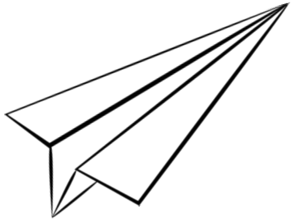
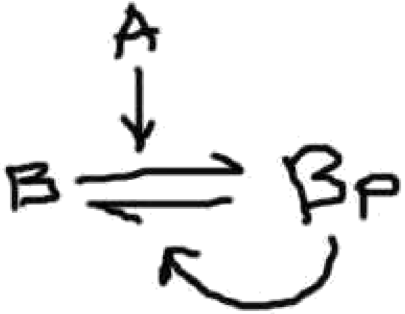
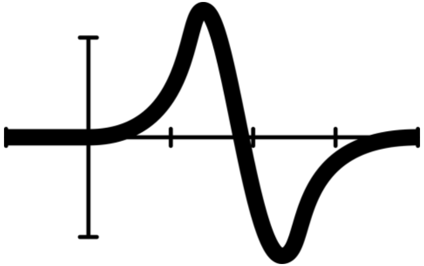






$$\frac{dc}{dt} = k_1 c(1-c)$$

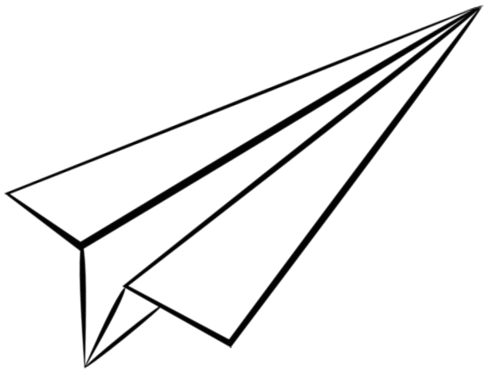
$$\int_{c_0}^{c} \frac{dc}{c(1-c)} = \int_0^t k_1 \cdot dt$$

How to Start Modeling

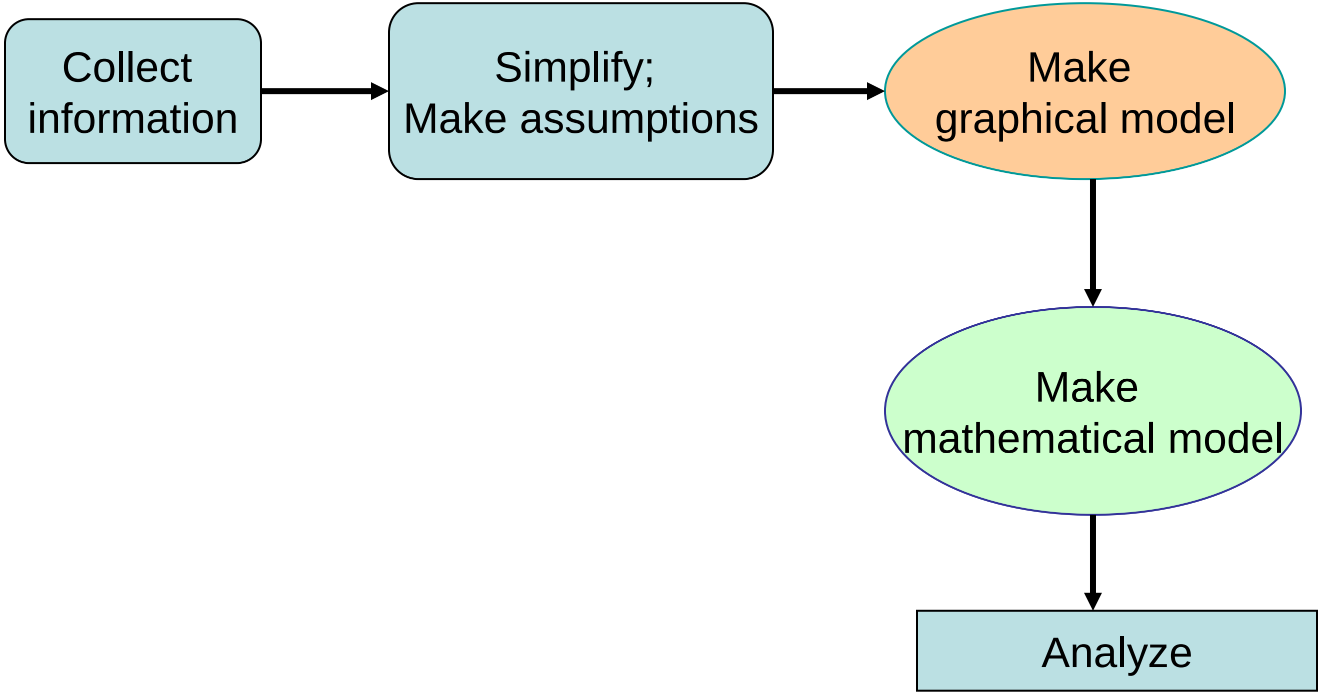
All models are wrong

Models are simplified representation of reality

Models answer specific questions

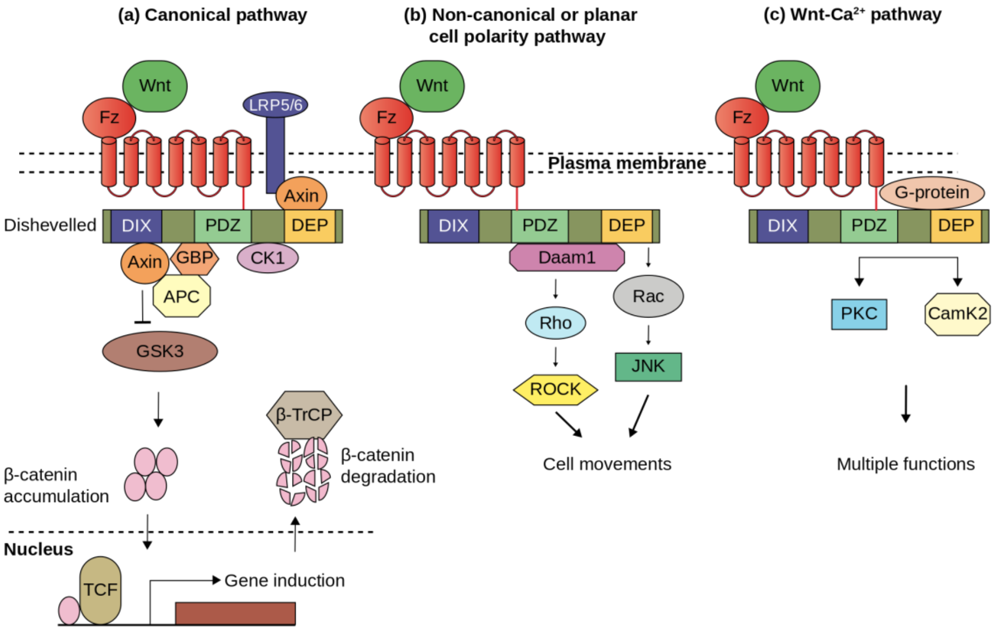


Steps in modeling



Graphical models:

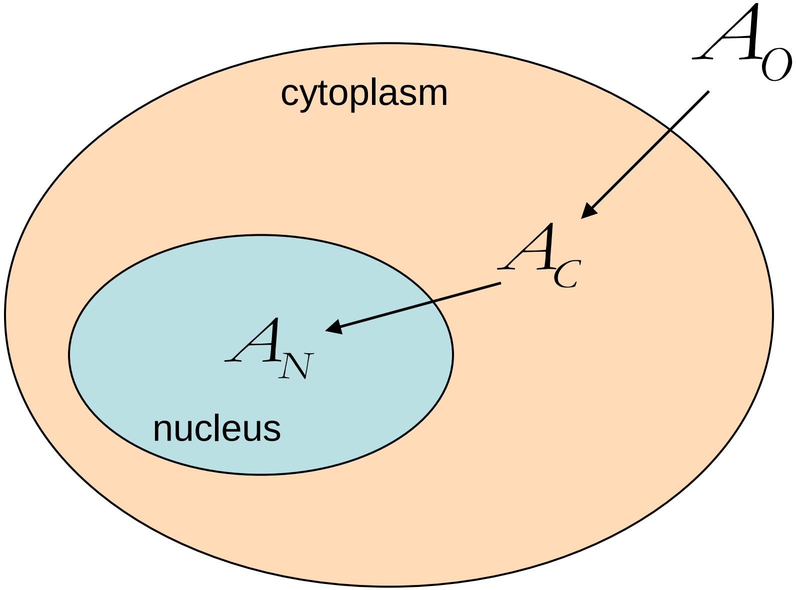
Simplified visual representation of a complex process



Creating consistent graphical models:

1. Define the boundary and compartments

2. Show all the players and name them

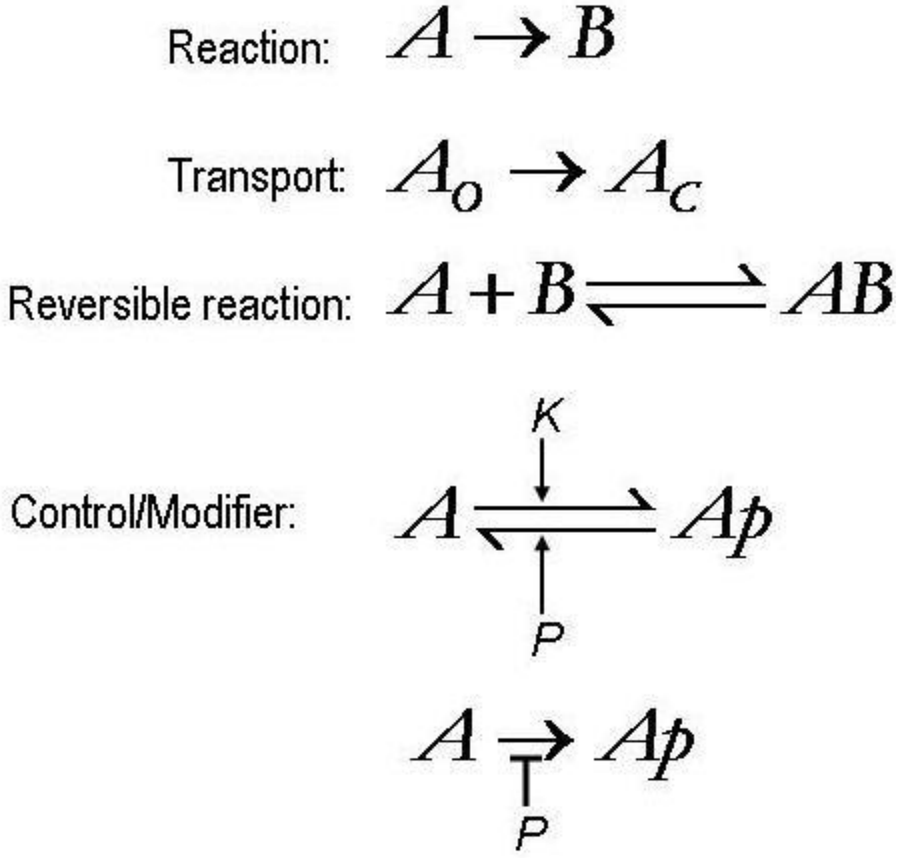


Creating consistent graphical models:

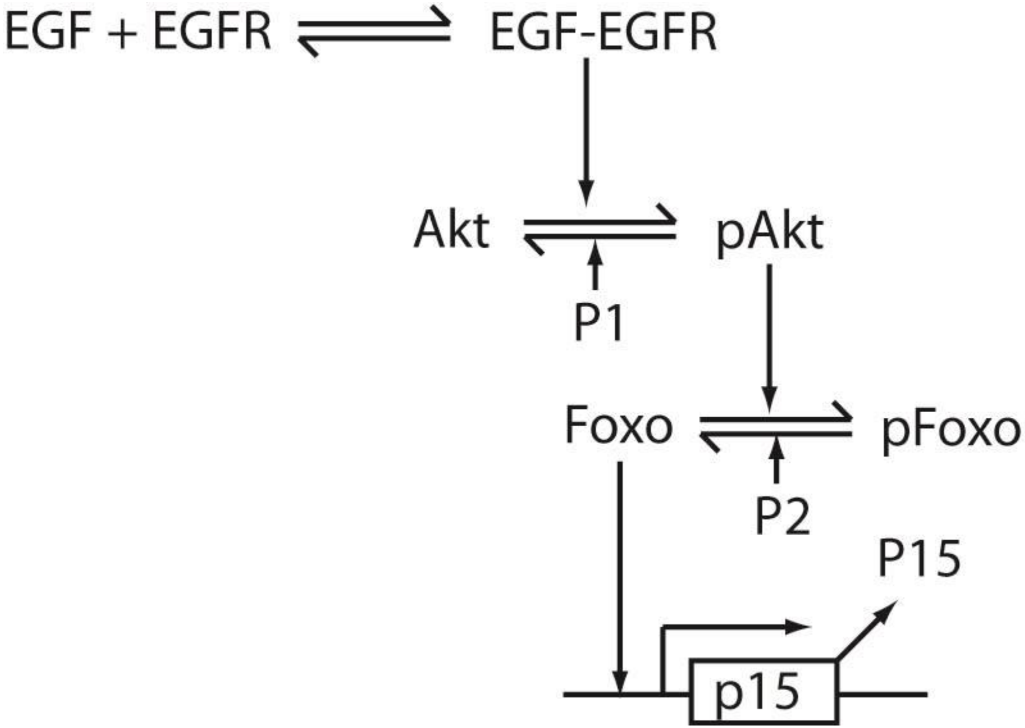
1. Define the boundary and compartments

2. Show all the players and name them

3. Representing molecular events



Example of a graphical model:



Mathematical model:

Ordinary differential equations (ODEs)

Partial differential equations (PDEs)

Ordinary Differential Equations

Basic school-level knowledge of Calculus would be useful

ODE: derivative of the function

$$\frac{dx}{dt} = t$$ is an ODE and it is a derivative of the function,

$$x = f(t) = \frac{t^2}{2} + C$$ (C is a constant)

Ordinary Differential Equations

Linear ODE:

$$\frac{dx}{dt} = a.x + b \qquad \frac{dx}{dt} = a(t).x + b(t)$$

The dependent variable and its derivative should have power of one and there should be no product of the dependent variable and its derivative

Non-linear ODE:

$$\frac{dx}{dt} = 2.x^2 + 4 \qquad x\frac{dx}{dt} = 3.x + t$$

Ordinary Differential Equations

Order of an ODE:

The order of a differential equation is equal to the highest derivative in the equation.

1st order:

$$\frac{dx}{dt} = a.x + b$$

2nd order:

$$\frac{d^2x}{dt^2} = a.x + b$$

Ordinary Differential Equations

Coupled system of ODEs:

Set of connected ODEs with multiple dependent variables and one independent variable

One ODE for each dependent variable

$$\frac{dx}{dt} = a.x + by$$

$$\frac{dy}{dt} = c.y + d.z$$

$$\frac{dz}{dt} = -k.x.z$$

Model using ODEs:

Ordinary differential equations are used to represent rates of processes

A reversible chemical reaction:

$$A \underset{k2}{\overset{k1}{\rightleftharpoons}} B$$

Rate of change of concentration of *B* with time,

$$\frac{d[B]}{dt} = k_1.[A] - k_2.[B]$$

Rate of change of concentration of *A* with time,

$$\frac{d[A]}{dt} = -k_1.[A] + k_2.[B]$$

Key assumptions for ODE-based models:

1. The system is homogenous (or well mixed).

2. Size of the system (*i.e.* number of each components) is large

Law of Mass Action (simplified & brief) : rate of a reaction is proportional to the product of molar concentrations of the reactants raised to powers.

$$aA + bB \xrightarrow{k_1} mM + nN$$

$$\text{Rate of reaction} = -\frac{1}{a}.\frac{d[A]}{dt} = -\frac{1}{b}.\frac{d[B]}{dt} = \frac{1}{m}.\frac{d[M]}{dt} = \frac{1}{n}.\frac{d[N]}{dt} = k_1.[A]^{a'}.[B]^{b'}$$

Key points:

1. Collect relevant information
2. Keep the model simple & specific
3. Make appropriate assumptions for simplifications
4. Create graphical model
5. Create mathematical model: choose correct mathematical approach
6. Key assumptions for ODE model: Homogeneity & large system size