

Introduction to mathematical modelling with ODEs

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2. Dynamics

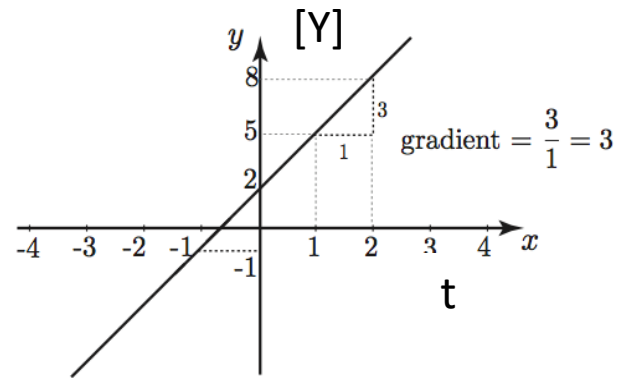
The nervous system and the automatic machine are fundamentally alike in that they are devices, which make decisions on the basis of decisions they made in the past.

Norbert Wiener

Rates as derivatives

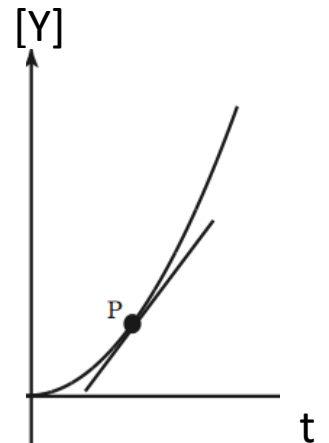
- To model reactions we need to express the rates mathematically as differential equations
- A system of differential equations can then be solved computationally

$$\text{rate} \approx \frac{[Y]_f - [Y]_s}{\Delta t}$$



$$\text{rate} \approx \frac{\Delta[Y]}{\Delta t}$$

$$\frac{\Delta[Y]}{\Delta t} \rightarrow \frac{d[Y]}{dt}$$

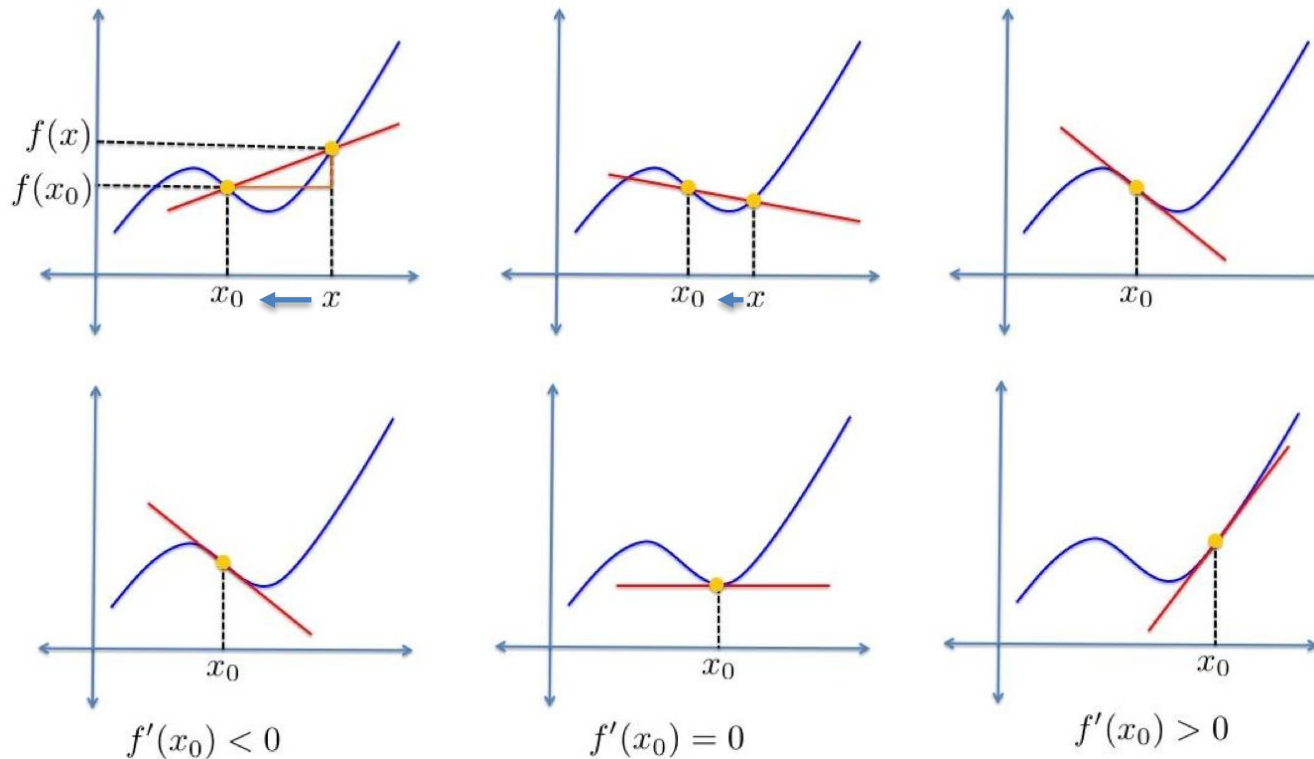


Differentiation

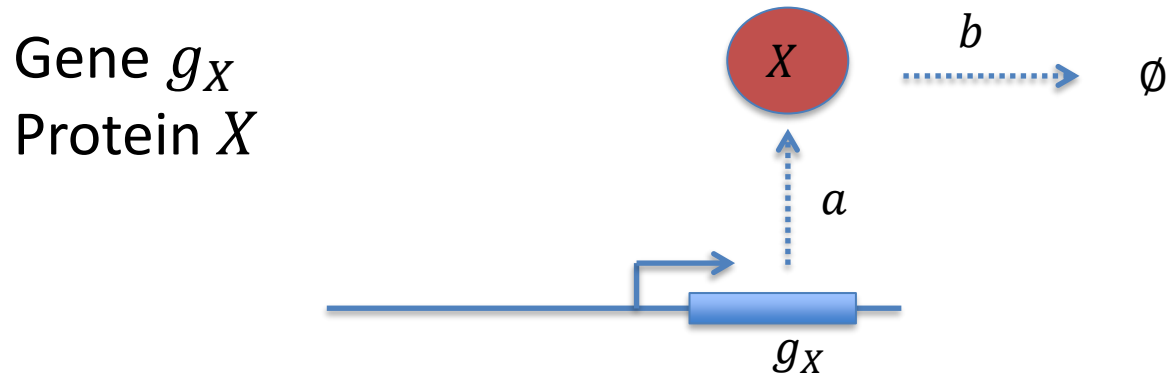
$$f'(x) = \frac{df(x)}{dx} = \lim_{x \rightarrow x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

Means: “The gradient of the function as x gets infinitely close to x_0 ”

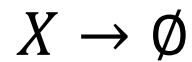
Or you can think about it as the tangent to the curve at x



Gene expression



- For simplicity, combine transcription and translation
- Include degradation of X



Input-output principle

- What is rate of change of X ?

$$\text{Rate of change of } X = \text{Rate of production} - \text{Rate of degradation}$$

(input) - (output)

- Rate of production = ag_X
- Rate of degradation = bX (mass action arguments)

$$\frac{dX}{dt} = ag_X - bX$$

What about the gene?

$$\frac{dX}{dt} = ag_X - bX$$

- We notice that the number of gene X doesn't change in the reaction (it is conserved). We can assume a number for gene X, often we can write

$$g_X = 1$$

- Which gives

$$\frac{dX}{dt} = a - bX$$

Expression for $X(t)$

- We have an equation for $\frac{dX}{dt}$, how do we obtain $X(t)$?
- $X(t)$ means “ X as a function of t ”
- Need to perform **integration**
- In this simple case we can do it **analytically** (mathematically)
 - using dsolve in MATLAB or Python, DSolve in Mathematica etc.

$$X(t) = \frac{a}{b} - \frac{e^{-bt}(a - X_0 b)}{b}$$

Steady states

- In our model, X settles down to a constant value
- Once reached there is **no change** in the system
- This is known as a **steady state**
- **At a steady state**

$$\frac{dX}{dt} = 0$$

- For our gene expression model this means we need to solve the following for X

$$a - bX = 0$$

- Which gives

$$X = \frac{a}{b}$$

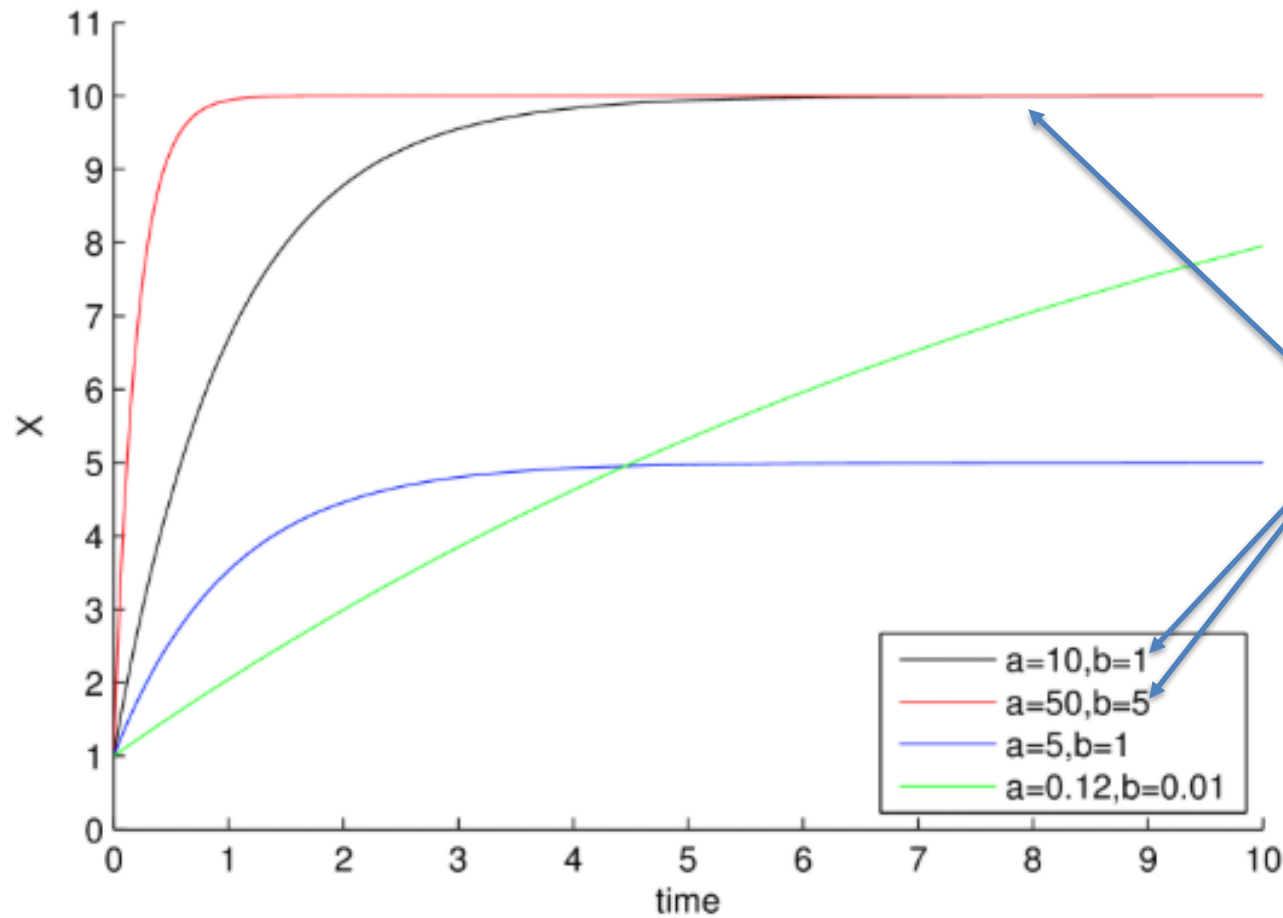
Steady states

- Steady states are very important for understanding a system
- They tell us about the long-term behaviour
- Often we are only interested in the steady states
- Take a look again at the solution $X(t)$

$$X(t) = \frac{a}{b} - \frac{e^{-bt}(a - X_0b)}{b}$$

- What happens as $t \rightarrow +\infty$?
 - (t tends to infinity or gets very large)

Gene expression model



Long term behavior is the same ($\frac{10}{1} = \frac{50}{5} = 10$)