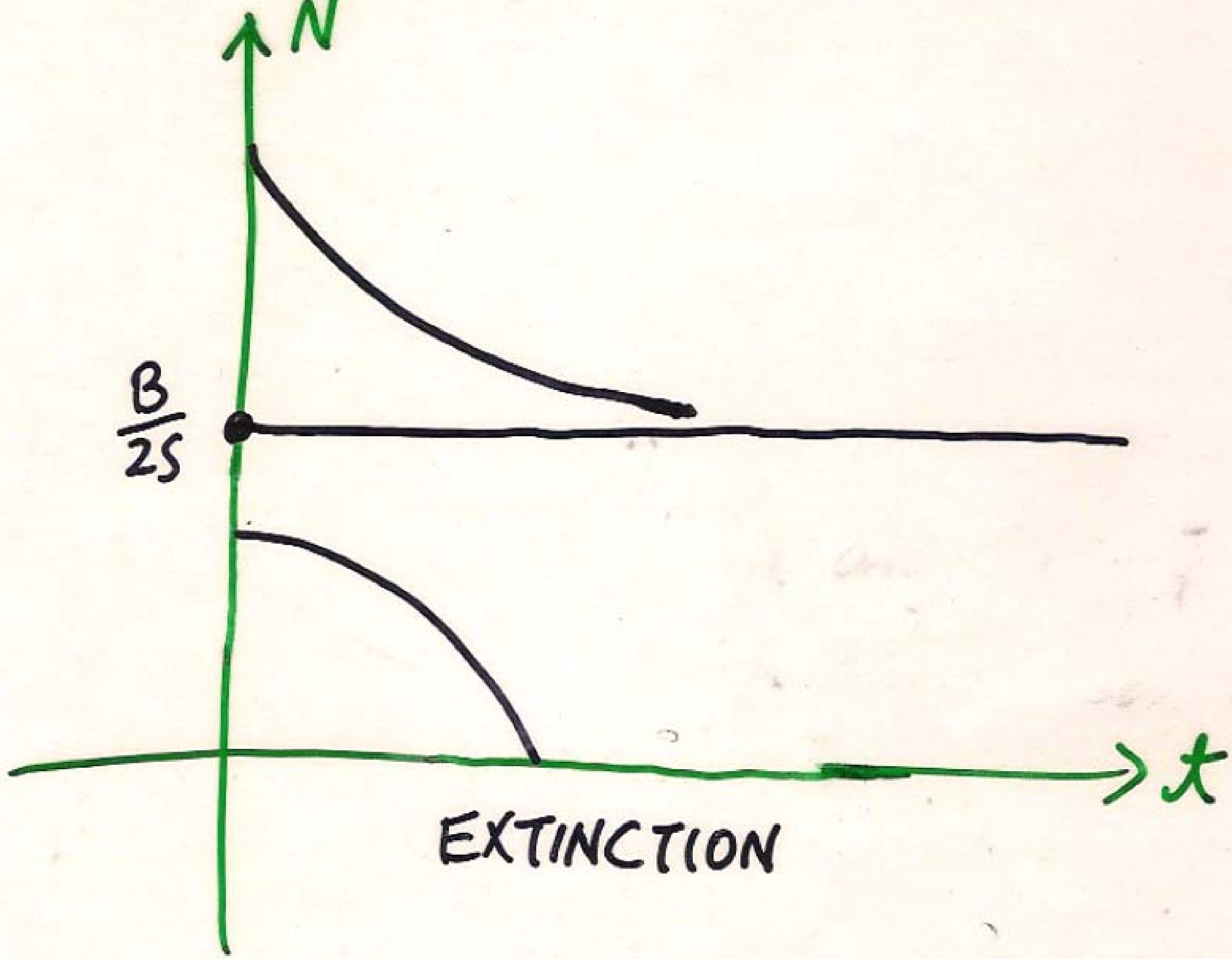
$$\therefore \int_{\hat{N}}^{0} \frac{dN}{BN - SN^2 - E} = \int_0^T dt = T$$

i.e. $$\boxed{T = \int_0^{\hat{N}} \frac{dN}{SN^2 - BN + E}}$$

Case 3:



black : $E = \frac{B^2}{4S}$
$\frac{dN}{dt}$
unstable equilibrium
N
$\frac{B}{2S}$
$-E$



see next page for concavity and inflection points.

as before,

$$\frac{d^2N}{dt^2} = (B - 2SN)(BN - SN^2 - E)$$

$$= -S(B - 2SN)\left(N - \frac{B}{2S}\right)^2$$

$$= 2S^2\left(N - \frac{B}{2S}\right)^3$$

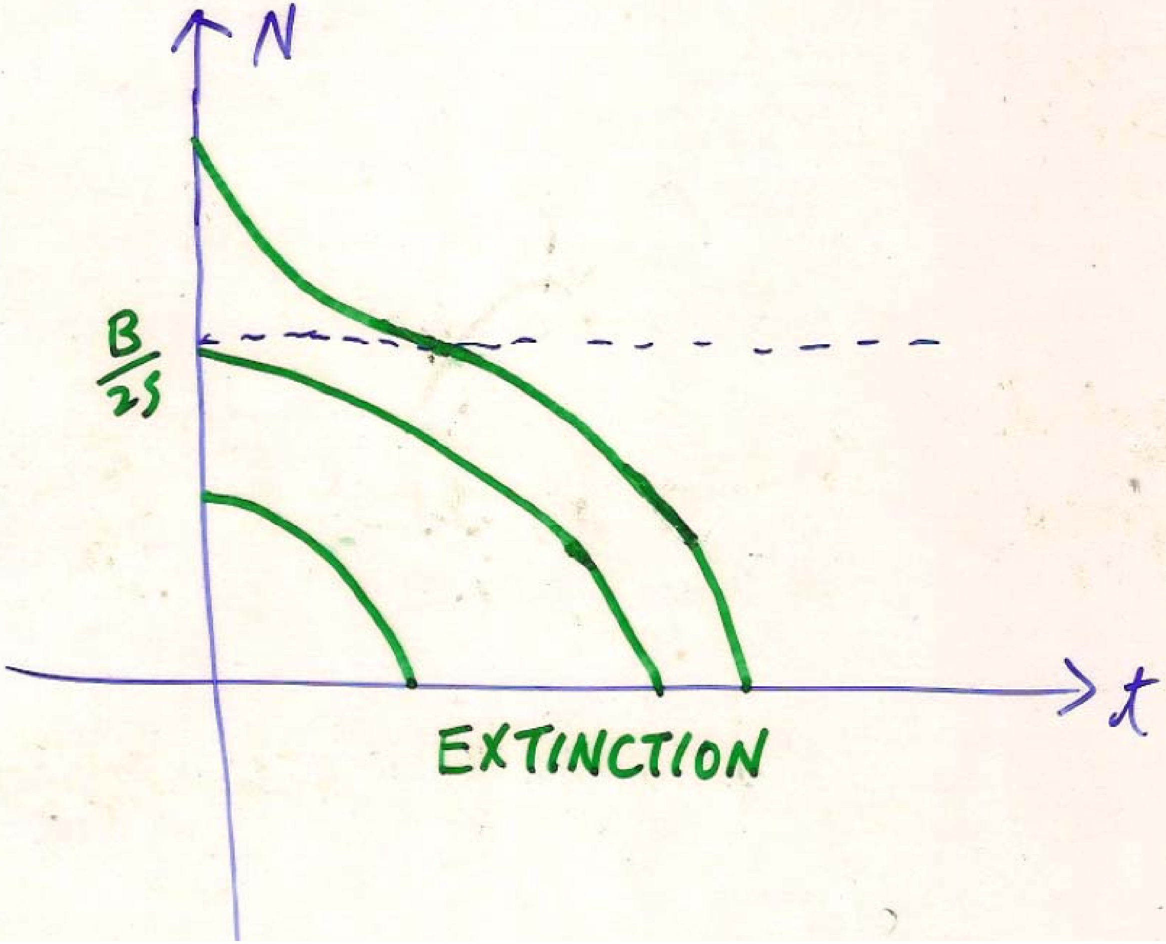
$\frac{d^2N}{dt^2}$	$-$		$+$
		$\frac{B}{2S}$	
N against t graph	concave down	$\uparrow$	concave up

NOT considered as a point of inflection because any non-equilibrium solution curves cannot cross here.

Clearly, the first and third cases are bad! The first case was $E > \frac{B^2}{4s}$. So we want the second case, with $E < \frac{B^2}{4s}$, and we want STABLE equilibrium, that is, a population which fluctuates around $\beta_2 = \frac{B+\sqrt{B^2-4Es}}{2s}$.

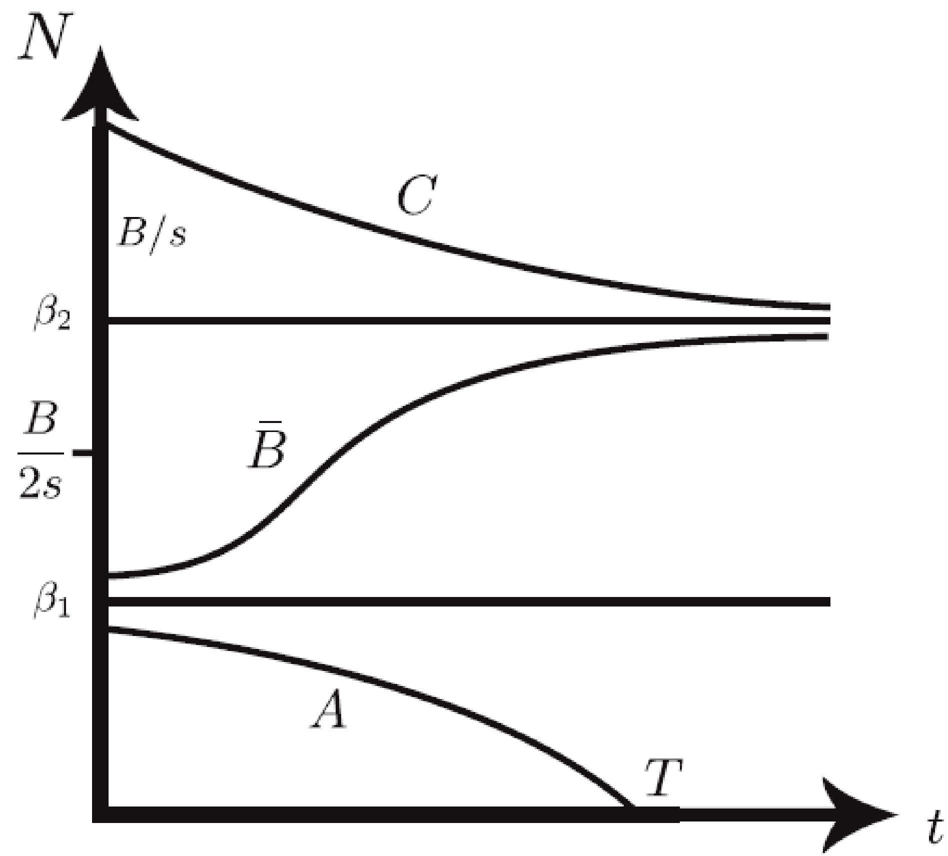
Let's imagine you are a modeller for the Peruvian State Fishing Regulatory Organisation. What do you predict?

Overfishing is bad! Pretty obvious! But what is NOT so obvious is the shape of the graph in the first case, $E > \frac{B^2}{4s}$. Note that it is downhill all the way, BUT at first the rate of decline is DECREASING, *ie* the graph is CONCAVE UP. (For the top curve in the next picture)


N
B
2S
t
EXTINCTION

Now it is not surprising that fish stocks decline when you start to harvest them - notice that, EVEN IN THE "GOOD" CASE the curve marked C is concave up and decreasing.

(See the next picture)



N
B/s
C
β_2
$\frac{B}{2s}$
$\bar{B}$
β_1
A
T
t

(Notice that $\beta_2 = \frac{B+\sqrt{B^2-4Es}}{2s} < \frac{B+\sqrt{B^2-0}}{2s} = \frac{B}{s}$ = carrying capacity in the absence of harvesting (recall $N_\infty = \frac{B}{s}$). So even the stable equilibrium population under harvesting is less than the carrying capacity!)

So the mere fact that the fish numbers are declining is not a danger signal in itself. In fact, UNTIL YOU GET TO THE POINT OF INFLECTION, the graph might fool you into thinking that the population will settle down eventually to some non-zero asymptotic value!

MORAL OF THE STORY: CONCAVE UP $\boxed{\text{NOW}}$ DOESN'T MEAN YOU NEED NOT PANIC! Any decline must be monitored carefully. The point is that since $D = sN$, a reduction in N drives the death rate DOWN, so paradoxically AT FIRST overfishing may SEEM to BENEFIT the fish!! But not for long!

3.6. MODEL OF A PLUG FLOW REACTOR

In chemical engineering, a PLUG FLOW REACTOR is like a long tube into which you push some mixture of chemicals which move through the tube while they react with each other. These devices can be very complicated objects, and we are not going to pretend to describe how they really work.

But we can set up a very simple MATHEMATICAL MODEL of such a gadget, with the understanding that a REALISTIC model would be very much more complicated!

For example, you push in hydrogen and oxygen at one end, and get water coming out the other end. Since Oxygen is cheap and Hydrogen is expensive, we assume that we pump in a lot of Oxygen compared to the Hydrogen, so there is plenty of Oxygen all the way along the PFR. The question we want to answer is: what happens to the concentration of

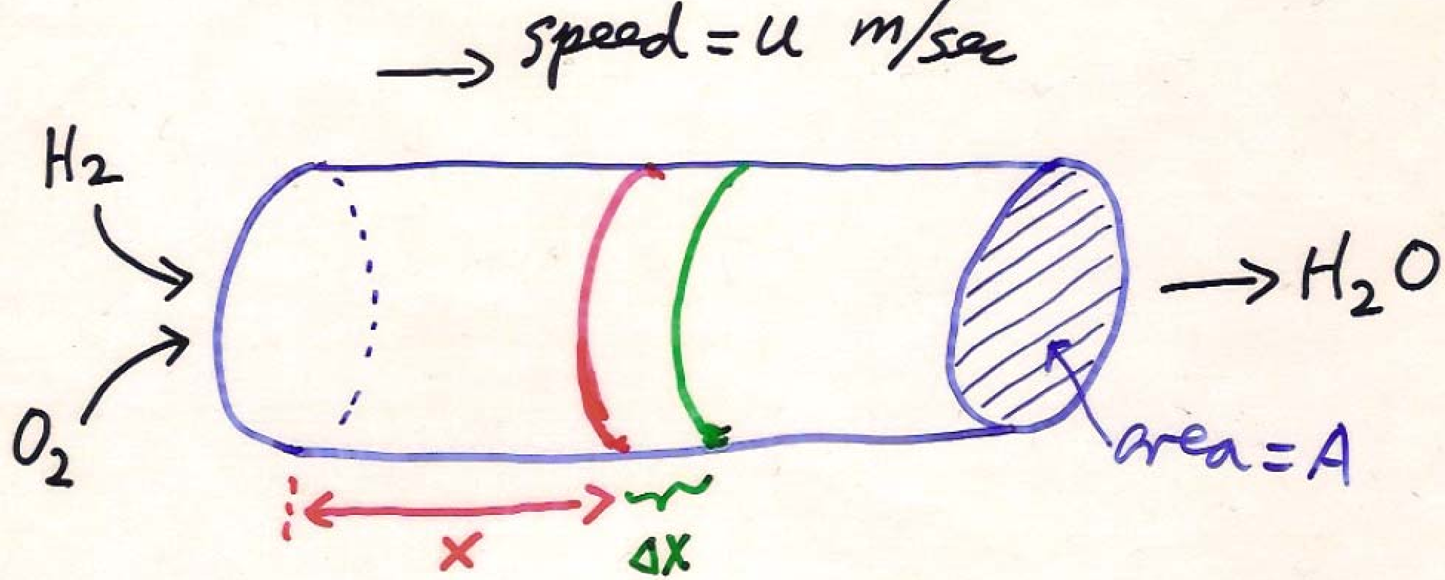
Hydrogen as a function of position in the PFR? Of course it will decrease, but how rapidly? Assume

[a] That everything flows through the PFR at constant speed u, and the cross-sectional area is A, a constant.

[b] That there is no mixing upstream or downstream $\rightarrow$ everything that happens in a small region of the PFR is controlled by chemical reactions IN that region and by flows in and out from the neighbouring regions.

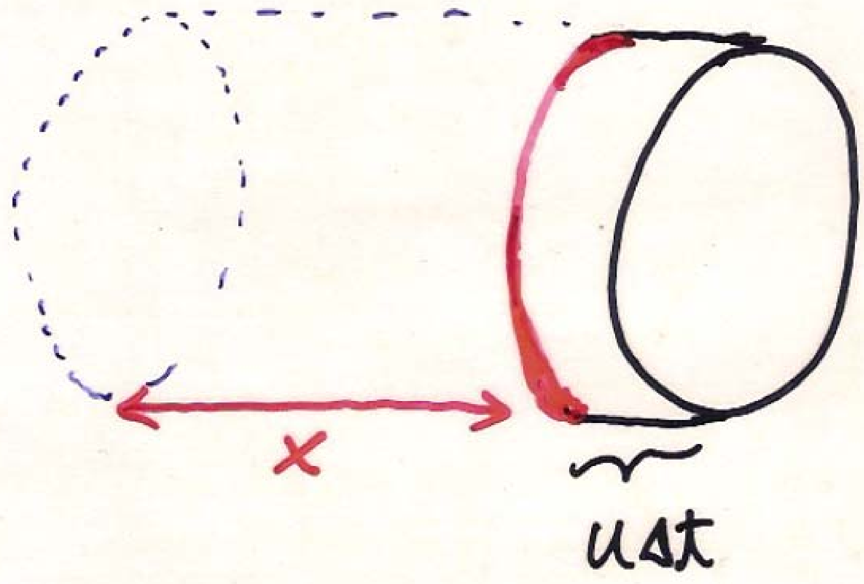
[c] All temperatures are constant in time.

Now at a point x along the PFR, how many molecules of H_2 are passing by per second? Let $C_{H_2}(x)$ be the CONCENTRATION of hydrogen (molecules per cubic metre) at x.



Let $C_{H_2}(x)$ = no. of molecules of H_2/m^3 at x.

Consider a small time increment Δt.



Let ΔN_{H_2} = no. of H_2 molecules inside the small cylinder shown above.

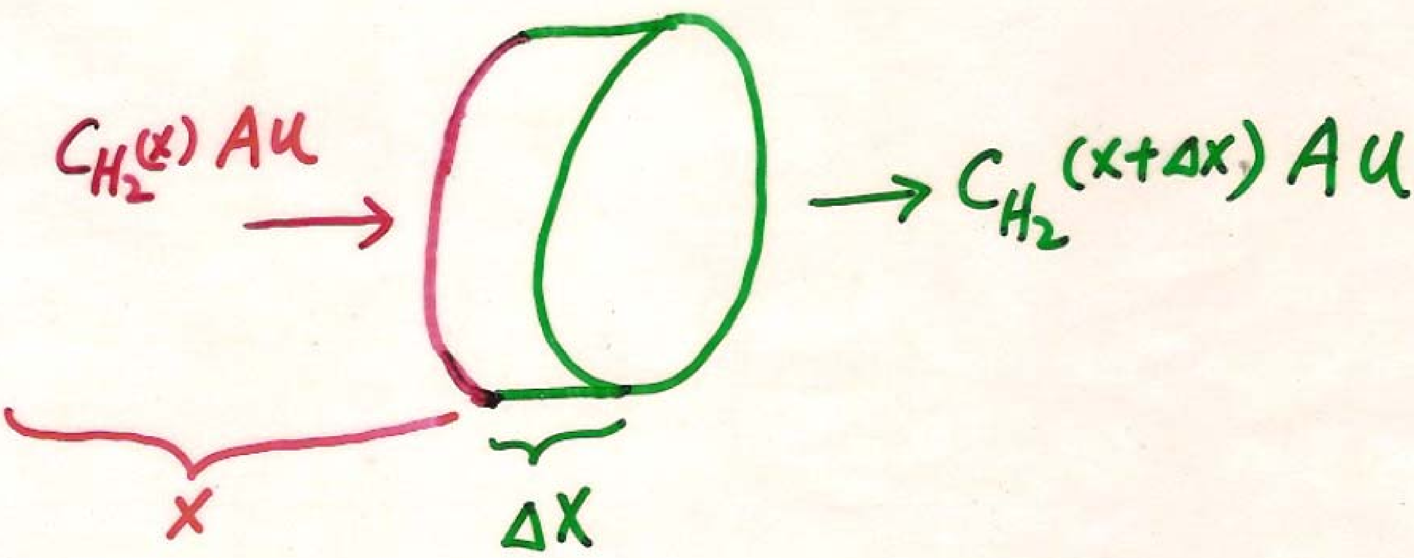
Vol. of small cylinder $= A \times u \Delta t$

$$\therefore \quad \Delta N_{H_2} = C_{H_2}(x) \{ A u \Delta t \}$$

$$\therefore \quad \frac{\Delta N_{H_2}}{\Delta t} = C_{H_2}(x) A u$$

$$\Delta t \to 0 \implies \frac{d N_{H_2}}{dt} = C_{H_2}(x) A u$$

Now we go back to the cross section of length Δx.



Let r = rate/m^3

= no. of reactions per second per m^3

of the chemical reaction

$$2H_2 + O_2 \longrightarrow 2H_2O$$

Observe that one reaction uses up

2 H_2 molecules.

$\therefore$ no. of molecules of H_2 used in the cross section of length Δx is

$$2 r A \Delta x \text{ per second}$$

$\because$ no. of H_2 molecules flow in rate

$$= C_{H_2}(x) A u \text{ per second}$$

and no. of H_2 molecules flow out rate

$$= C_{H_2}(x+\Delta x) A u \text{ per second}$$

$$\therefore C_{H_2}(x) A u - C_{H_2}(x+\Delta x) A u = 2 r A \Delta x$$

($\because$ flow in rate − flow out rate = used up rate)

Let $C_{H_2}(x+\Delta x) - C_{H_2}(x) = \Delta C_{H_2}$

$$\therefore -\Delta C_{H_2} A u = 2 r A \Delta x$$

$$\therefore \frac{\Delta C_{H_2}}{\Delta x} = -\frac{2r}{u}$$

$$\Delta x \to 0 \implies \frac{d C_{H_2}}{dx} = -\frac{2r}{u}$$

Now r depends on many things, for example the concentration of H_2, the temperature, etc etc etc. Let's construct a simple MODEL of this situation. It's pretty clear that the main thing that controls the rate of a reaction is the concentration, and it's also clear that the higher the concentration, the faster the reaction will go — so the rate should be an increasing function of the concentration, and of course it should be zero when the concentration is zero. So the SIMPLEST POSSIBLE model we can think of is given by the equation

$$r = kC_{H_2}(x),$$

where k [units 1/sec — check this!] is a positive constant [because we always assume here that the temperature is constant — in general k will depend on the temperature of course]. That is, we assume that the rate is [approximately!] proportional to the concentration. Then

$$\boxed{\frac{dC_{H_2}}{dx} = -\frac{2kC_{H_2}}{u}}$$

This is the differential equation of our model of the plug flow reactor.

$$\frac{dC_{H_2}}{C_{H_2}} = -\frac{2k}{u}\,dx$$

$$\Rightarrow \quad C_{H_2} = A e^{-\frac{2k}{u}x}$$

at $x=0$, $C_{H_2} = C_{H_2}(\text{entrance})$

$$\therefore \quad C_{H_2} = \left\{ C_{H_2}(\text{entrance}) \right\} e^{-\frac{2k}{u}x}$$

Let T = time taken for the chemicals to go through the reactor

L = length of reactor

Then at $x = L$, $C_{H_2} = C_{H_2}(\text{exit})$

and $L = uT$

$\therefore C_{H_2}(\text{exit}) = C_{H_2}(\text{entrance})\, e^{-2kT}$

What this relation is really telling us is that Plug Flow Reactors are a good idea, because they are very efficient. As you know, the exponential function decreases very rapidly, so the Hydrogen is being turned into water very efficiently — almost none of it is left by the time you come to the end of the PFR. Notice too that the important parameter here is the

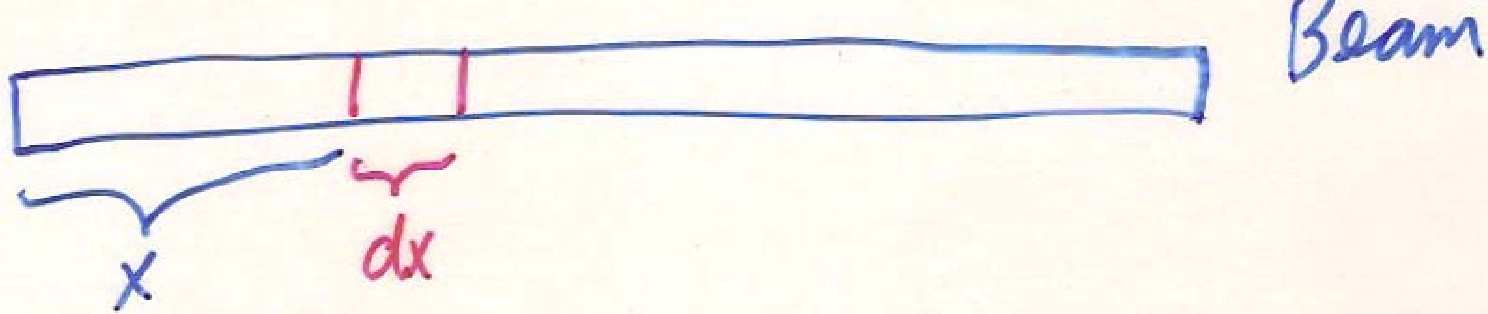
TIME the mixture spends inside the PFR. Finally, remember where that 2 came from — it came from the chemical formula for the reaction. So you have to know your Chemistry to use one of these things.

So PFRs are good, unless they blow up of course..... remember that we deliberately left out temperature.

3.7. CANTILEVERED BEAMS: A MODEL OF A BALCONY.

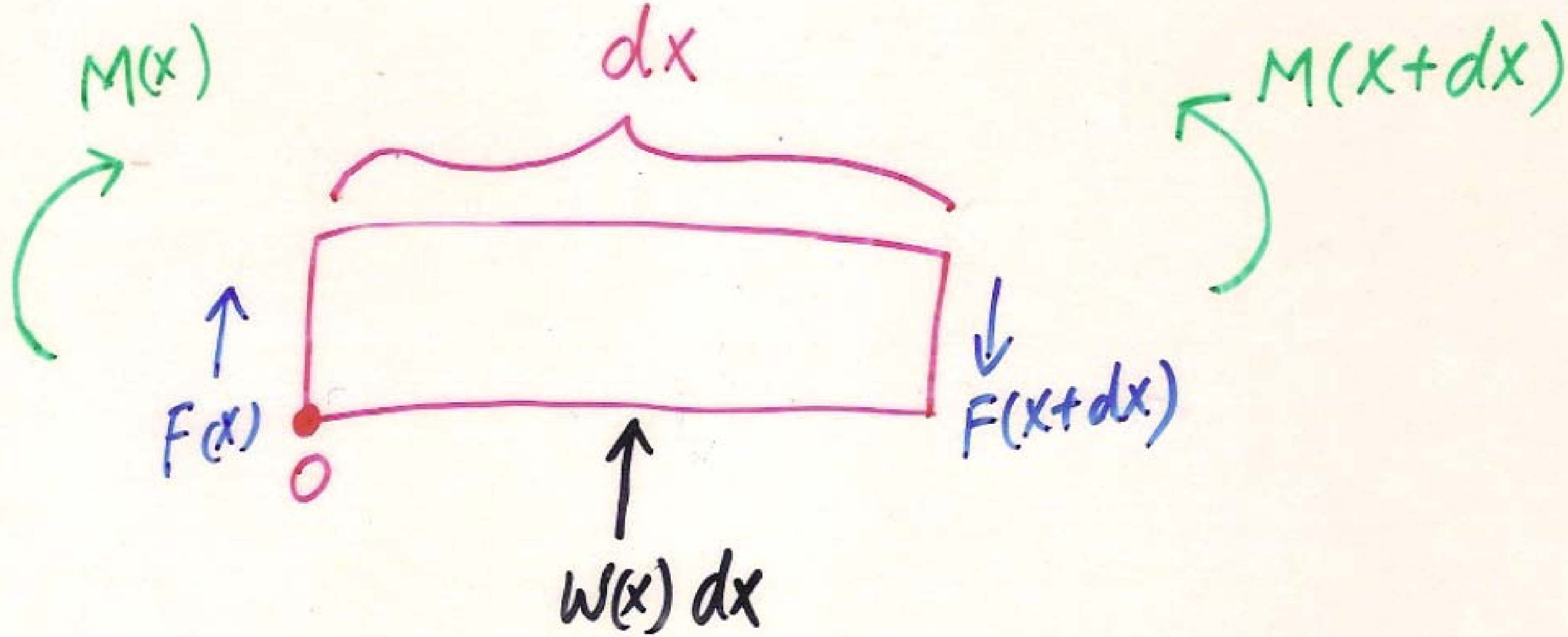
Let's build a simple mathematical MODEL of a balcony. Balconies are tricky to make: let's see why! A BEAM is a long, thin object used in buildings etc, which bends when subjected to loads.

Take a small element as shown.


Beam
x
dx

Then the element is subjected to both FORCES and TORQUES. All of these must balance out if you don't want the beam to move.

Both F, the SHEARING FORCE, and M, the TORQUE or BENDING MOMENT, are functions of x. We assume that there is a force, called the LOAD, acting on the beam. This load is also a function of x.



M(x)
dx
M(x+dx)
F(x)
0
F(x+dx)
W(x) dx

$F(x)$ = shearing force
$M(x)$ = torque

} internal to the beam

$w(x)$ = load (unit: force per unit length)

↑

external to the beam

Equating force

$$\Rightarrow F(x) + w(x)\,dx = F(x+dx)$$

$$\Rightarrow w(x)\,dx = F(x+dx) - F(x)$$

$$\simeq \frac{dF}{dx}\,dx$$

$$\Rightarrow \frac{dF}{dx} = w(x) \quad \text{------} \quad (1)$$

Equating moment at O

$$\Rightarrow \quad M(x) + F(x+dx)\,dx = M(x+dx) + w(x)\,dx\left(\tfrac{1}{2}dx\right)$$

$$\Rightarrow \quad M(x) + \left(F(x) + \frac{dF}{dx}dx\right)dx \simeq \left(M(x) + \frac{dM}{dx}dx\right) + \frac{1}{2}w(x)(dx)^2$$

$$\Rightarrow \quad F(x)\,dx \simeq \frac{dM}{dx}dx$$ ($\because (dx)^2$ is much smaller when dx is small)

$$\Rightarrow \quad \frac{dM}{dx} = F(x) \quad \text{------} \quad (2)$$

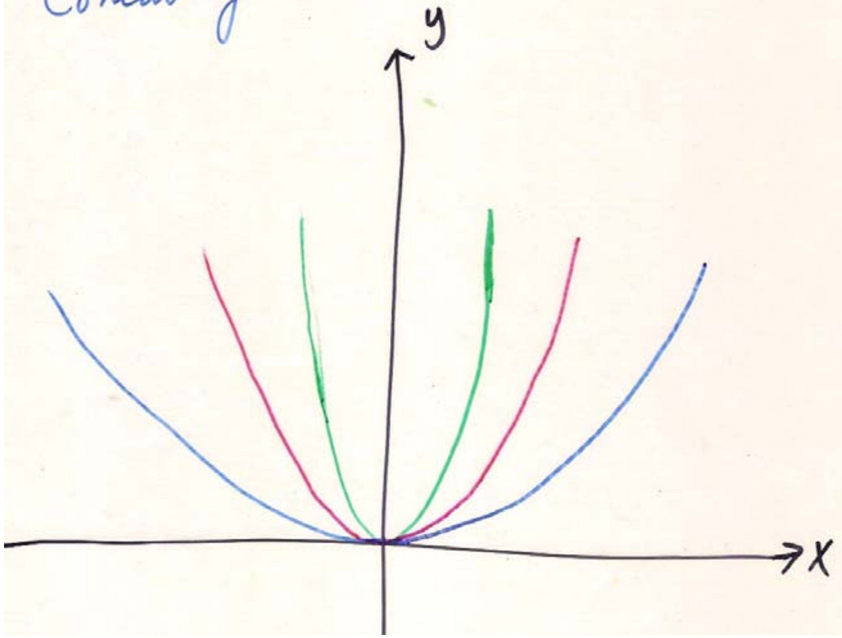
(2) $\Rightarrow \dfrac{d^2M}{dx^2} = \dfrac{dF}{dx}$

$= w(x)$ (by (1))

We obtain

$$\boxed{\frac{d^2M}{dx^2} = w(x)} \quad \text{-----} \quad (3)$$

Concavity



Green: $y = 10x^2 \Rightarrow \frac{d^2y}{dx^2} = 20$

Red: $y = x^2 \Rightarrow \frac{d^2y}{dx^2} = 2$

Blue: $y = \frac{1}{10}x^2 \Rightarrow \frac{d^2y}{dx^2} = \frac{1}{5} = 0.2$

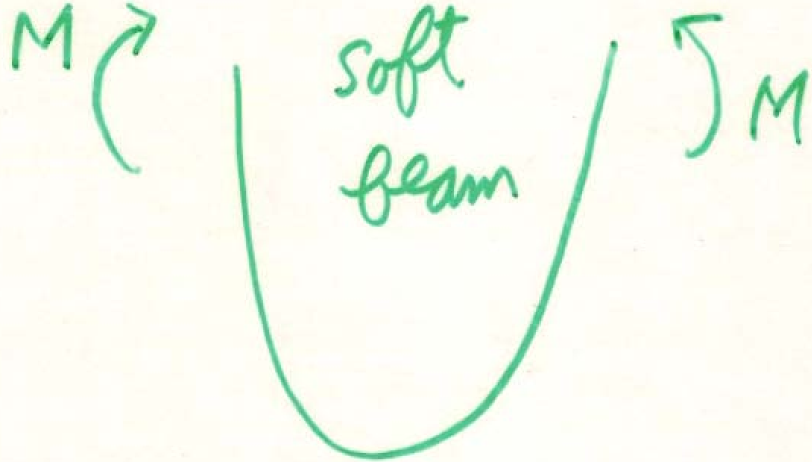
Observe: large $\frac{d^2y}{dx^2} \Rightarrow$ more bending of the curve.

stiff beam

small bending

$\Rightarrow$ small $\dfrac{d^2y}{dx^2}$

$\Rightarrow$ large $\dfrac{M}{d^2y/dx^2}$



large bending

$$\Rightarrow \text{large } \frac{d^2y}{dx^2}$$

$$\Rightarrow \text{small } \frac{M}{d^2y/dx^2}$$

The expression $\frac{M}{d^2y/dx^2}$ measures

the stiffness of a beam.

It is shown in physics that

the stiffness satisfies the equation

$$\frac{M}{d^2y/dx^2} = E\,I$$

Young's modulus

second moment of area of the beam

for a given beam, these are constants

$$\therefore \quad \frac{d^2y}{dx^2} = \frac{M}{EI} \quad \text{----} \; (4)$$

$$\therefore \frac{d^4y}{dx^4} = \frac{d^2}{dx^2}\left(\frac{d^2y}{dx^2}\right)$$

$$= \frac{d^2}{dx^2}\left(\frac{M}{EI}\right) \quad \text{(by 4)}$$

$$= \frac{1}{EI}\frac{d^2M}{dx^2}$$

$$= \frac{1}{EI} w(x)$$

$$\boxed{\frac{d^4y}{dx^4} = \frac{w(x)}{EI}} \quad \text{-----} \; 5$$

So the deflection of the beam is governed by the FOURTH-ORDER ODE

$$\boxed{\frac{d^4y}{dx^4} = \frac{w(x)}{EI}}$$

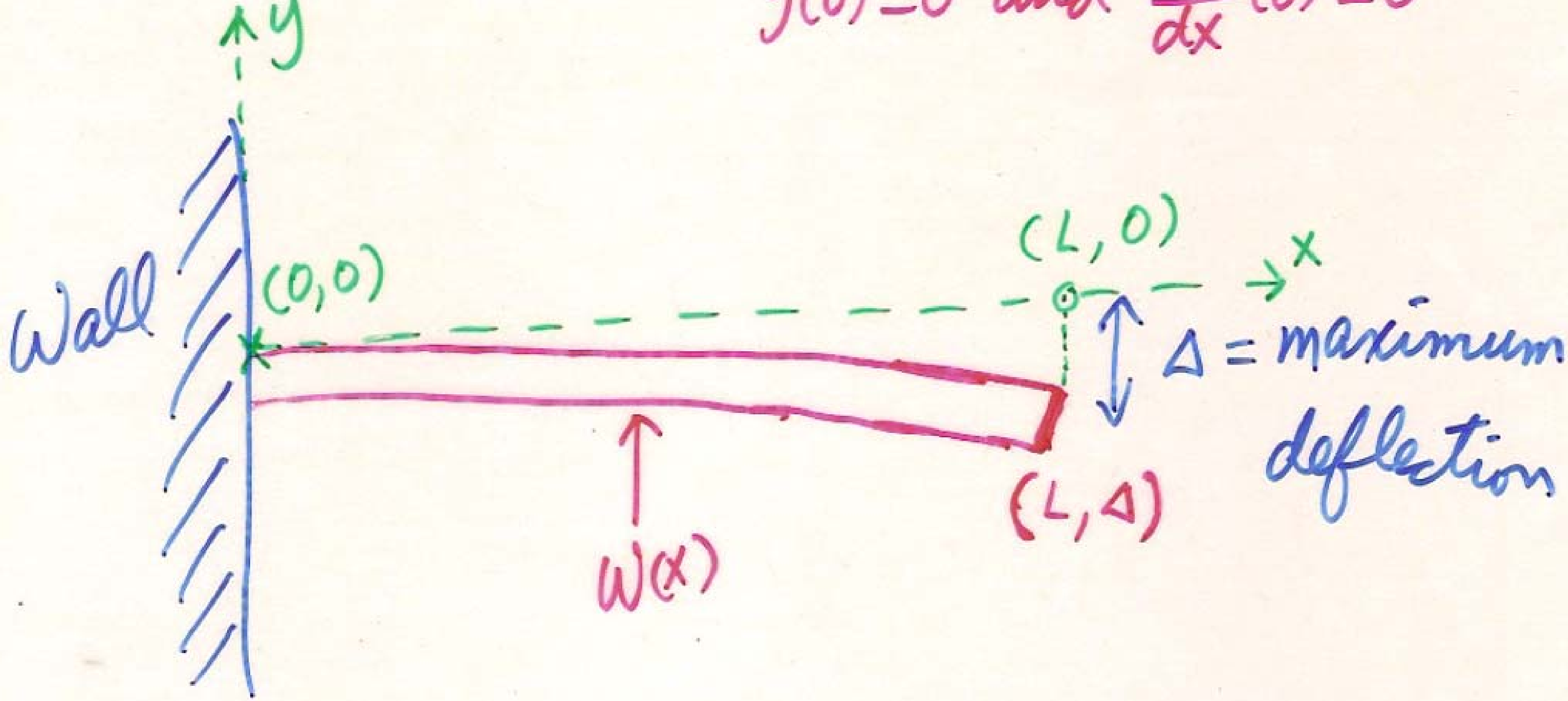
EXAMPLE. A CANTILEVER is a beam stuck into a wall, as shown. Suppose it bends under its own weight. We assume that it has a uniform mass per unit length, so the load function is $w(x) = \text{constant} = -\alpha$. (Remember that w is positive in the UPWARD direction.)

QUESTION: What is Δ, the maximum deflection?

Cantilever

For the red curve, we have

$y(0)=0$ and $\frac{dy}{dx}(0)=0$



Assume that the beam has uniform mass per unit length $= \alpha$. (a constant)

Assume that the deflection is caused by the beam's own weight, i.e. no other external force acting on it.

Recall that the load function $w(x)$ is positive in the upward direction and the weight of the beam acts downwards

$$\therefore \quad w(x) = -\alpha$$

In this case we have

$$\frac{d^4y}{dx^4} = \frac{w(x)}{EI} = -\frac{\alpha}{EI} \quad (\text{by } 5)$$

$$\therefore \frac{d^3y}{dx^3} = -\frac{\alpha}{EI}x + A \quad \text{- - - -} \quad 6$$

Recall that $\frac{d^2y}{dx^2} = \frac{M}{EI}$ (see 4)

$$\therefore \frac{d^3y}{dx^3} = \frac{1}{EI}\frac{dM}{dx}$$

$$= \frac{1}{EI} F(x) \qquad (\text{by } ②)$$

Observe : $F(x) =$ shearing force at x

$\therefore F(L) = 0$ ($\because$ there is no beam beyond L)

Setting $x = L$ in (6)

$$\Rightarrow \frac{1}{EI} F(L) = -\frac{\alpha L}{EI} + A$$

$$\Rightarrow A = \frac{\alpha L}{EI}$$

$\therefore$ (6) becomes

$$\frac{d^3y}{dx^3} = -\frac{\alpha}{EI}x + \frac{\alpha L}{EI}$$

$$\therefore \frac{d^2y}{dx^2} = -\frac{\alpha}{2EI}x^2 + \frac{\alpha L}{EI}x + B \quad \text{----} (7)$$

Recall: $\dfrac{d^2y}{dx^2} = \dfrac{M}{EI}$ (see 4)

Observe: $M(L)=0$ ($\because$ there is no beam beyond L)

Setting $x=L$ in 7

$$\Rightarrow 0 = -\frac{\alpha}{2EI}L^2 + \frac{\alpha L^2}{EI} + B$$

$$\Rightarrow B = -\frac{\alpha L^2}{2EI}$$

$\therefore$ 7 becomes

$$\frac{d^2y}{dx^2} = -\frac{\alpha}{2EI}x^2 + \frac{\alpha L}{EI}x - \frac{\alpha L^2}{2EI}$$

$$\therefore \frac{dy}{dx} = -\frac{\alpha}{6EI}x^3 + \frac{\alpha L}{2EI}x^2 - \frac{\alpha L^2}{2EI}x + C \quad \cdots 8$$

Recall: for the red curve, we have

$$\frac{dy}{dx}(0) = 0$$

$$\therefore \; (8) \Rightarrow C = 0$$

$$\Rightarrow \frac{dy}{dx} = -\frac{\alpha}{6EI}x^3 + \frac{\alpha L}{2EI}x^2 - \frac{\alpha L^2}{2EI}x$$

$$\Rightarrow y = -\frac{\alpha}{24EI}x^4 + \frac{\alpha L}{6EI}x^3 - \frac{\alpha L^2}{4EI}x^2 + D$$

---- (9)

Recall: for the red curve, we have

$$y(0)=0$$

$$\therefore \text{(9)} \Rightarrow D=0$$

$$\boxed{y=-\frac{\alpha}{24EI}x^4+\frac{\alpha L}{6EI}x^3-\frac{\alpha L^2}{4EI}x^2}$$

This is the equation of the red curve.

When $x = L$, we have $y = \Delta$

$$\therefore \quad \Delta = -\frac{\alpha}{24EI}L^4 + \frac{\alpha}{6EI}L^4 - \frac{\alpha}{4EI}L^4$$

$$\therefore \quad \boxed{\Delta = -\frac{\alpha L^4}{8EI}}$$

and so we obtain the famous CANTILEVER DEFLECTION FORMULA

$$\Delta = -\frac{\alpha L^4}{8EI}.$$

The negative answer of course reflects the fact that the cantilever always bends DOWNWARDS. Check that the answer MAKES SENSE: the deflection is larger for larger loads α, of course that makes sense. The deflection is smaller if EI is large, that is, if the beam is very stiff: that too makes sense. Finally, the deflection is greater if the beam is very long [large L], which also makes sense.

There is still a surprise here though: notice that if you make your cantilever twice as long, the downwards deflection does not double − − − it increases by a factor of SIXTEEN! So watch out if you want to build balconies etc. [The power of 4 here is a relic of the fact that we solved a FOURTH-order ODE.]