Computational Methods (PHYS 2030)

Instructors: Prof. Christopher Bergevin (cberge@yorku.ca)

Schedule: Lecture: MWF 11:30-12:30 (CLH M)

Website: http://www.yorku.ca/cberge/2030W2018.html

York University
Winter 2018
Lecture 4

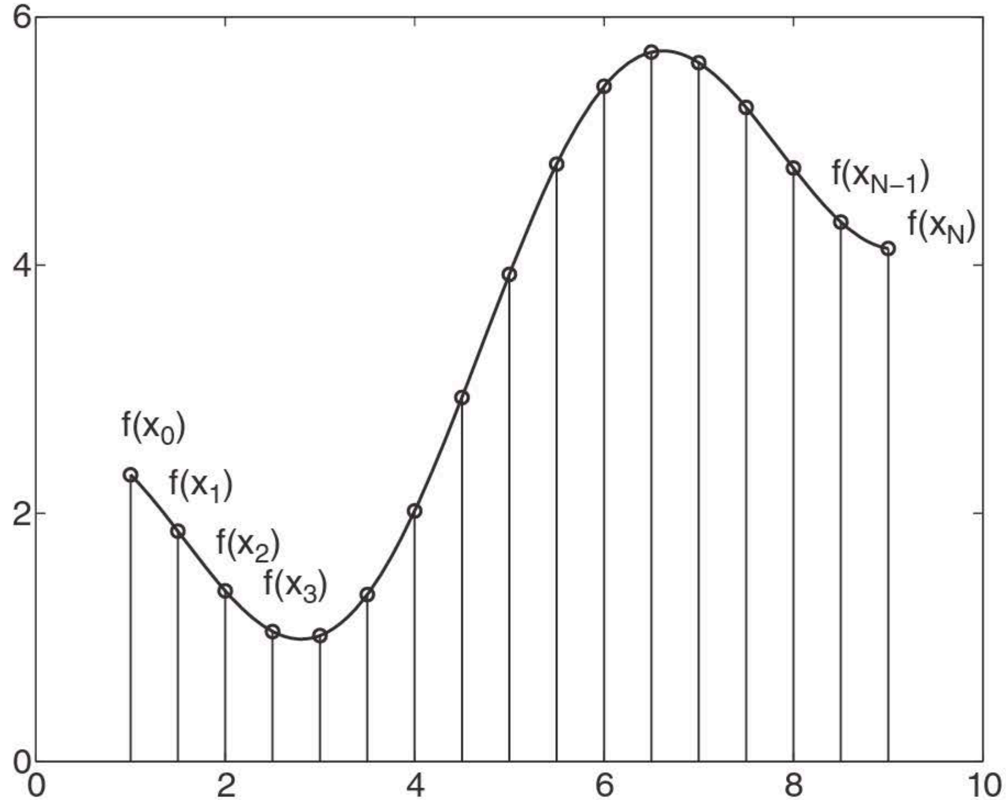


Figure 4.3: Graphical representation of the integration process. The integration interval is broken up into a finite set of points. A quadrature rule then determines how to sum up the area of a finite number of rectangles.

Kutz (2013)

Newton-Cotes Formulae

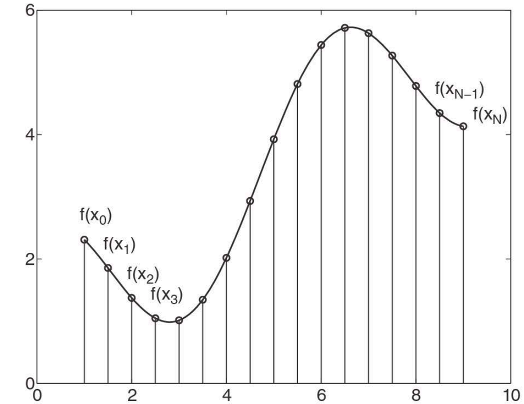


Figure 4.3: Graphical representation of the integration process. The integration interval is broken up into a finite set of points. A quadrature rule then determines how to sum up the area of a finite number of rectangles.

$$\text{Trapezoid rule} \int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12} f''(c) \tag{4.2.6a}$$

$$\text{Simpson's rule} \int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90} f''''(c) \tag{4.2.6b}$$

$$\text{Simpson's 3/8 rule} \int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80} f''''(c) \tag{4.2.6c}$$

$$\text{Boole's rule} \int_{x_0}^{x_4} f(x)dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) - \frac{8h^7}{945} f^{(6)}(c). \tag{4.2.6d}$$

Note that these formulae have an extra ‘error’ term

$$P_n(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0 \tag{4.2.4}$$

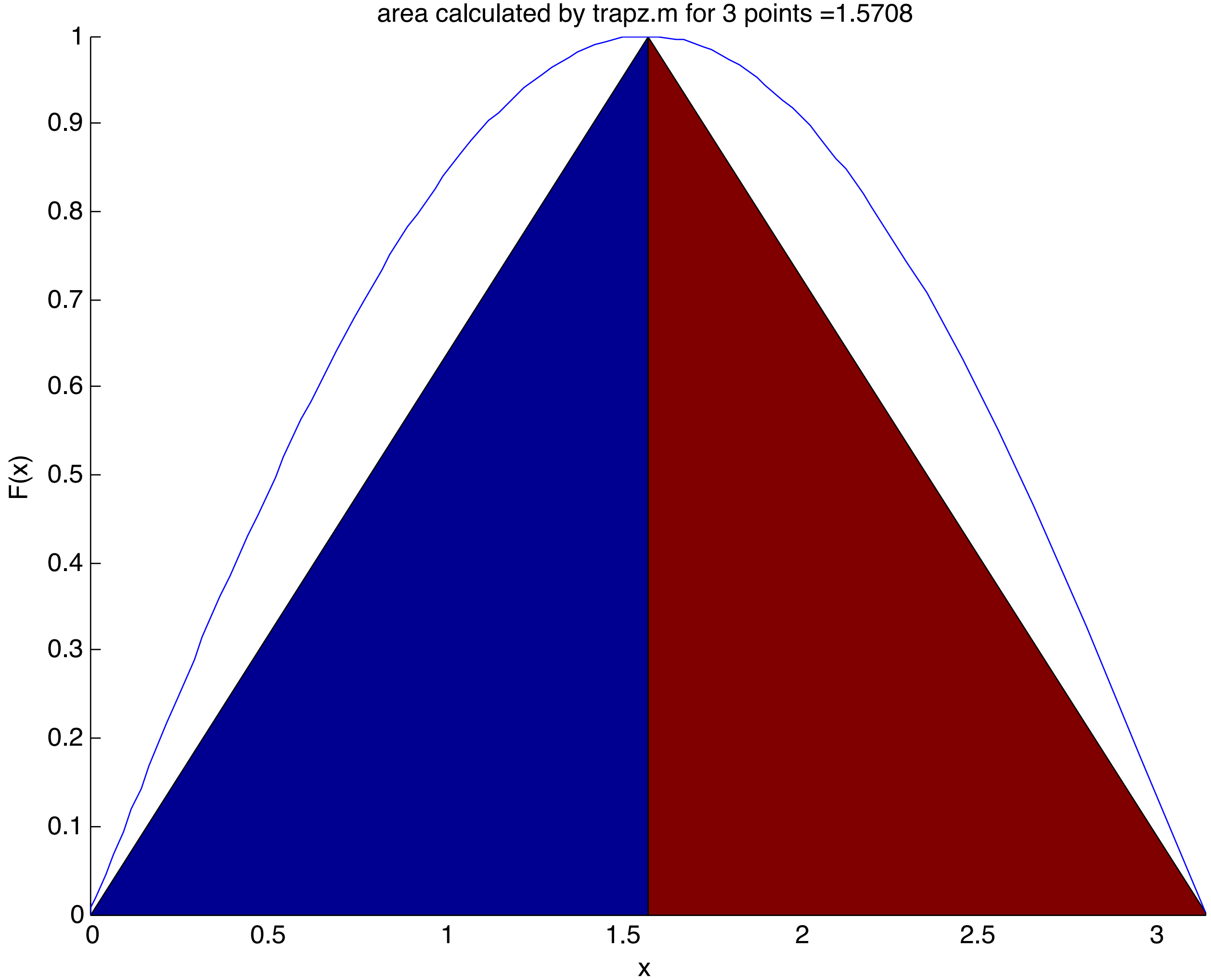
→ Ultimately, we are approximating via a series of polynomials (and we decide how high we want to go!)

Kutz (2013)

```
% Numerical integration example - original source:
% http://ef.engr.utk.edu/ef230-2011-01/modules/matlab-integration/

clear;
% ----------------------
% User parameters
F = @(x)(sin(x)); % function to integrate
%F = @(x)(exp(-x.^2/2)); % function to integrate
xL= [0 pi]; % integration limits

N= 5;    % Method A - # of points for LEFT and RIGHT
pts= [3 4 5 10 25]; % Method B - # of points to consider integrating (via trapz function)
dur= 1;     % Method B - pause duration [s] for trapz loop
% ----------------------

% ***************
% Show the curve
figure(1);
fplot(F,[xL(1),xL(2)]) % a quick way to plot a function
xlabel('x'); ylabel('F(x)');

% ***************
% Method A
% Approximate the integral via brute force LEFT and RIGHT Riemann sums
sumL= 0; sumR=0;
delX= (xL(2)-xL(1))/N;    % step-size
x= linspace(xL(1),xL(2),N+1);  % add one since N is # of 'boxes' and is really N-1
for nn=1:N
    sumL= sumL + F(x(nn))*delX;
    sumR= sumR + F(x(nn+1))*delX;
end
disp(['left-hand rule yields =',num2str(sumL),' (for ',num2str(N),' steps)']);
disp(sprintf('right-hand rule yields = %g', sumR));

% ***************
% Method B
% Approximate the integral via trapz for different numbers of points
for np=pts
    figure(2); clf % clear the current figure
    hold on % allow stuff to be added to this plot
    x = linspace(xL(1),xL(2),np); % generate x values
    y = F(x); % generate y values
    a2 = trapz(x,y); % use trapz to integrate
    % Generate and display the trapezoids used by trapz
    for ii=1:length(x)-1
        px=[x(ii) x(ii+1) x(ii+1) x(ii)];   py=[0 0 y(ii+1) y(ii)];
        fill(px,py,ii)
    end
    fplot(F,[xL(1),xL(2)]); xlabel('x'); ylabel('F(x)');
    disp(['area calculated by trapz.m for ',num2str(np),' points =',num2str(a2)]);
    title(['area calculated by trapz.m for ',num2str(np),' points =',num2str(a2)]);
    pause(dur);   % wait a bit
end

% ***************
% Method C
a1 = quad(F,xL(1),xL(2)); % use quad to integrate
msg = ['area calculated by quad.m = ' num2str(a1,10)]; disp(msg);
```

What three different methods are being used? Which ones are a 'black box'?

Trapezoid method (Method B)
np= 3

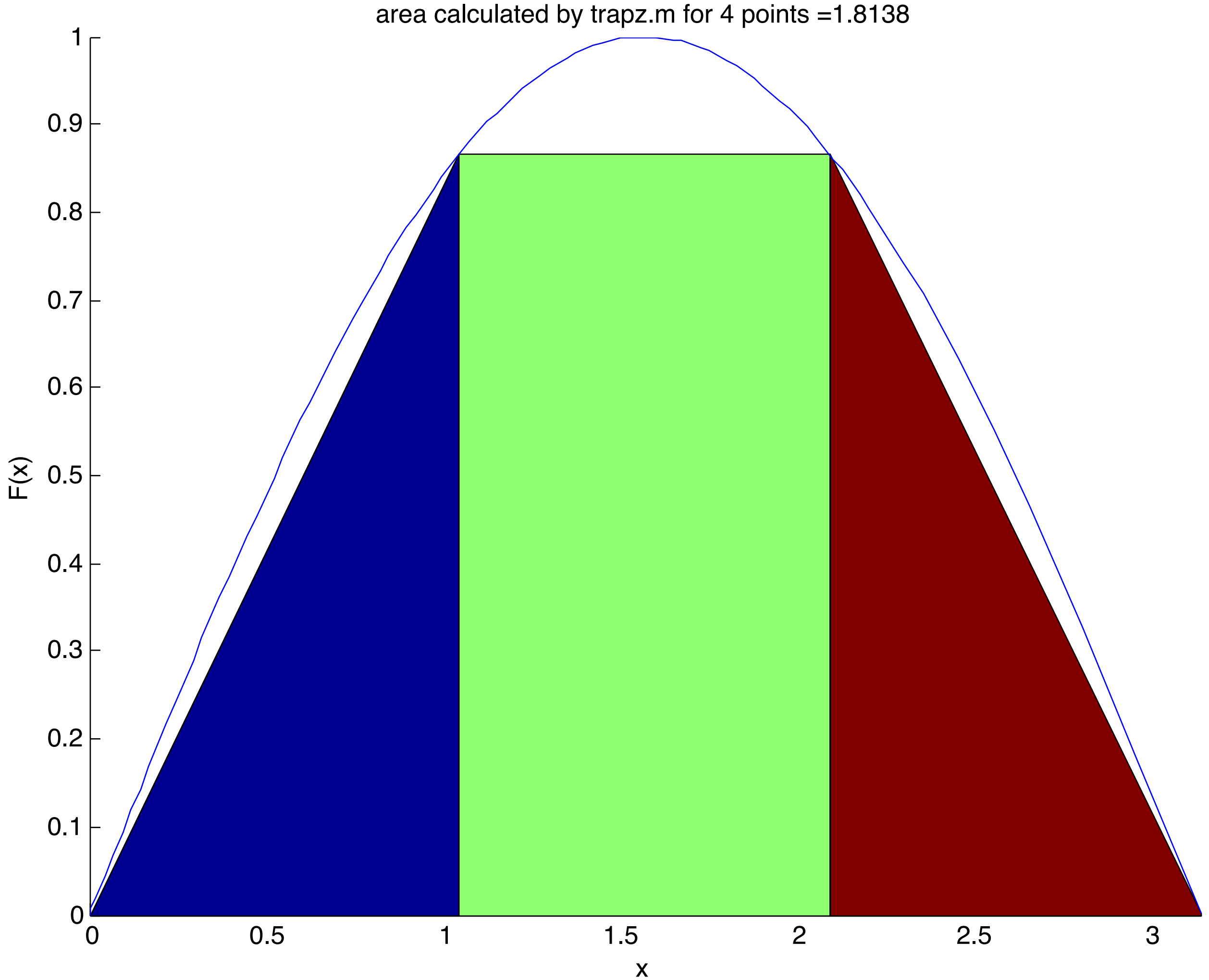


→ Are these rectangles? Why not?

→ Three points means how many ‘rectangles’?

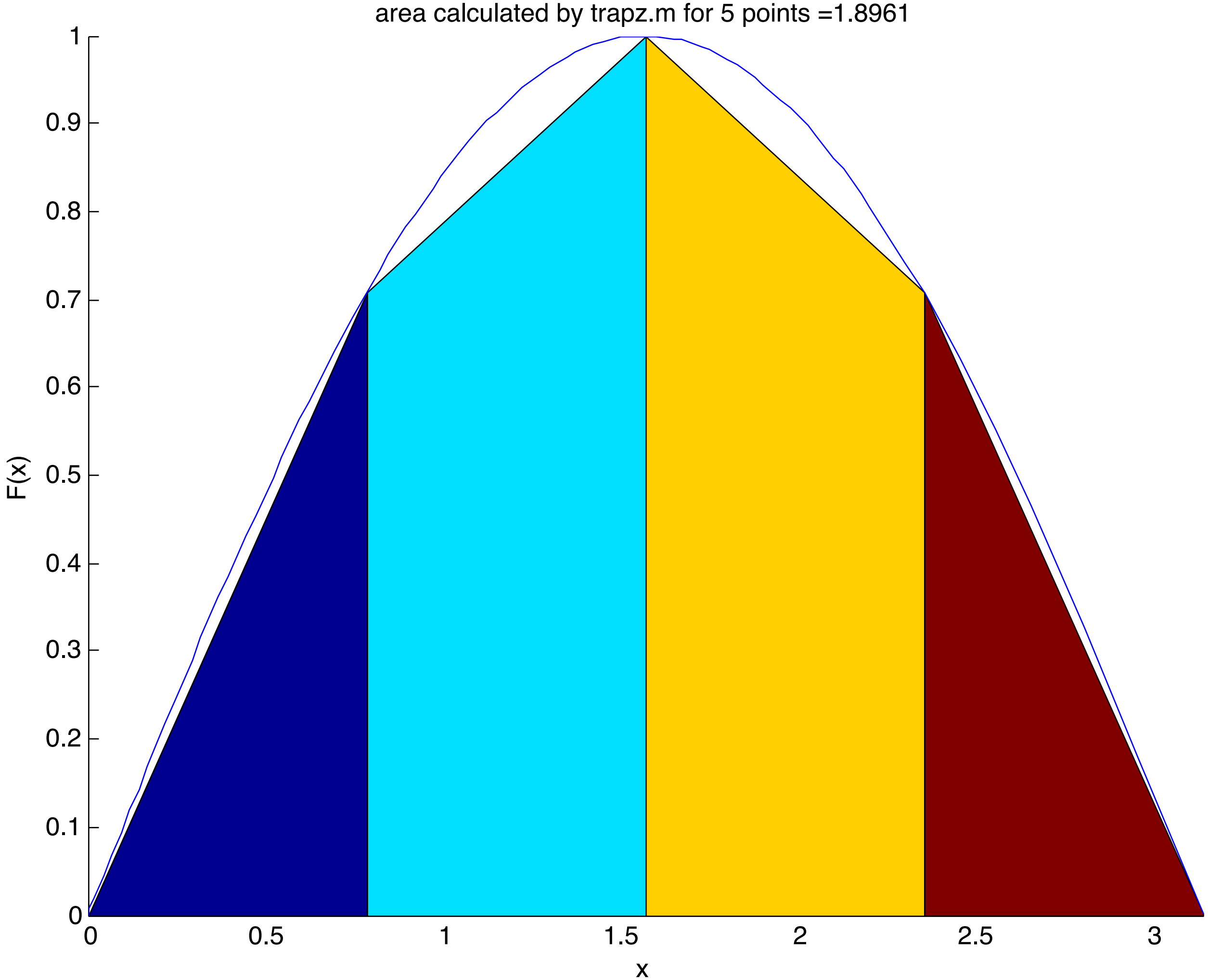
Trapezoid method (Method B)

np= 4

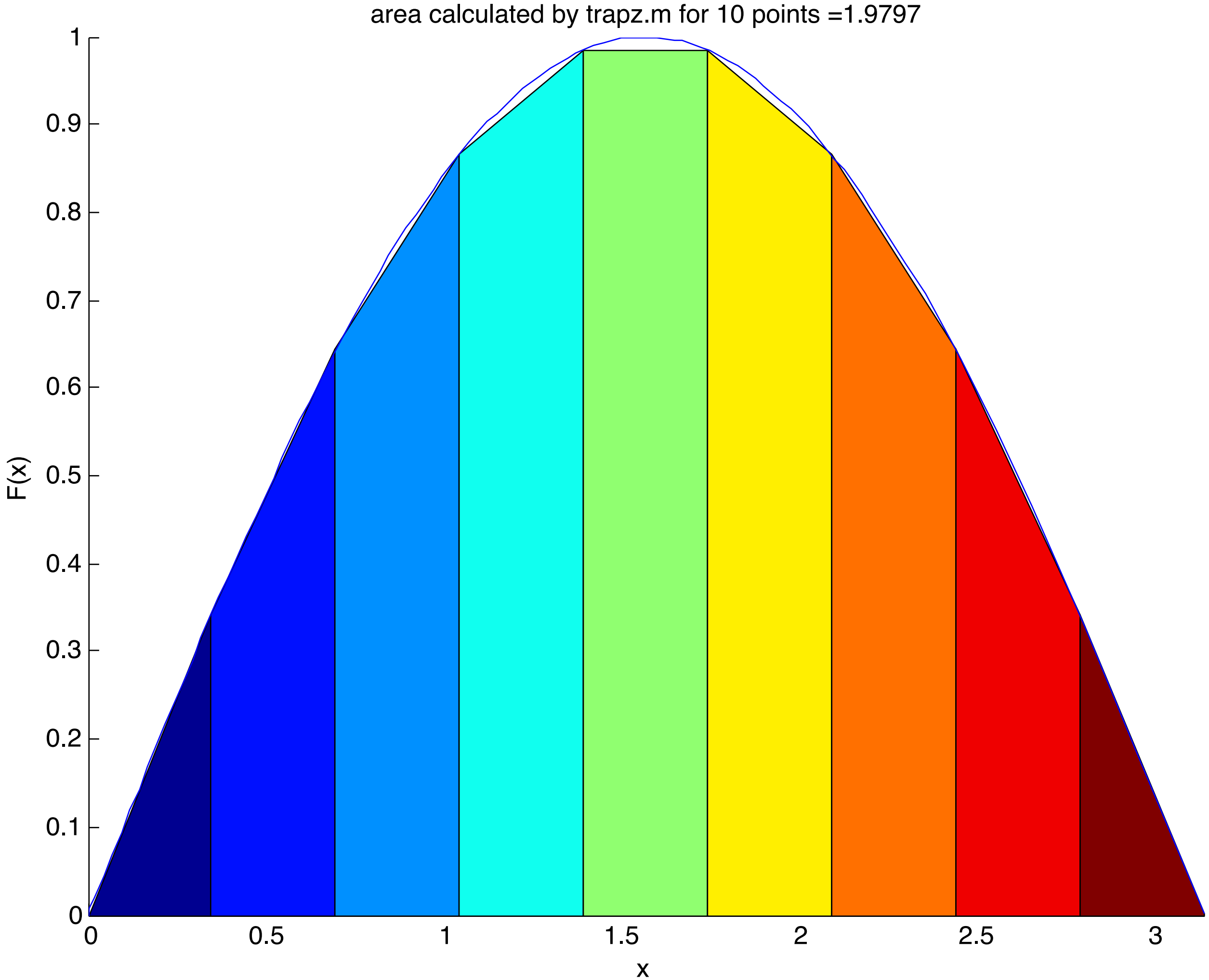


→ What is the associated 'error'?

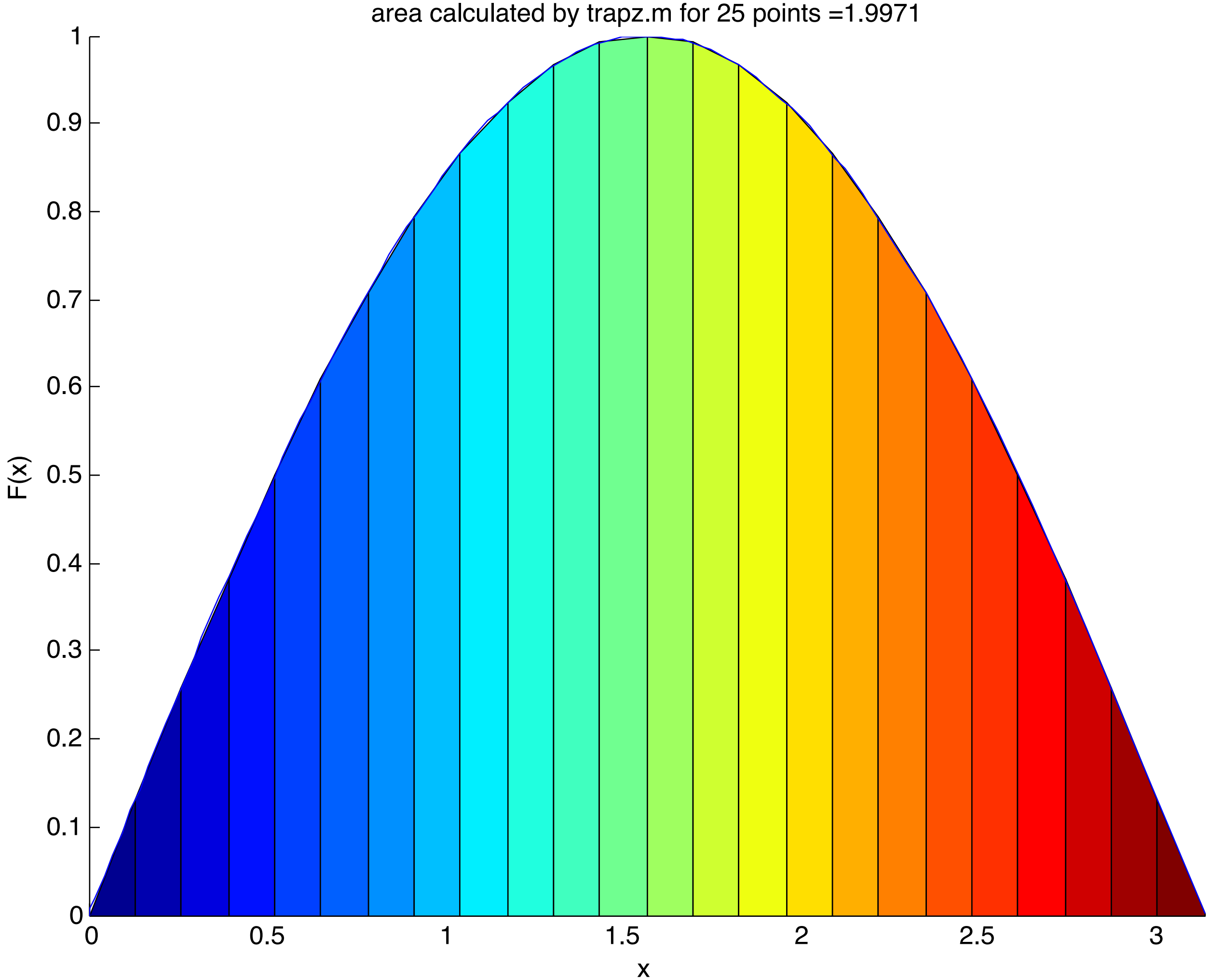
Trapezoid method (Method B)
np= 5



Trapezoid method (Method B)
np= 10



Trapezoid method (Method B)
np= 25



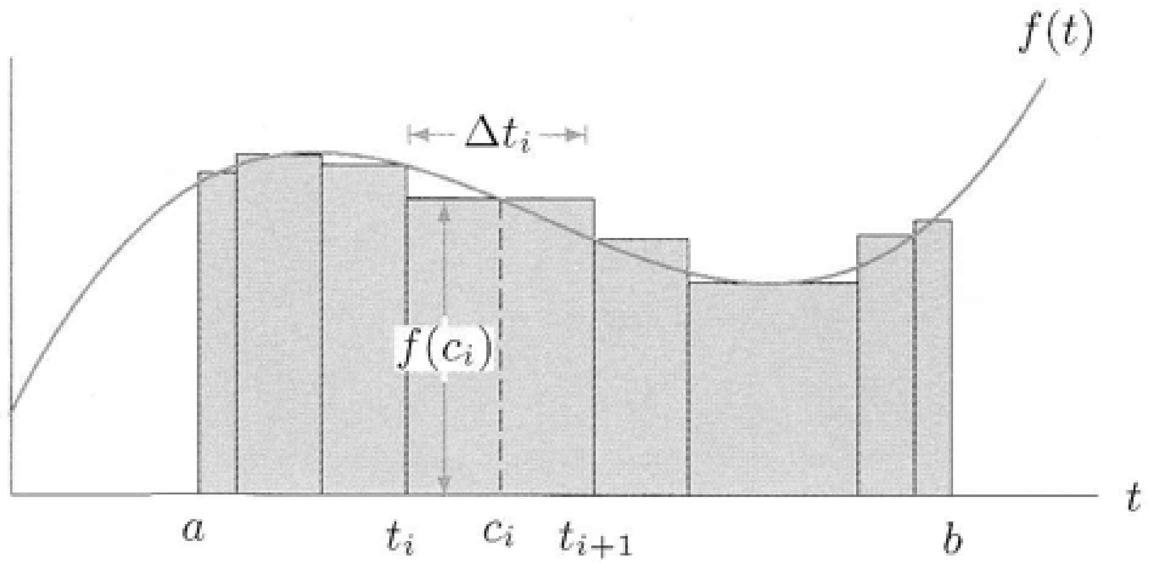
```
>> INTexample1
left-hand rule yields =1.9338 (for 5 steps)
right-hand rule yields = 1.93377
area calculated by trapz.m for 3 points =1.5708
area calculated by trapz.m for 4 points =1.8138
area calculated by trapz.m for 5 points =1.8961
area calculated by trapz.m for 10 points =1.9797
area calculated by trapz.m for 25 points =1.9971
area calculated by quad.m = 1.999999996
>>
```

→ Why do the LEFT and RIGHT Riemann sums yield the same values?

→ Are LEFT and RIGHT better than TRAP?

→ How many 'points' does quad.m use?

<u>Background</u>: Riemann sums



→ Note that Δt need not be constant (this is helpful computationally!)

Hughes-Hallett et al. (2005)

Summary

$$\int_a^b f(x)dx \approx \sum_{j=0}^{N} f(x_j)h$$

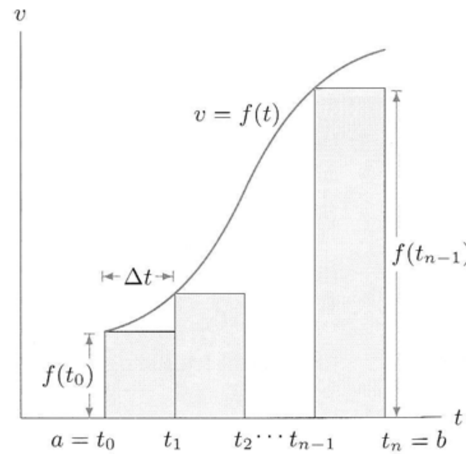


Figure 5.8: Left-hand sums

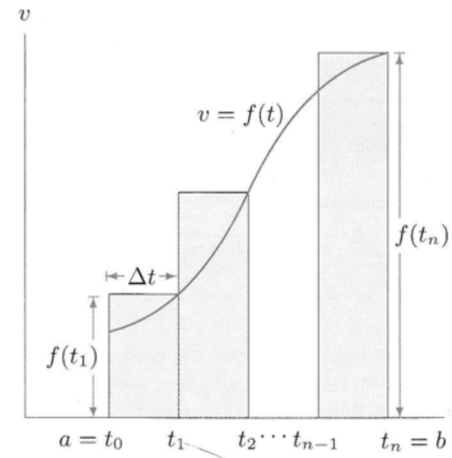
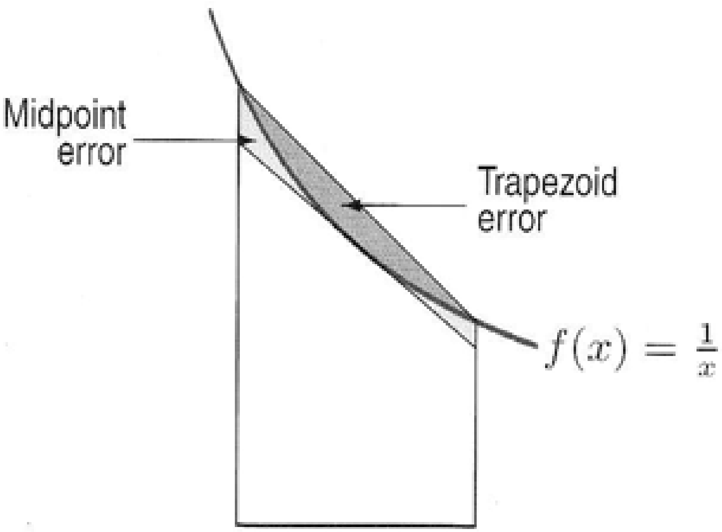
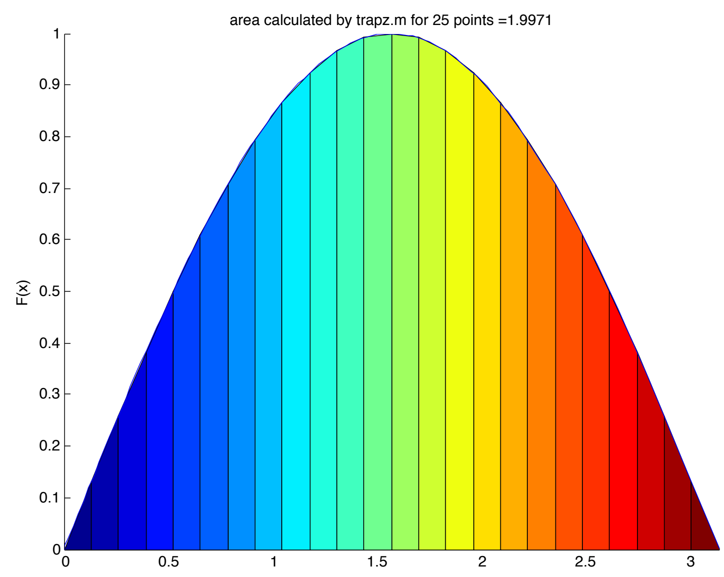


Figure 5.9: Right-hand sums





Trapezoid rule $\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12} f''(c)$ (4.2.6a)

Simpson's rule $\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90} f''''(c)$ (4.2.6b)

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Benjamin A. Stickler · Ewald Schachinger

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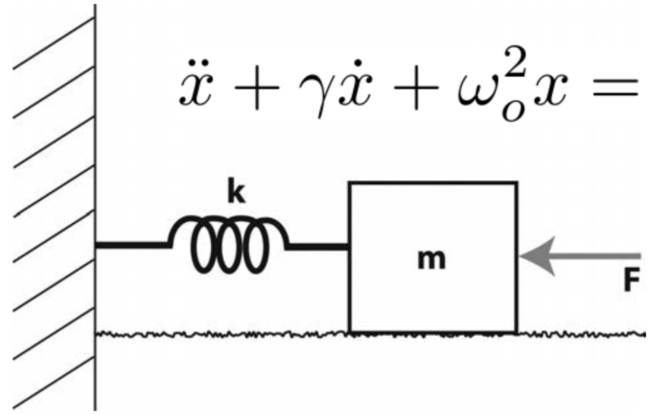
Motivation: Differential equations

→ A very common/useful tool in our toolbox....

Harmonic oscillator

$$\ddot{x} + \gamma \dot{x} + \omega_o^2 x = 0$$



Note: This just a specific case of Newton's 2nd law (F=ma)!

Wave equation

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2}$$

Laplace's equation

$$\Delta f = \nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 0$$

Maxwell's equations

$$\nabla \cdot \mathbf{E} = \frac{\rho_v}{\varepsilon} \qquad \text{(Gauss' Law)}$$

$$\nabla \cdot \mathbf{H} = 0 \qquad \text{(Gauss' Law for Magnetism)}$$

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} \qquad \text{(Faraday's Law)}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \varepsilon \frac{\partial \mathbf{E}}{\partial t} \qquad \text{(Ampere's Law)}$$

Several basic flavors apparent:

- Ordinary (ODE)
- Partial (PDE)
- Scalar vs. Vector

<u>Motivation</u>: Systems of differential equations

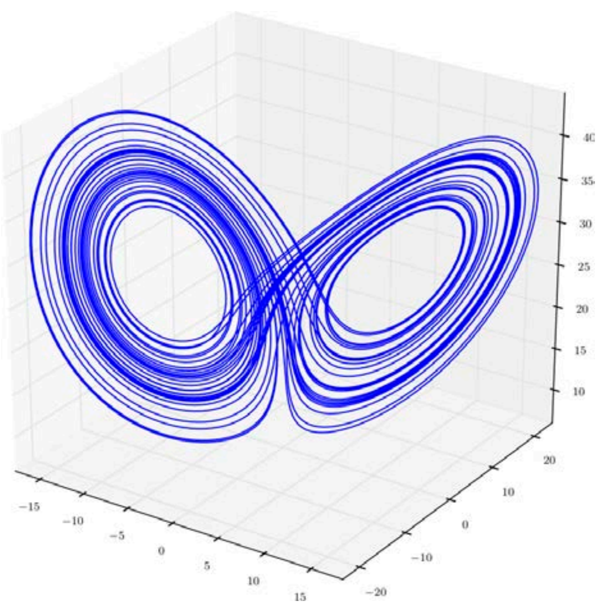
Lorenz equations

$$\frac{dx}{dt} = \sigma(y - x)$$

$$\frac{dy}{dt} = rx - y - xz$$

$$\frac{dz}{dt} = xy - bz$$

→ Chaos!



SIR model
('compartmental' model in epidemiology)

S = the number of *susceptibles*, the people who are not yet sick but who could become sick

I = the number of *infecteds*, the people who are currently sick

R = the number of *recovered*, or *removed*, the people who have been sick and can no longer infect others or be reinfected.

$$\frac{dS}{dt} = -\beta IS$$

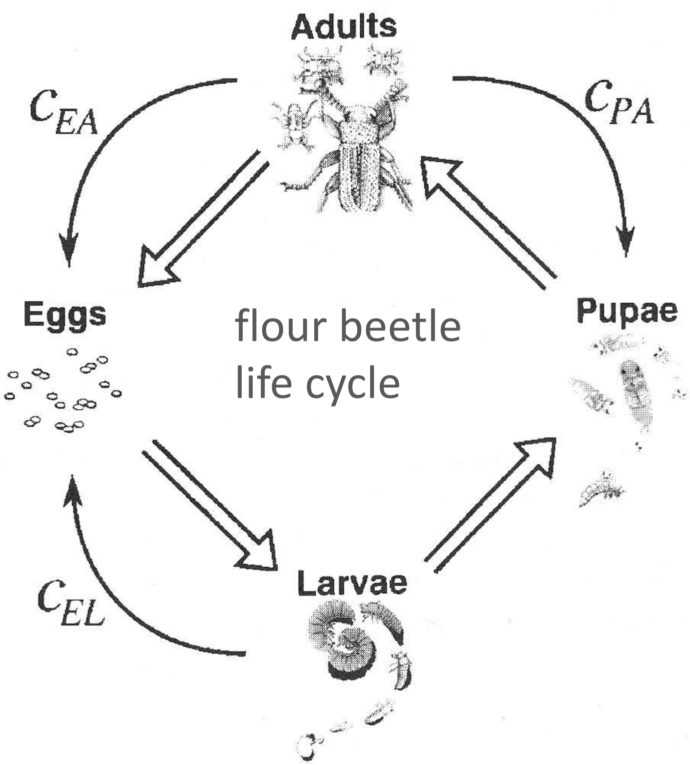
$$\frac{dI}{dt} = \beta IS - \gamma I$$

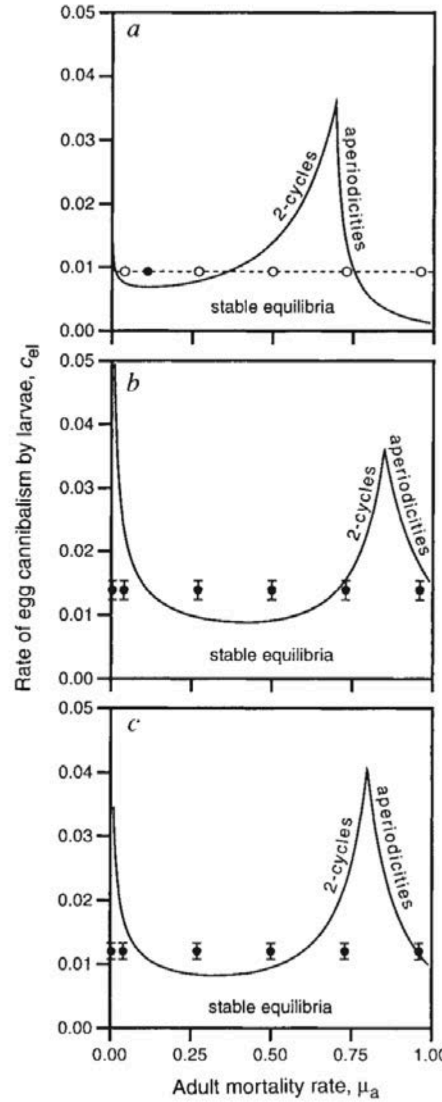
$$\frac{dR}{dt} = \gamma I$$

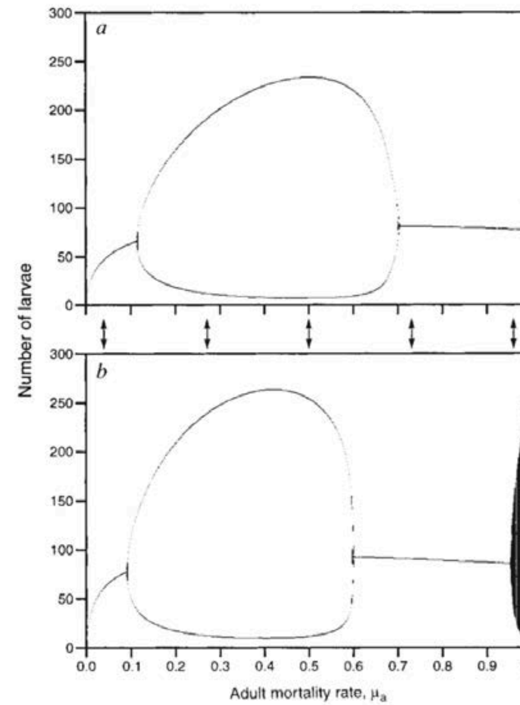
Motivation: Systems of differential equations

Discrete LPA Model (Cushing, Costantino, et al.)

$$L_{t+1} = bA_t \exp(-c_{el}L_t - c_{ea}A_t)$$
$$P_{t+1} = (1-\mu_l)L_t$$
$$A_{t+1} = P_t \exp(-c_{pa}A_t) + (1-\mu_a)A_t$$







→ Chaos!

Costatino et al. (1995)

Basic idea(s)

→ Differential equations are very common/useful tool in our toolbox....

In a nutshell, we are very good at describing how things *change*....

$$\frac{d\mathbf{y}}{dt} = f(t, \mathbf{y}) \tag{7.1.1}$$

... but less good at finding solutions to the the corresponding equations

Idea: Since equations tell us how things change, numerically integrate to find solution(s)

$$\frac{d\mathbf{y}}{dt} = f(t, \mathbf{y}) \quad \Rightarrow \quad \frac{\mathbf{y}_{n+1} - \mathbf{y}_n}{\Delta t} \approx f(t_n, \mathbf{y}_n). \tag{7.1.4}$$

Approximation:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta t \cdot f(t_n, \mathbf{y}_n). \tag{7.1.5}$$

Kutz (2013)

From the outset: General useful concepts/definitions

- Linear versus nonlinear → Very important distinction!
(we will get a sense of why throughout 2030)

- Slope fields

- Equilibria (i.e., fixed points) and stability

- Phase plane analysis (for systems of ODEs)

- Existence & uniqueness theorem (e.g., many ODEs that have solutions have an infinite number of them!)

- '*Initial condition*' versus '*boundary condition*' problems

→ For additional background, look into 'dynamical systems theory'
(e.g., http://en.wikipedia.org/wiki/Dynamical_system)

Ex.

Question: How fast does a person learn?

(very) Simple model: Rate a person learns = Percentage of task not yet learned

y is the percentage learned as a function of time t

$$\frac{dy}{dt} = 100 - y$$

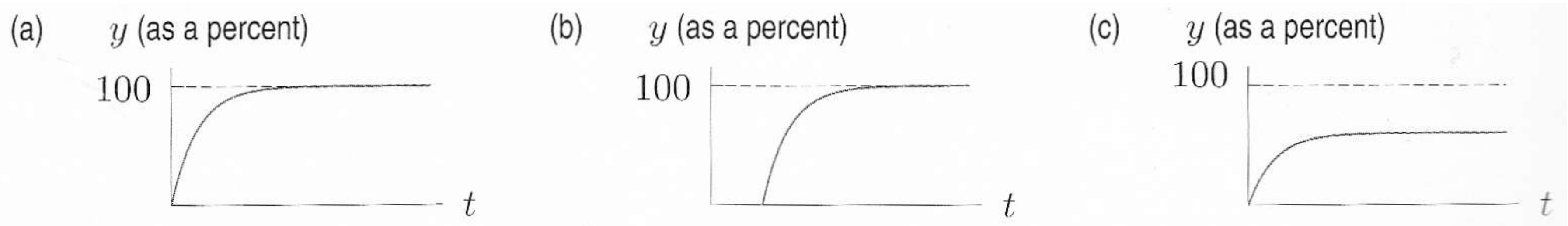


Figure 11.1: Possible graphs showing percentage of task learned, y, as a function of time, t

Solution
(e.g., via separation of variables)

$$y(t) = 100 - Ce^{-t}$$

Hughes-Hallett et al. (2005)

Ex.

$$\frac{dy}{dt} = 100 - y$$

$$y(t) = 100 - Ce^{-t}$$

→ Note that our 'model' (redundantly) allows for y greater than 100

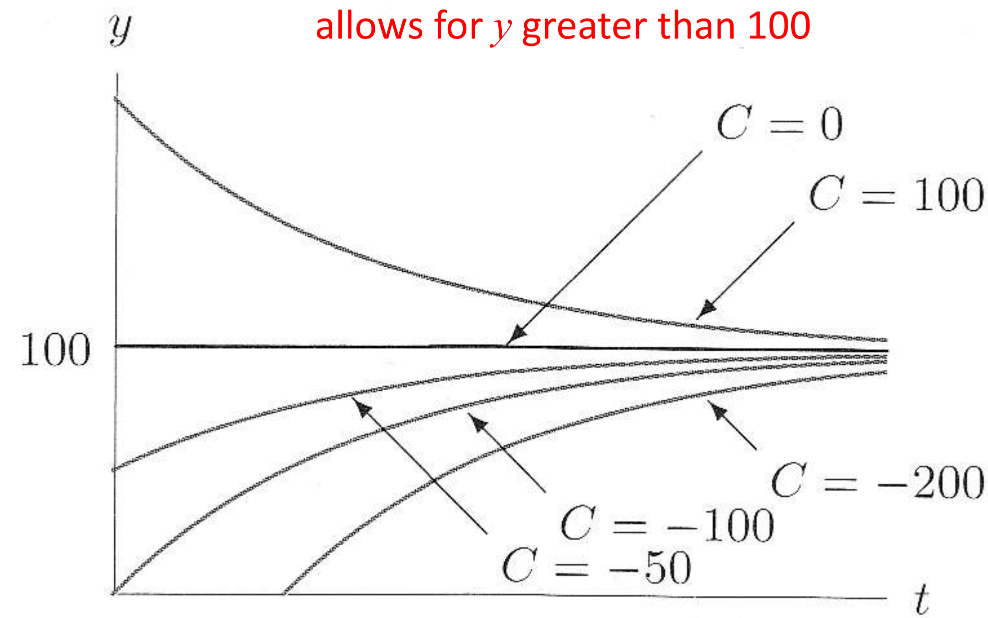


Figure 11.2: Solution curves for $dy/dt = 100 - y$: Members of the family $y = 100 + Ce^{-t}$

- Equilibrium points?

Values of $y(t)$ where $dy/dt = 0$

$y(t) = 100$

- Stability?

Do solutions move towards or away from the equilibrium if starting nearby?

stable (solution move towards $y(t) = 100$ with increasing t)

- What determines the value of C?

initial conditions (think about E&U theorem!)

Hughes-Hallett et al. (2005)

Some further common examples

Solution

Exponential growth/decay

$$\frac{dP}{dt} = kP$$

$$P = P_0 e^{kt}$$

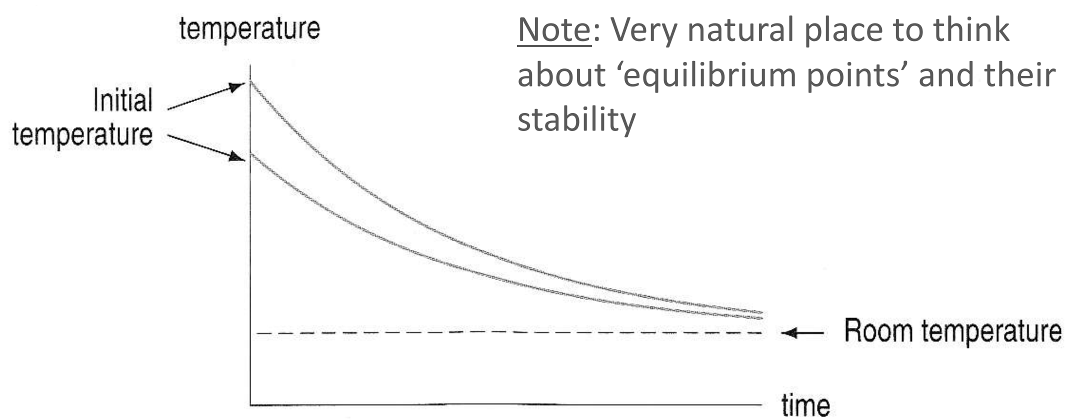
Newton's law of heating/cooling

"Newton proposed that the temperature of a hot object decreases at a rate proportional to the difference between its temperature and that of its surroundings. Similarly, a cold object heats up at a rate proportional to the temperature difference between the object and its surroundings."

$$\frac{dT}{dt} = \alpha(T_o - T)$$

Solution

$$T(t) = T_0 + Ce^{-\alpha t}$$



Note: Very natural place to think about 'equilibrium points' and their stability

Hughes-Hallett et al. (2005)

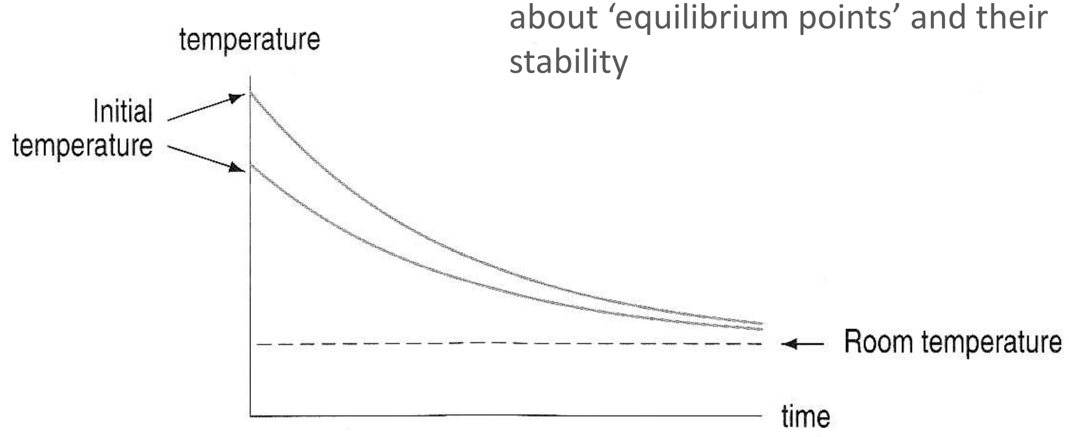
Stability

Newton's law of heating/cooling

$$\frac{dT}{dt} = \alpha(T_o - T)$$

Solution

$$T(t) = T_0 + Ce^{-\alpha t}$$



Note: Very natural place to think about 'equilibrium points' and their stability

- An **equilibrium solution** is constant for all values of the independent variable. The graph is a horizontal line.
- An equilibrium is **stable** if a small change in the initial conditions gives a solution which tends toward the equilibrium as the independent variable tends to positive infinity.
- An equilibrium is **unstable** if a small change in the initial conditions gives a solution curve which veers away from the equilibrium as the independent variable tends to positive infinity.

Hughes-Hallett et al. (2005)

<u>Post-class exercises</u>

- What is the difference between ordinary differential equations (ODEs) and partial differential equations (PDEs)?

When a murder is committed, the body, originally at 37°C, cools according to Newton's Law of Cooling. Suppose that after two hours the temperature is 35°C, and that the temperature of the surrounding air is a constant 20°C.

(a) Find the temperature, H, of the body as a function of t, the time in hours since the murder was committed.

(b) Sketch a graph of temperature against time.

(c) What happens to the temperature in the long run? Show this on the graph and algebraically.

(d) If the body is found at 4 pm at a temperature of 30°C, when was the murder committed?