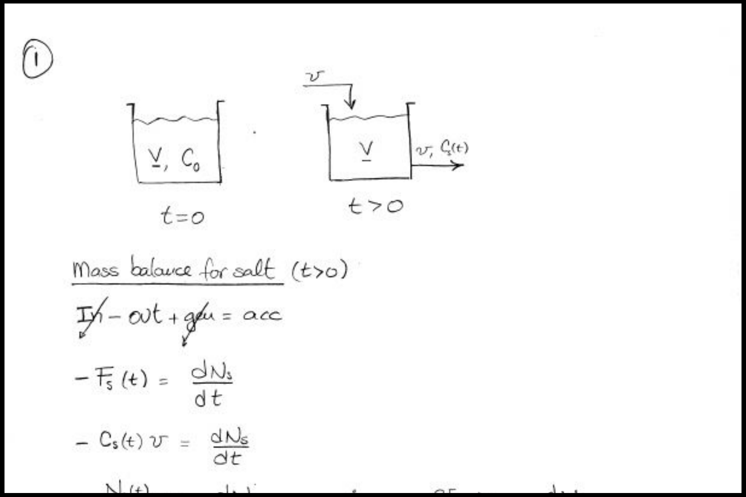
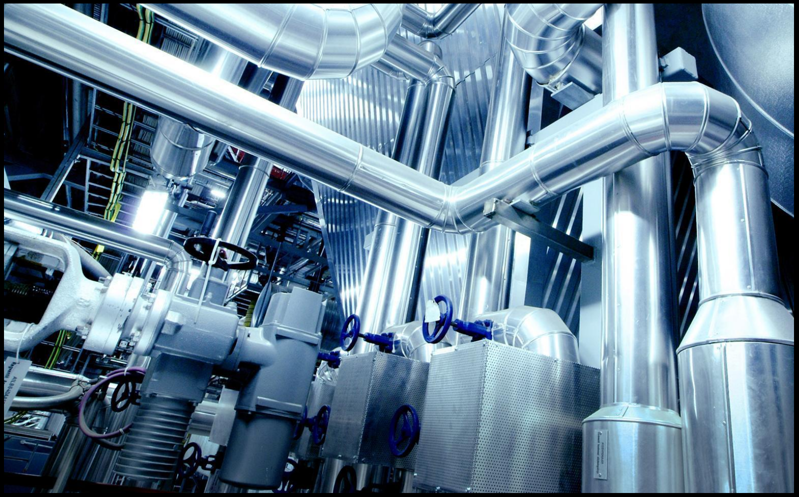




ChE352
Numerical Techniques for Chemical Engineers
Professor Stevenson

Lecture 9

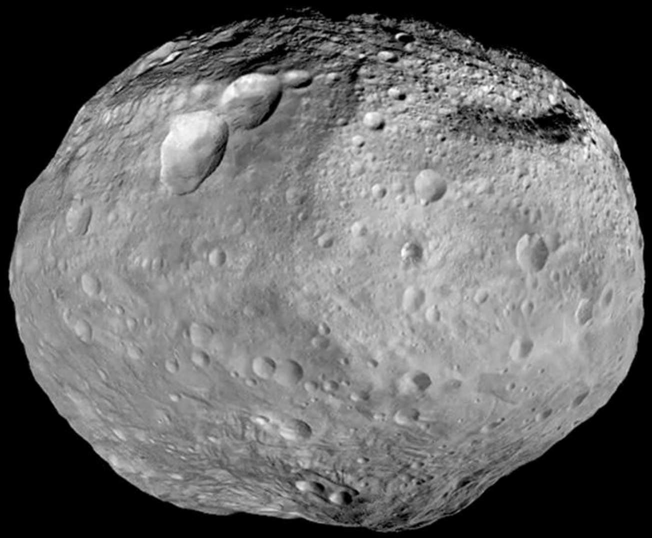
Homework #5: groups of 2-3

Please sort yourselves into groups of 2-3 before the next homework, and send me the names (each group only has to send once)

Classical dynamics: Asteroids

Given an asteroid with a position, velocity, and forces, how does it move?

Position = x
Velocity = dx/dt
Force = $m(d^2x/dt^2)$



If we know the ***initial values*** of the variables, we can find their values at later times too using a form of numerical integration

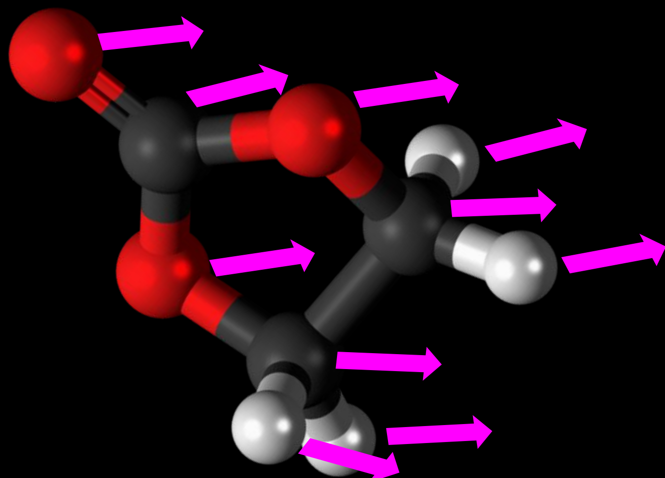
Classical dynamics: Molecules

Given a set of atoms with positions, velocities, and forces, how do they move?

Position = $\mathbf{x}$

Velocity = $d\mathbf{x}/dt$

Force = $m(d^2\mathbf{x}/dt^2)$



Each atom has its own vectors $\mathbf{x}$, $d\mathbf{x}/dt$, and $m(d^2\mathbf{x}/dt^2)$

If we know the ***initial values*** of the variables, we can find their values at later times too using a form of numerical integration

Initial Value Problems

$$\boxed{WE\ WANT\ y(t)}$$

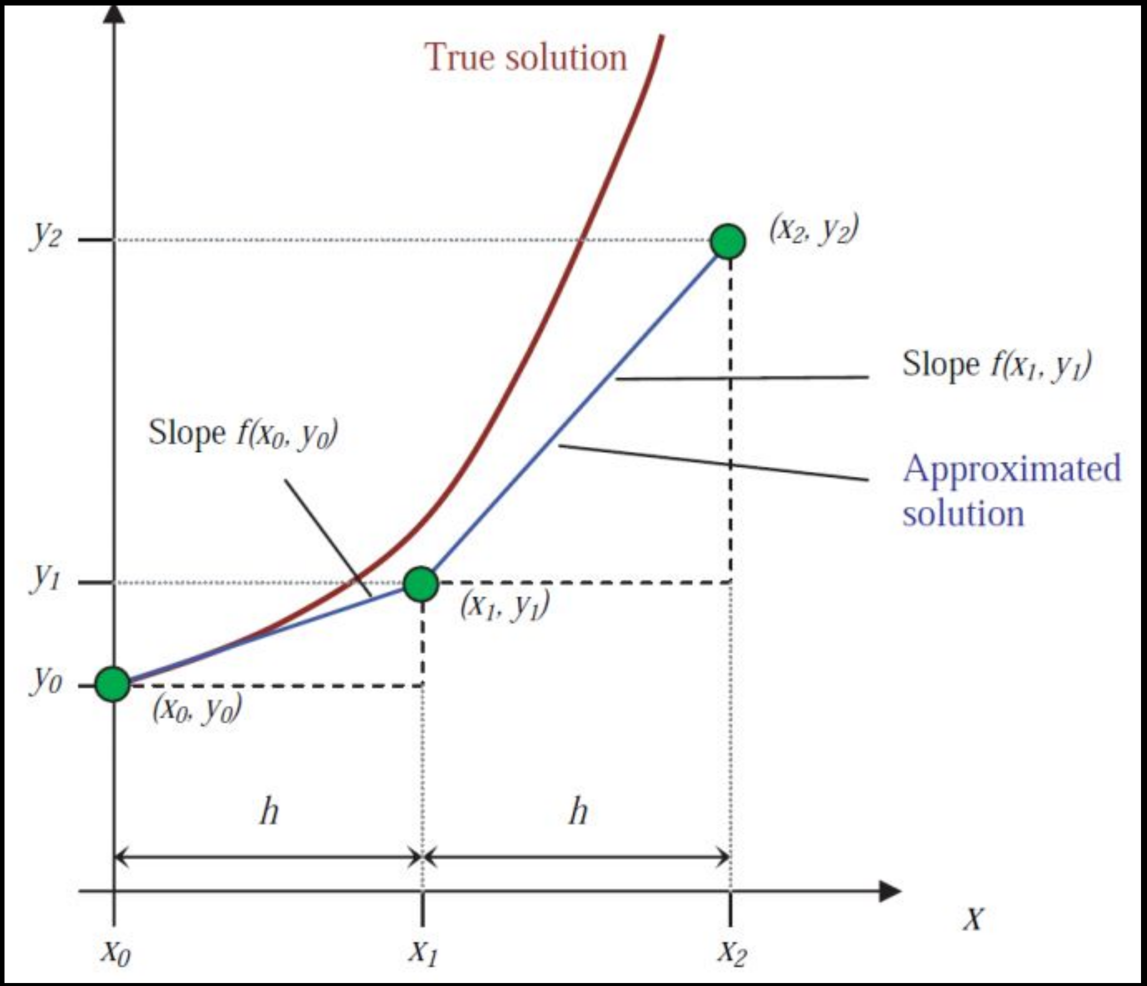
$$WE\ HAVE\quad \frac{dy}{dt} = f(t, y)$$

$$a \le t \le b, \quad y(a) = \alpha$$

$$t, y \in \mathbb{R}, \quad y : \mathbb{R} \to \mathbb{R}$$

$$f : \mathbb{R}^2 \to \mathbb{R}$$

$$f\ continuous$$



What is the *independent* variable in f(t, y)?

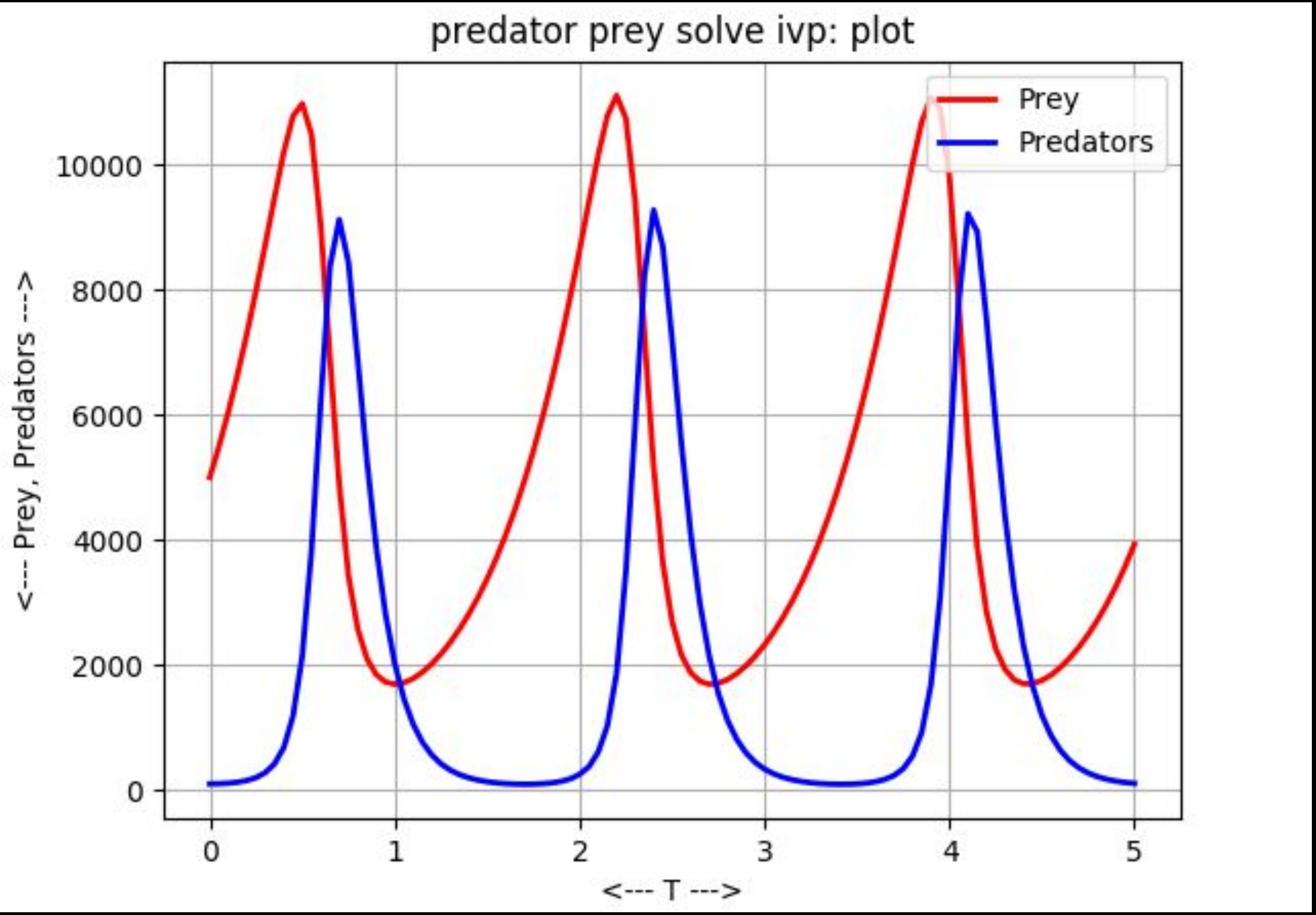
What about on this graph?

What makes it an IVP?

- When you know how a value starts, and you know how it changes, but you do not know the values after the start
- Classic example: predator/prey population
  - Easy to see how the derivatives are related
    - More prey ➜ more predators
    - More predators ➜ fewer prey
  - But how do these changes add up over time?
  - Example: exercise 5.7.5 (pg 221) in F&B

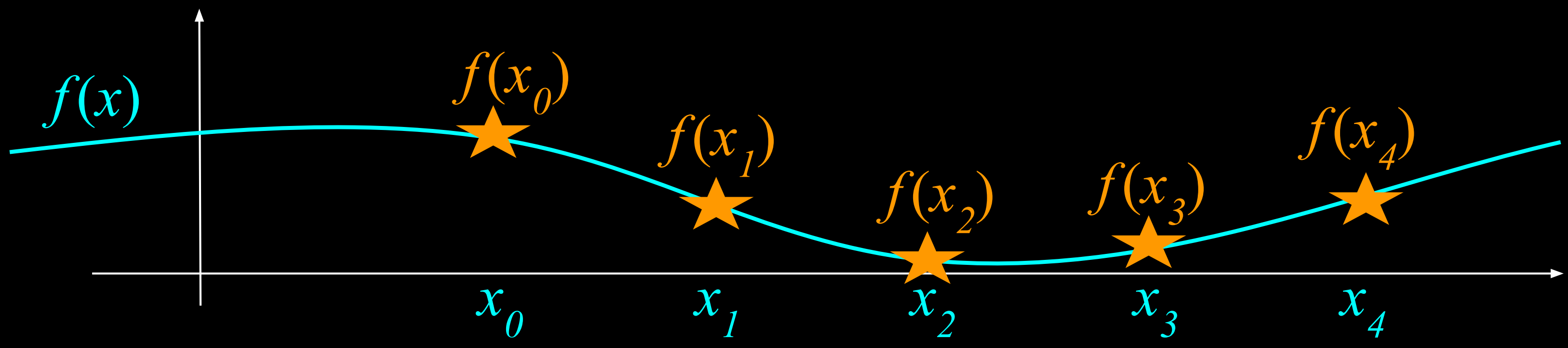
Predator/prey IVP

Either dynamic equilibrium, or both predator & prey go extinct, depending on IVP properties.



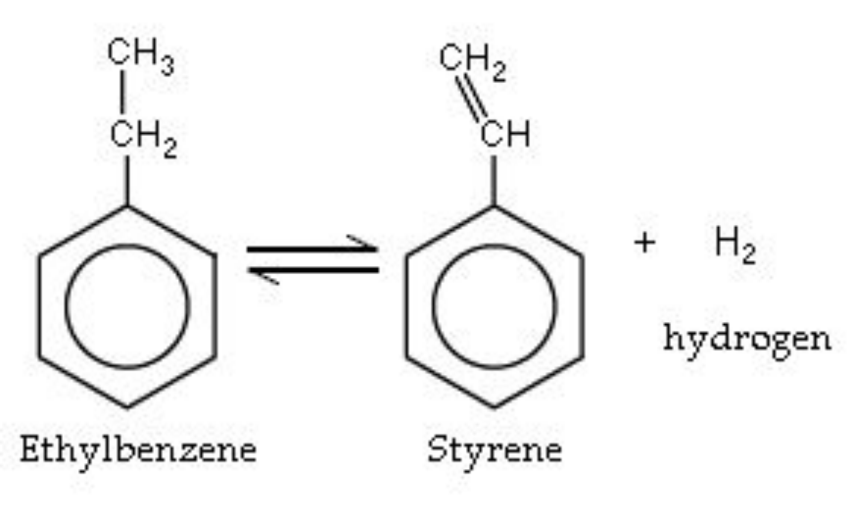
Functions vs function values

- We can use the values $f(x_i)$ without knowing the function $f(x)$ in total
- If we only need discrete $f(x_i)$ values, an array such that y[i] = $f(x_i)$ is fine



Example: Styrene Reactor Design

- Scenario: you're a chemical engineer for a company that makes styrofoam
- You notice a shortage of styrene ("S"), the monomer of styrofoam, so you want to make it from ethylbenzene ("EB"), a cheap oil refinery byproduct, instead of buying it



What do you call this kind of reaction?

Simplified reactor equations

First you would need to calculate the yield of S as a function of distance & reactor length (z, v)

$$EB \underset{k_r}{\overset{k_f}{\rightleftarrows}} S+H \quad \left(Catalytic\ dehydrogenation\ @650\ ^{o}C\right)$$

1st order 2nd order

$$\frac{dC_S}{d\tau} = R_S = k_f C_{EB} - k_r C_S C_H, \quad C_S\left(\tau=0\right) = C_S^o \quad \left[\tau = \frac{z}{v}\right]$$

$$\frac{dC_{EB}}{d\tau} = R_{EB} = -R_H = -R_S, \quad C_{EB}\left(\tau=0\right) = C_{EB}^o$$

What variables here give the yield of S?

Can we solve for yield analytically?

What aspects of reality are missing?

More realistic equations: ϱ varies

$$\frac{dN_S}{dz} = \frac{k_f N_{EB}}{v} - \frac{k_r N_S N_H}{v} = R_S^{'}, \quad N_S\left(z=0\right) = vC_S^o$$

$$\frac{dN_{EB}}{dz} = -R_S^{'}, \quad N_{EB}\left(z=0\right) = vC_{EB}^o \quad \left[N_i = \text{molar flux of species i}\right]$$

$$\frac{dP}{dz} = -\frac{\rho v^2}{d_p}\left(\frac{1-\varepsilon}{\varepsilon^3}\right)\left[\frac{150\left(1-\varepsilon\right)}{\mathrm{Re}_p} + 1.75\right], \quad P\hat{V} = ZRT \quad \Rightarrow \quad \rho = \frac{PM}{ZRT}$$

$$v = \frac{ZRT}{P}\left(N_{EB} + N_S + N_H + N_W\right)$$

Still doesn't account for temperature change, side products (benzene and toluene), coking...

Can we solve this analytically?

"Well-posed" IVPs

- An IVP (in 1D) is well-posed if:

initial condition

$$\frac{dy}{dt} = f(t, y) \quad for \quad a \le t \le b \quad with \quad y(a) = \alpha$$

and f, df are continuous for all relevant t & y:

$$1. \quad f : \mathbb{R}^2 \to \mathbb{R}, \quad f \ continuous$$

$$2. \quad \frac{\partial f}{\partial y} \quad is \ continuous$$

- A well-posed IVP has a unique solution y(t)
- Opposite is <u>ill-posed</u> (no unique solution)

Activity: Well-posed IVPs

Standard form of an IVP

$$\frac{dy}{dt} = f(t,y) \quad for \quad a \le t \le b \quad with \quad y(a) = \alpha$$

State the problem below in the standard form of an IVP (aka: define y, t, f, a, and α)

Styrene synthesis reaction (irreversible)

$$\frac{dC_{EB}}{d\tau} = -k_f C_{EB}, \quad C_{EB}(\tau = 0) = C_{EB}^o$$

Then, check whether your IVP meets the conditions for having a unique solution.

(Why do we care that the solution is unique?)

Answer: Well-posed IVPs

$$a = 0, \quad \alpha = C_{EB}^{o},$$

$$t = \tau, \quad y = C_{EB}, \quad \boxed{f(t,y) = -k_f y} = -k_f C_{EB} = R_{EB}$$

$$1. \quad f : \mathbb{R}^2 \to \mathbb{R} \quad (Yes?), \quad f \; continuous \quad (linear)$$

$$2. \quad \frac{\partial f}{\partial y} = -k_f \quad is \; continuous \quad (Yes.)$$

IVP is well-posed and has a unique solution

Error bounds for well-posed IVPs

A well-posed IVP solution y can be approximated with bounded error. If we define a perturbed problem z using the same function f(t, y):

$$\frac{dz}{dt} = f\left(t, z\right) + \delta\left(t\right) \quad for \quad a \le t \le b$$

$$with \quad z\left(a\right) = \alpha + \delta\left(a\right)$$

Then the difference (error) between z(t) and y(t) is always proportional to the size of δ(t)

Why does that help us?

How do we solve IVPs?

$$\frac{dy}{dt} = f(t, y) \quad for \quad a \le t \le b \quad with \quad y(a) = \alpha$$

Estimate a small step with a Taylor series!

1st-order Taylor expansion of y at point t_i:

$$y(t) = y(t_i) + (t - t_i)\, y'(t_i) + \frac{(t - t_i)^2}{2} y''(\xi_i)$$

If we define a step size $h = (t_{i+1} - t_i)$ and evaluate at a nearby point t_{i+1}:

$$y(t_{i+1}) = y(t_i) + hf(t_i, y(t_i)) + \frac{h^2}{2} y''(\xi_i)$$

What order is the error for solution y(b)?

Euler's Method

- Dropping the error term (proportional to h^2):

$$y(t_{i+1}) \approx y(t_i) + hf(t_i, y(t_i))$$

- Define a variable ***w*** for our approximation:

$$w \approx y \quad \rightarrow \quad w(t_{i+1}) = w(t_i) + hf(t_i, w(t_i))$$

- Simplifying notation:

$$w_i \equiv w(t_i) \quad \rightarrow \quad \boxed{w_{i+1} = w_i + hf(t_i, w_i)}$$

- "Asteroids" code:

```
x += dt * x_speed
x_speed += dt * x_acceleration
```

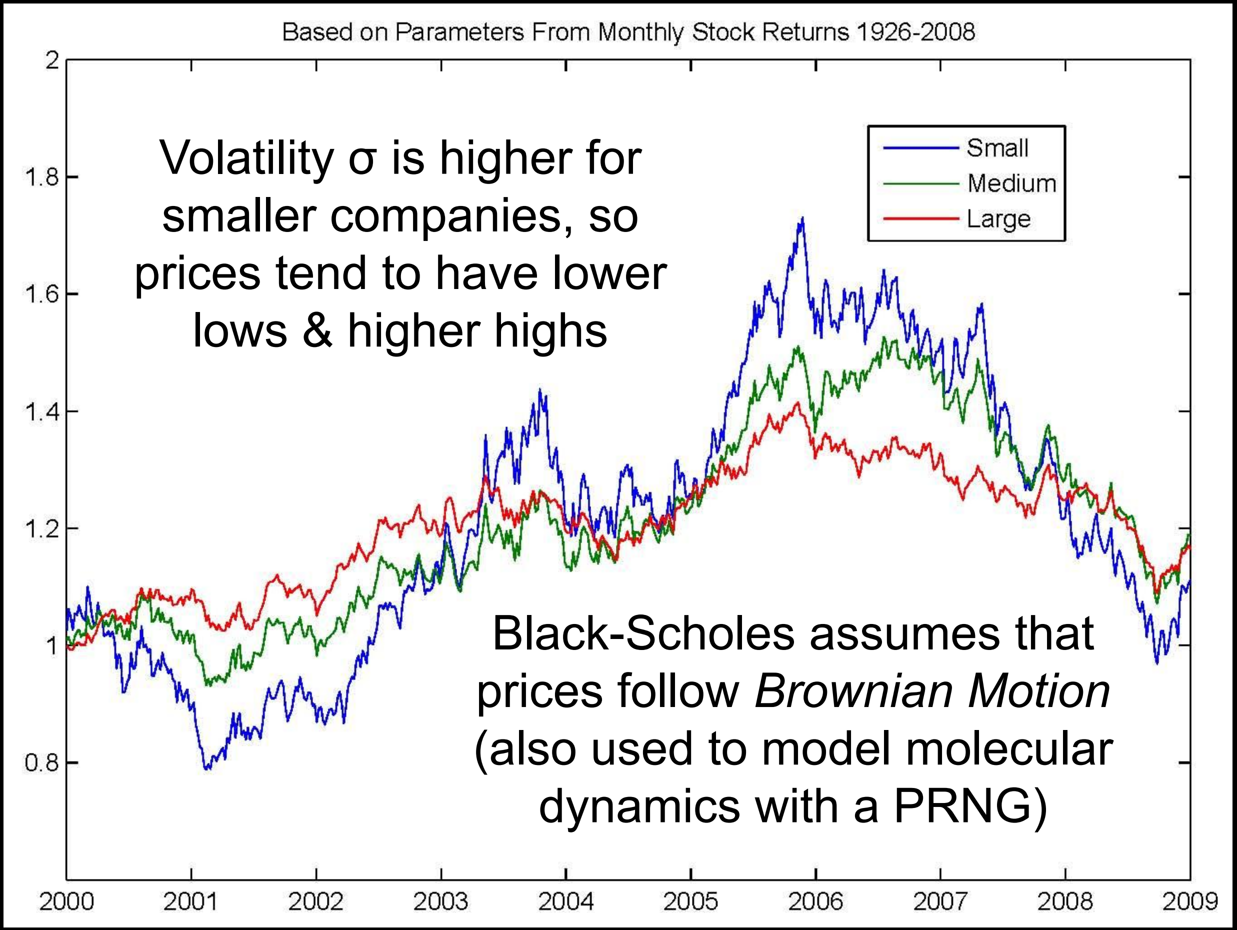
①Stock price IVPs ②??? ③Profit

- *Do not pick individual stocks unless you have money to set on fire*
- Those who *do* bet on stock prices (like hedge funds) do it with IVPs
- Typical model: the Black-Scholes equation

$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS\frac{\partial V}{\partial S} - rV = 0$$

S is the stock price, V is the price of an *option* to buy the stock at a future time, r is the risk-free interest rate, σ is the *volatility* of the stock price, t is time

①Stock price IVPs ②??? ③Profit



$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS\frac{\partial V}{\partial S} - rV = 0$$

Valentine's Math: PRNG Secrets

- Pseudo-Random Number Generator
- The output of a PRNG is repeatable as long as it has the same state (aka *seed*)
- If you and another person share a secret, you can each use it to seed a PRNG, giving *identical* random-looking outputs
- This lets you share secret messages
- https://www.kaggle.com/allaboutchemistry/prng-encryption