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 2

Pop Quiz: Determine the derivative of the following functions

$$f(x) = x^3 + C$$

$$f(x) = 1/(x^3 + C)$$

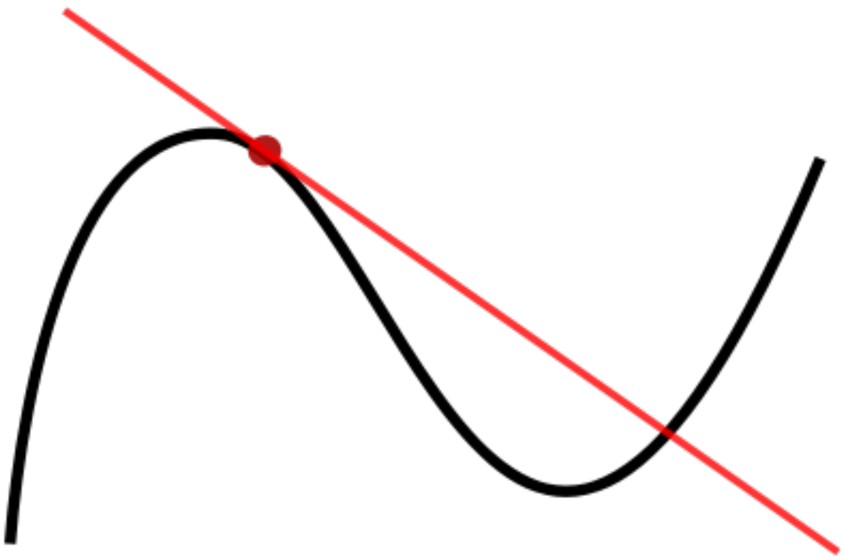
$$f(x) = \sin(x^3 + C)$$

$$f(x) = \arctan(x^3 + C)$$

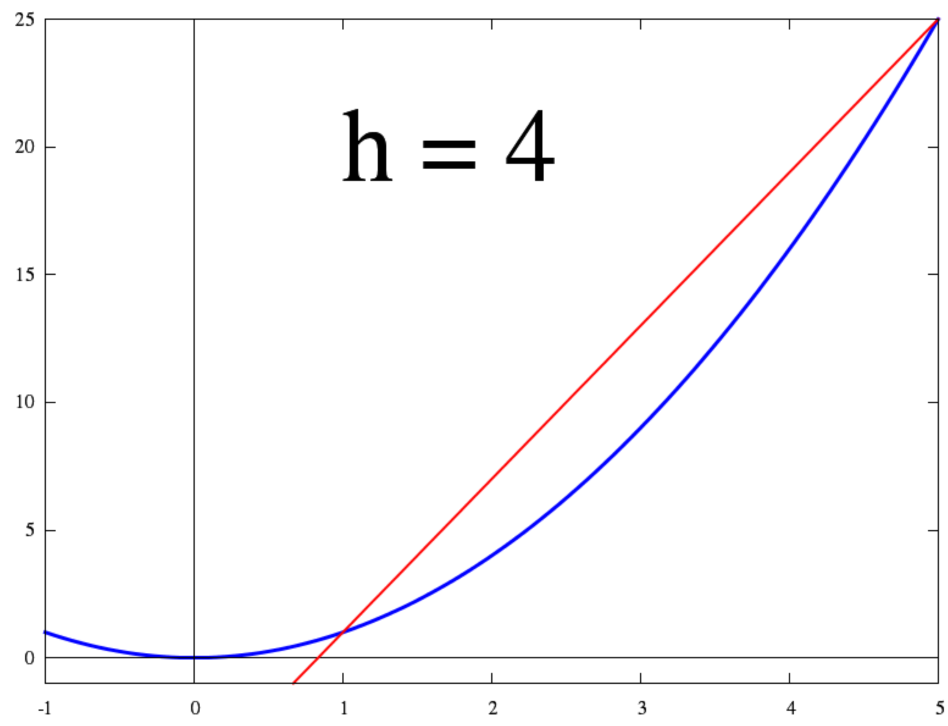
See how many you can do off the top of your head. Then, if you feel a burning need to use Google, count the number of keystrokes/clicks you use (i.e., minimize!)

Goal: Develop insight into numerical differentiation

- Consider some continuous and differentiable function $f(x)$



$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}.$$



Note: Here we are differentiating about some point (x=a)

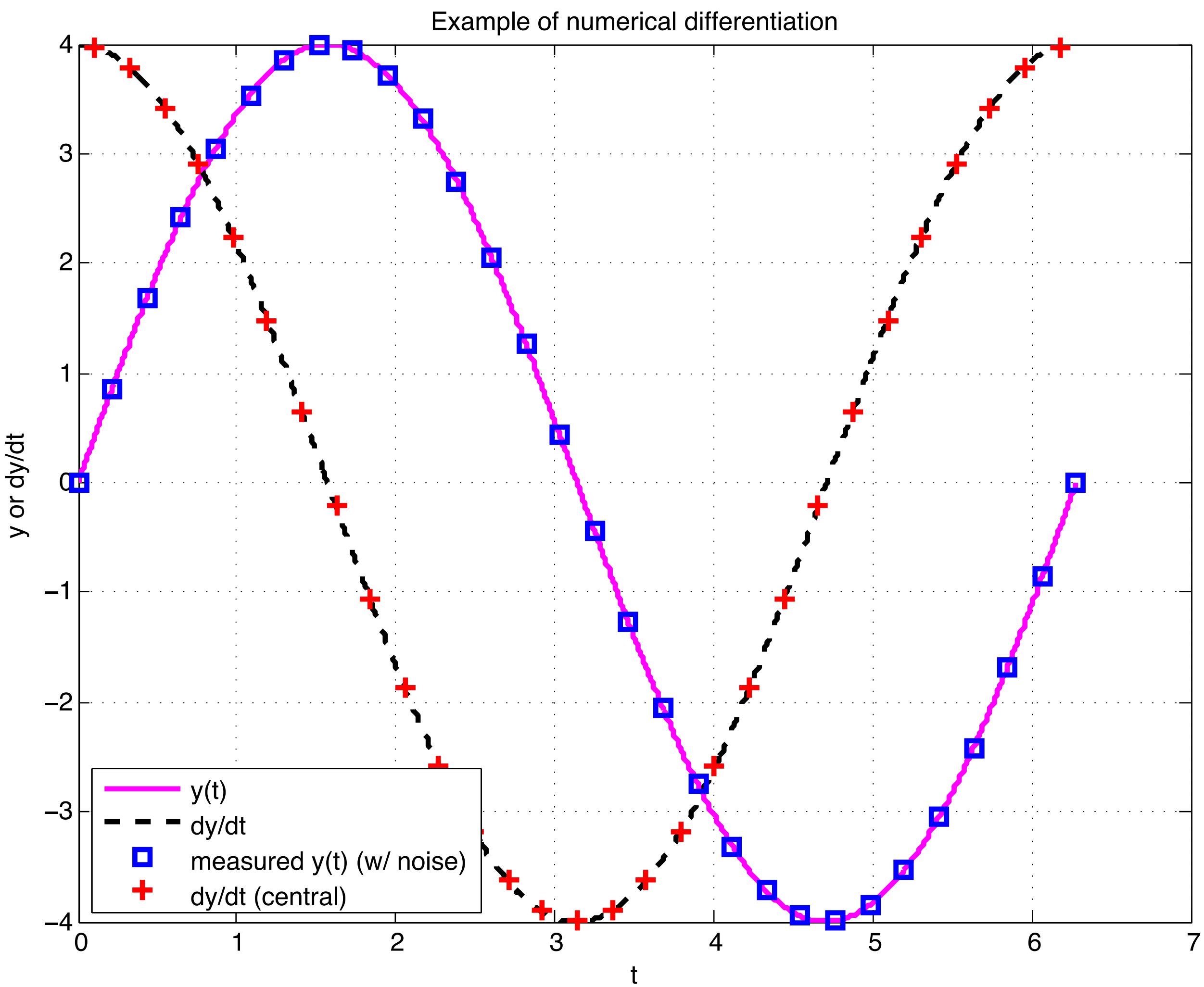
https://en.wikipedia.org/wiki/Derivative

```
% ### EXdiff1.m ###      09.04.14
% [source] http://ef.engr.utk.edu/ef230-2011-01/modules/matlab-integration/
% --> simple example of numerical differentiation compared to analytic solution
clear all; clf;
% --------------
% User parameters
np = 30; % number of points on a curve
Nfact= 0.00; % scale factor for additive noise
fType= 0; % choose function: 0-sinusoid, 1-arctan
% ----
% tStart= start point for time (ditto tEnd)
if fType==0
    func = @(t)4.*sin(t); % function
    dfunc = @(t)4.*cos(t); % derivative of function
    tStart= 0;  tEnd= 2*pi; loc= 'SouthWest';
elseif fType==1
    func = @(t)atan(t); % function
    dfunc = @(t)1./(1+t.^2); % derivative of function
    tStart= -2*pi;  tEnd= 2*pi; loc= 'NorthWest';
end
% ----
t = linspace(tStart,tEnd,np);  % determine time array
y = func(t)+ Nfact*randn(numel(t),1)';  % determined 'sampled' points (which can be noisy)
dydt = diff(y)./diff(t);    % compute derivative via numerical difference
% ----
% visualize
tt = linspace(tStart,tEnd,np*100);    % plot actual curve sans noise (oversample time here)
yy = func(tt);
plot(tt,yy,'m-','LineWidth',2); hold on; grid on;
yy = dfunc(tt);
plot(tt,yy,'k--','LineWidth',2);
plot(t,y,'bs','LineWidth',2);    % plot points and connecting lines
% central difference - plot numerical derivative at midpoint
ttCD = t(1:end-1) + diff(t)./2;
plot(ttCD,dydt,'r+','LineWidth',2,'MarkerSize',8);
xlabel('t'); ylabel('y or dy/dt'); title('Example of numerical differentiation');
legend('y(t)','dy/dt','measured y(t) (w/ noise)','dy/dt (central)','Location',loc);
```

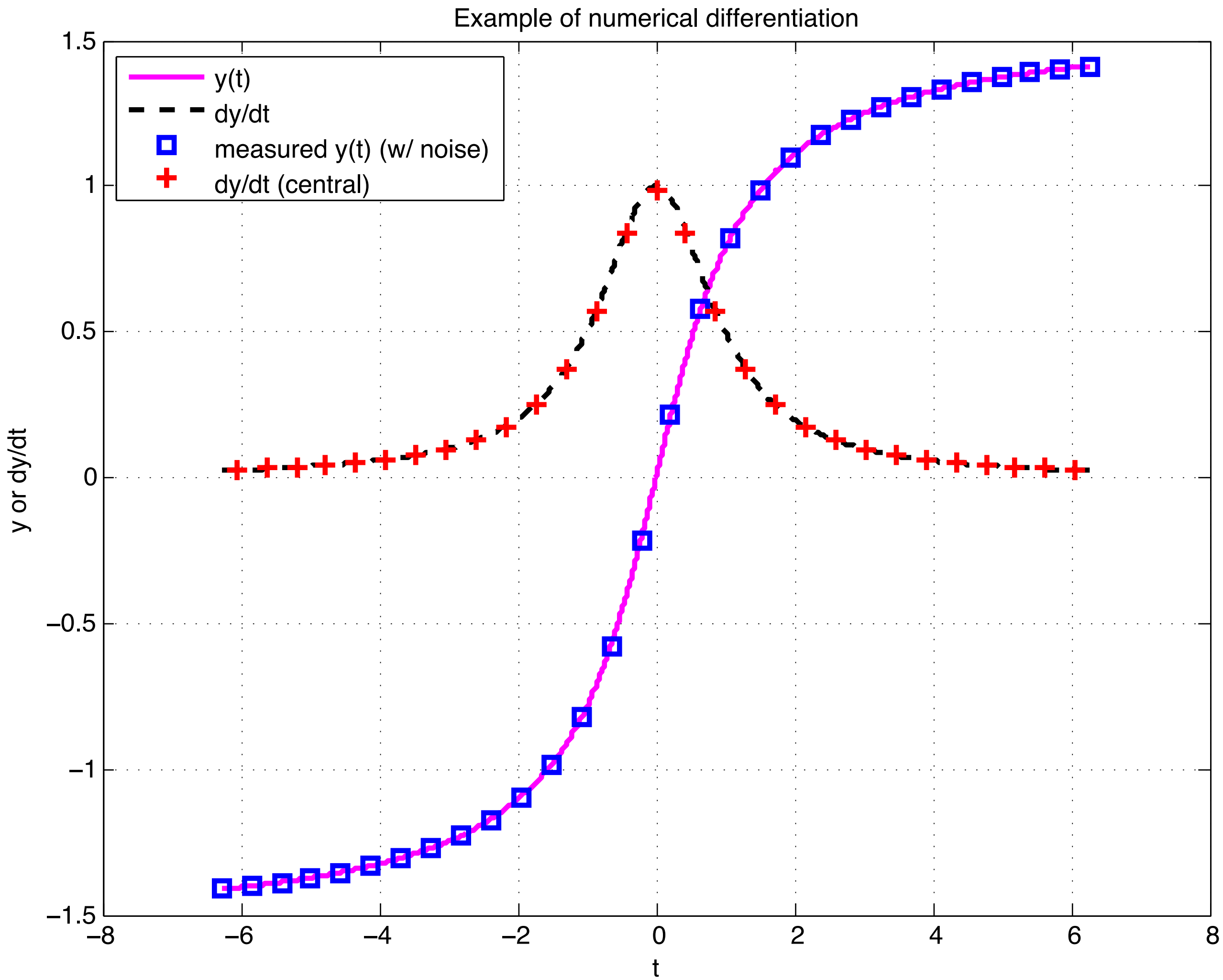
Very simple means to estimate slope

→ Where is that relevant line of code?

```
fType= 0;
```

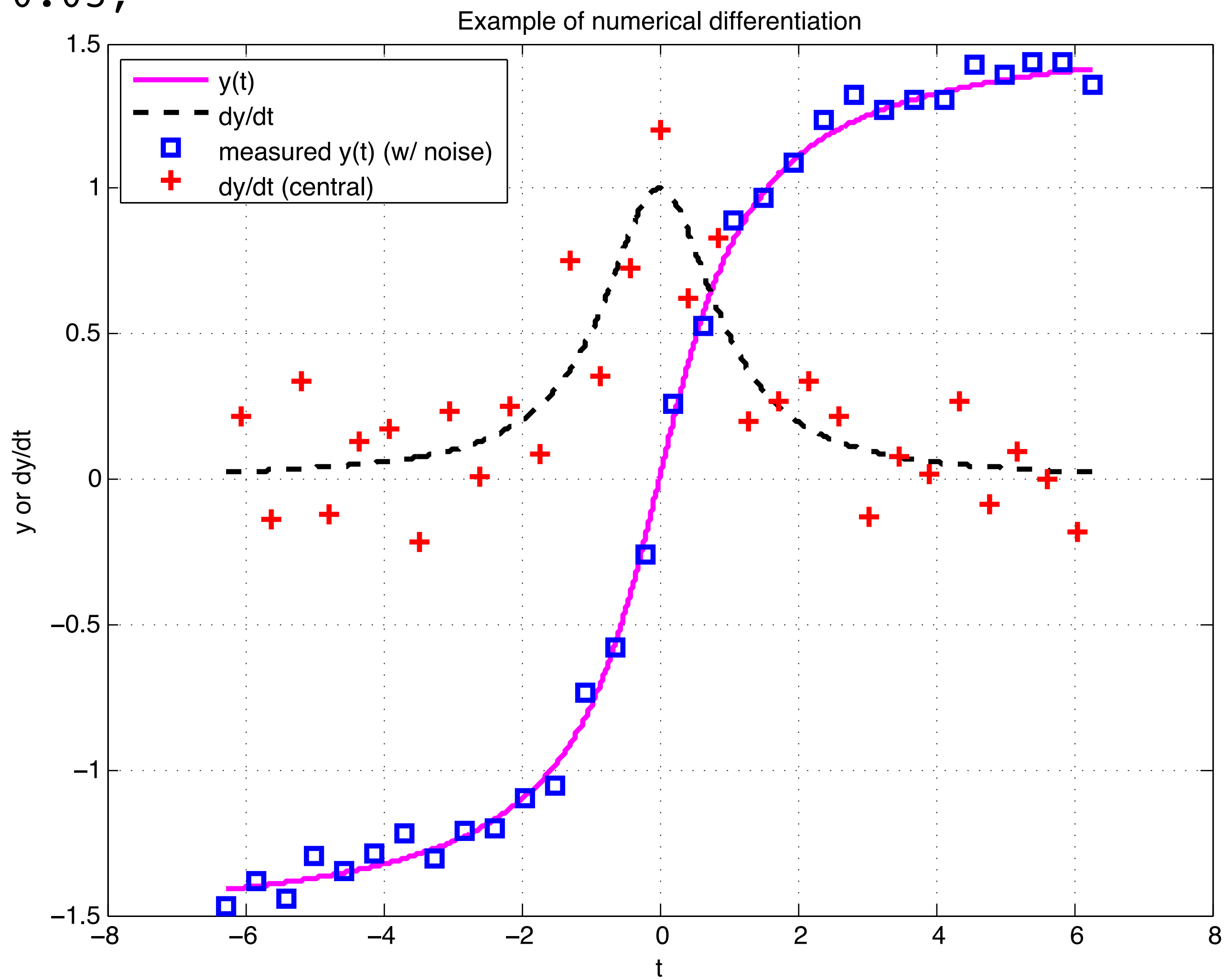

Example of numerical differentiation
4
3
2
1
0
−1
−2
−3
−4
y or dy/dt
0
1
2
3
4
5
6
7
t
y(t)
dy/dt
measured y(t) (w/ noise)
dy/dt (central)

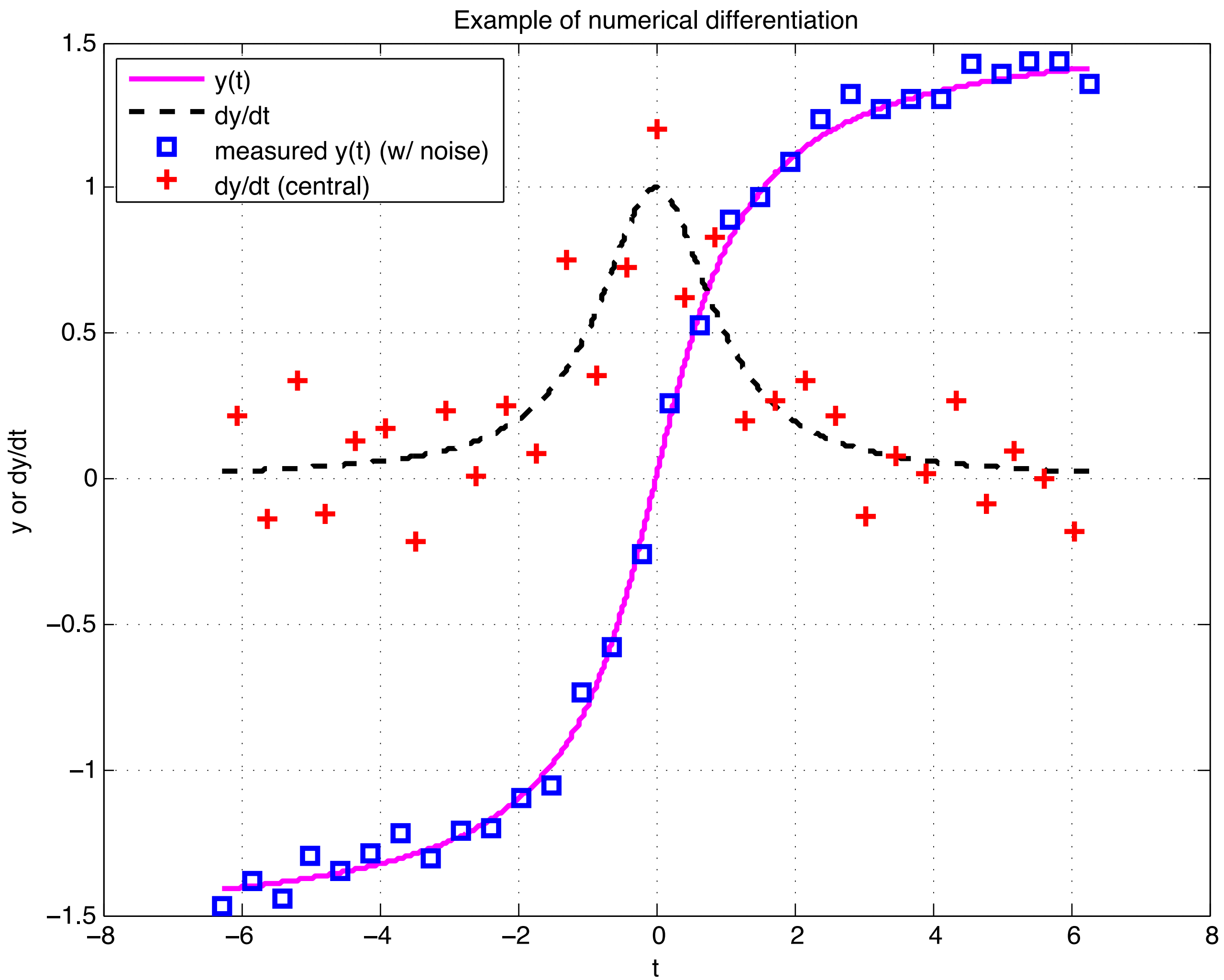
```
fType= 1;
```



Example of numerical differentiation
y(t)
dy/dt
measured y(t) (w/ noise)
dy/dt (central)
y or dy/dt
t
1.5
1
0.5
0
−0.5
−1
−1.5
−8
−6
−4
−2
0
2
4
6
8

```
fType= 1;
Nfact= 0.05;
```

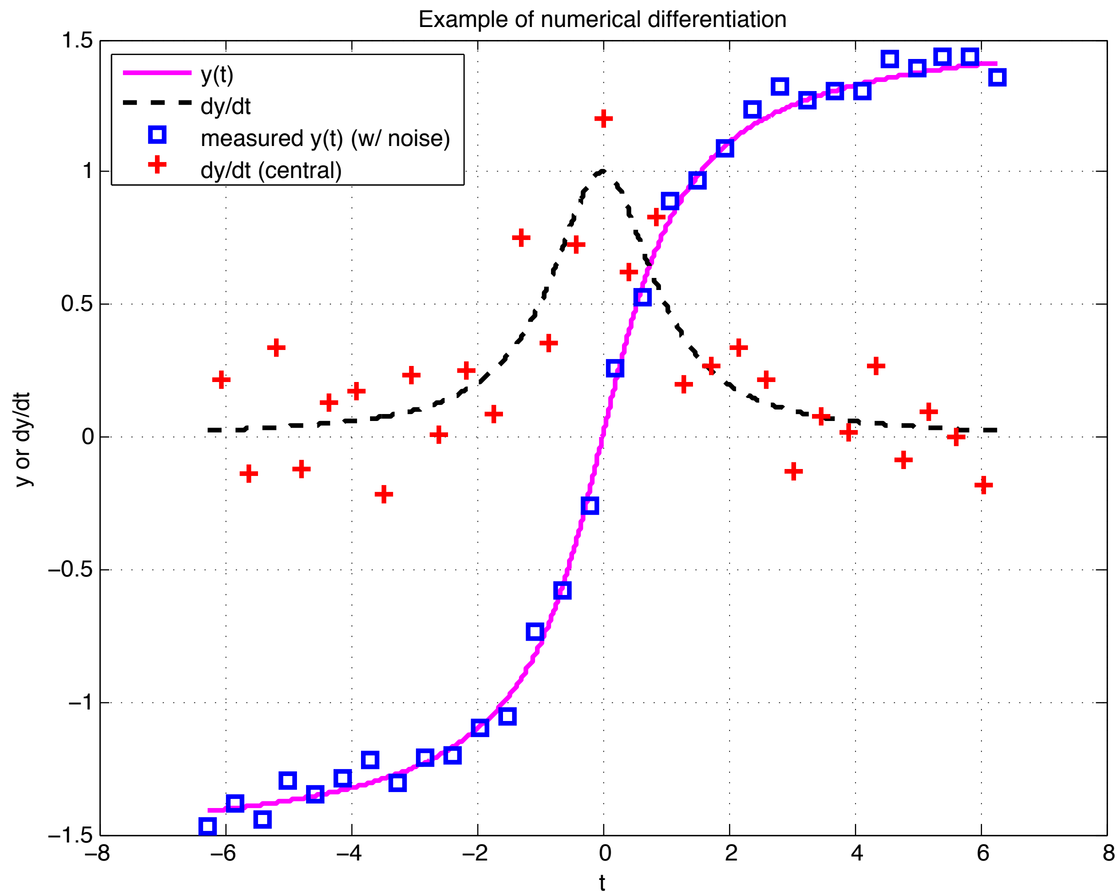




The “catch”:

(from the computational viewpoint):

- If we already know $f(x)$, we are all set (i.e., this is easy)
- But most of the time, we only have a discrete # of “data” from which we need to infer $f(x)$ (and thereby its derivative)
- Such can be heavily influenced by noise/uncertainty

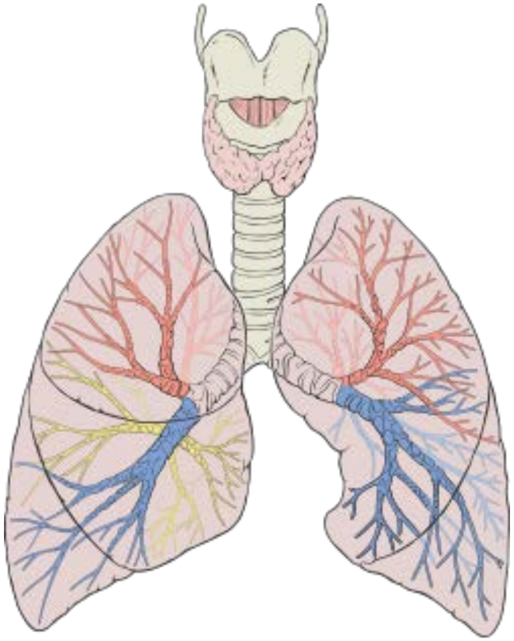


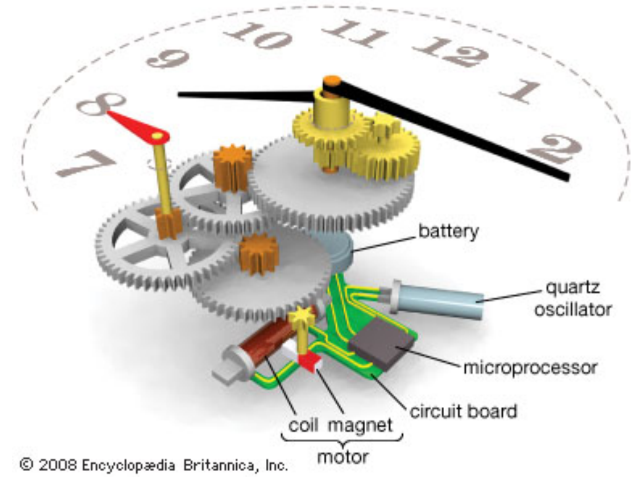
As we will see, your intuition is likely reversed:

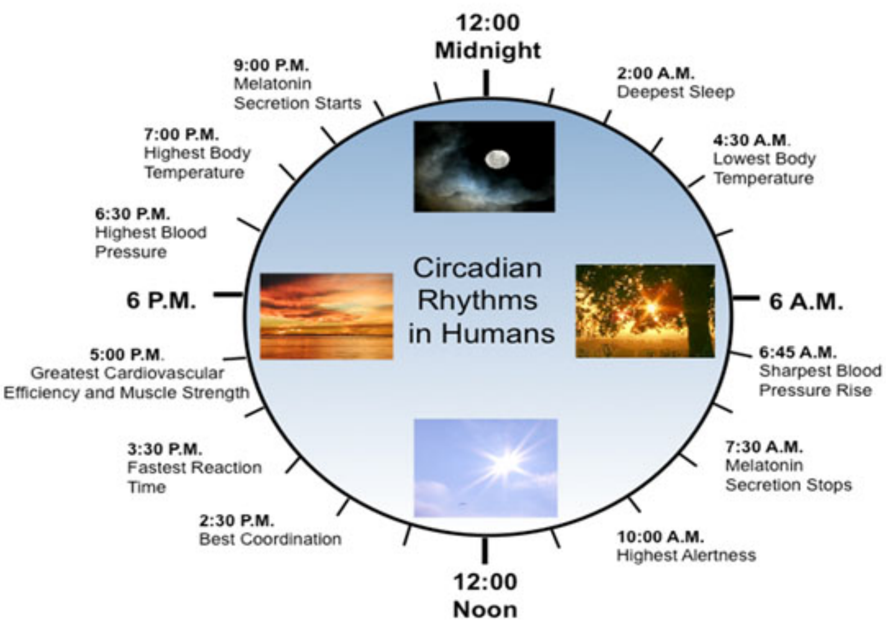
- Analytically, differentiation is 'easy' and integration is hard
- Numerically, the converse is true (differentiation = hard, integration = easy)

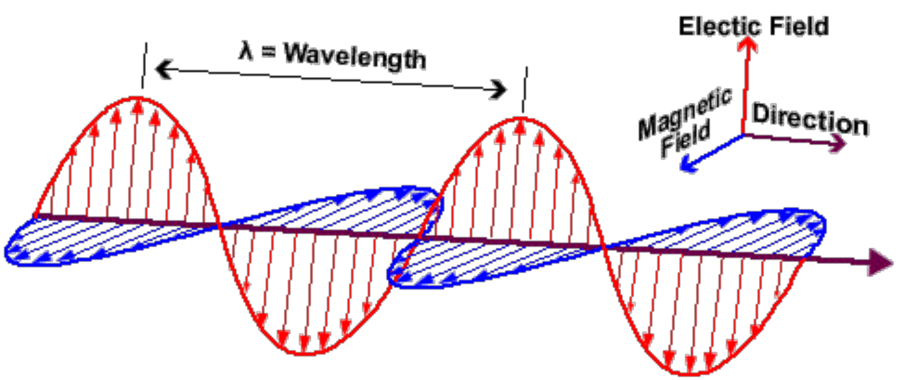
Goal: Develop insight into numerical differentiation

Things that oscillate....







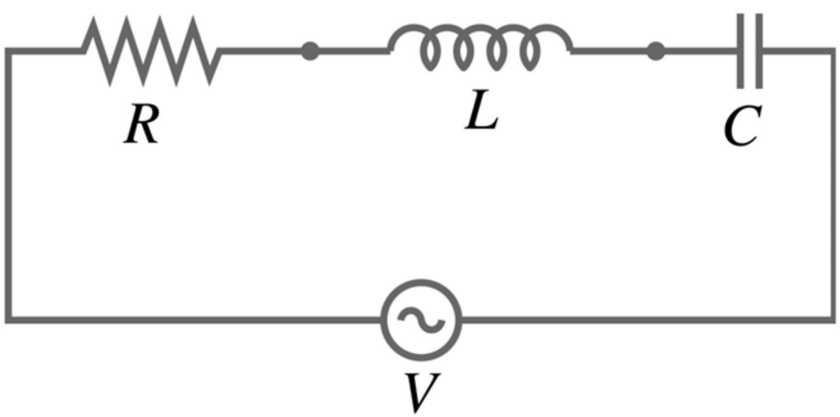


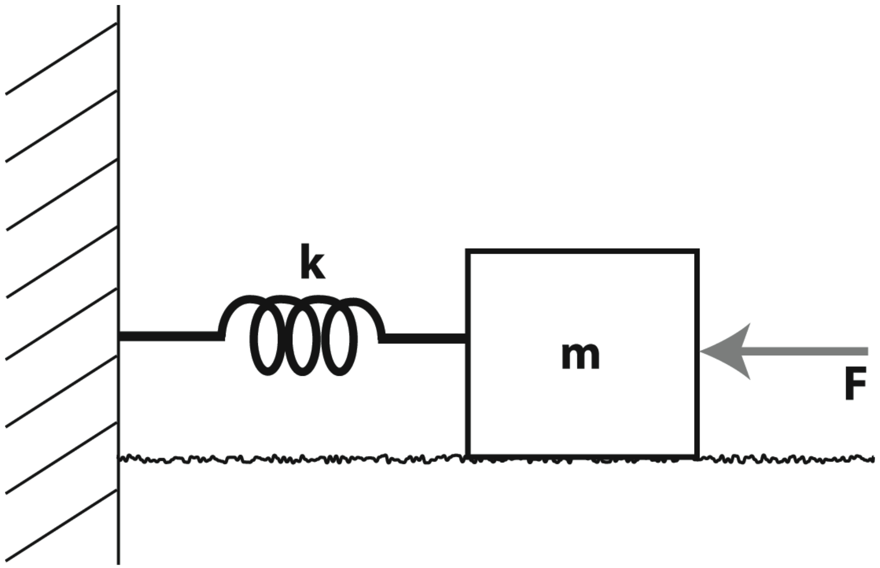
Things that oscillate....

Goal: Develop insight into numerical differentiation

→ We will use the harmonic oscillator as an (reoccurring) example

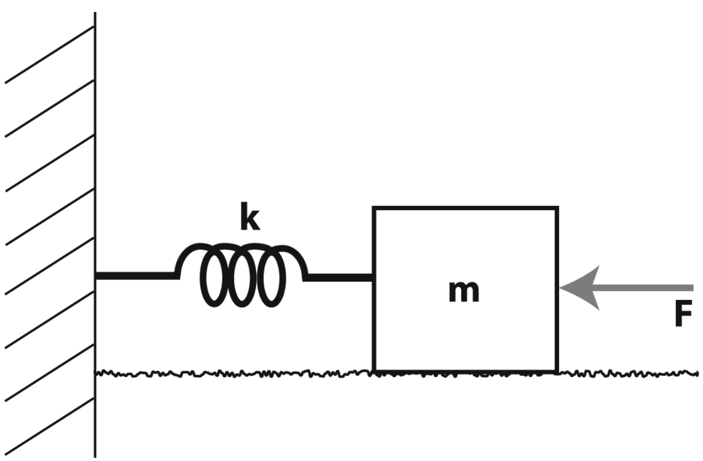
Ex. RLC circuit, mass-on-a-spring, quantum harmonic oscillator

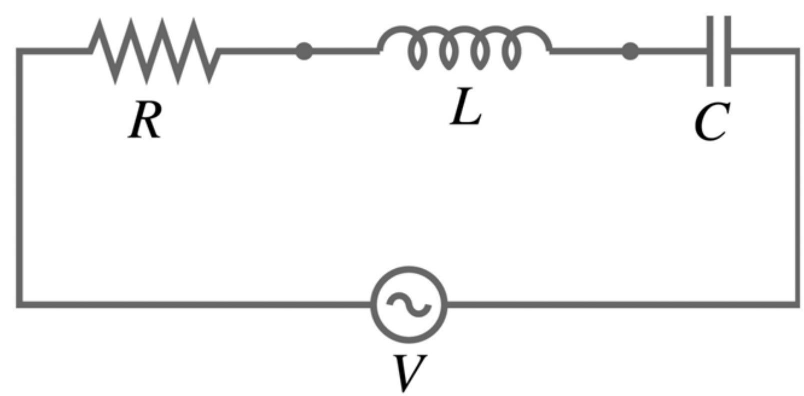




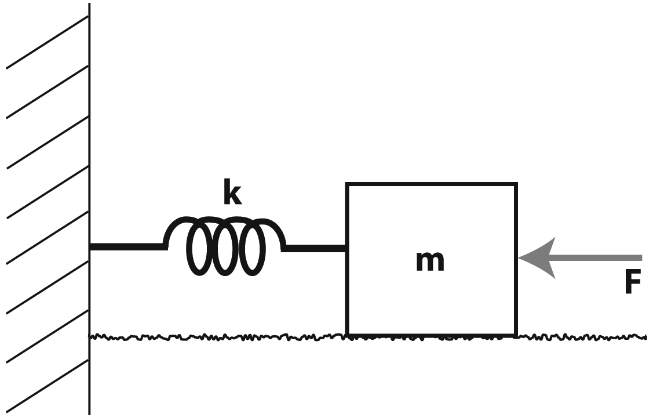
Ex. RLC circuit = Damped, Driven Harmonic Oscillator

Mechanical		Electrical	
F (force)	$\leftarrow\rightarrow$	V (potential)	state variables
v (velocity)	$\leftarrow\rightarrow$	I (current)	
x (position)	$\leftarrow\rightarrow$	q (charge)	
m (mass)	$\leftarrow\rightarrow$	L (inductance)	system properties
b (damping)	$\leftarrow\rightarrow$	R (resistance)	
k (spring)	$\leftarrow\rightarrow$	$1/C$ (capacitance)	





Theoretical considerations



Simplest case: Undamped, Undriven

$$F = ma = m\ddot{x} = -kx$$

Newton's Second Law
Hooke's Law

$$\ddot{x} + \frac{k}{m}x = 0$$

Second order ordinary differential equation
(no need worrying about how to "solve", yet...)

$$x(t) = A\cos\left(\omega_o t + \phi\right)$$

$\Rightarrow$ Solution is oscillatory!

$$\omega_o = \sqrt{k/m}$$

System has a *natural* frequency

Resonance

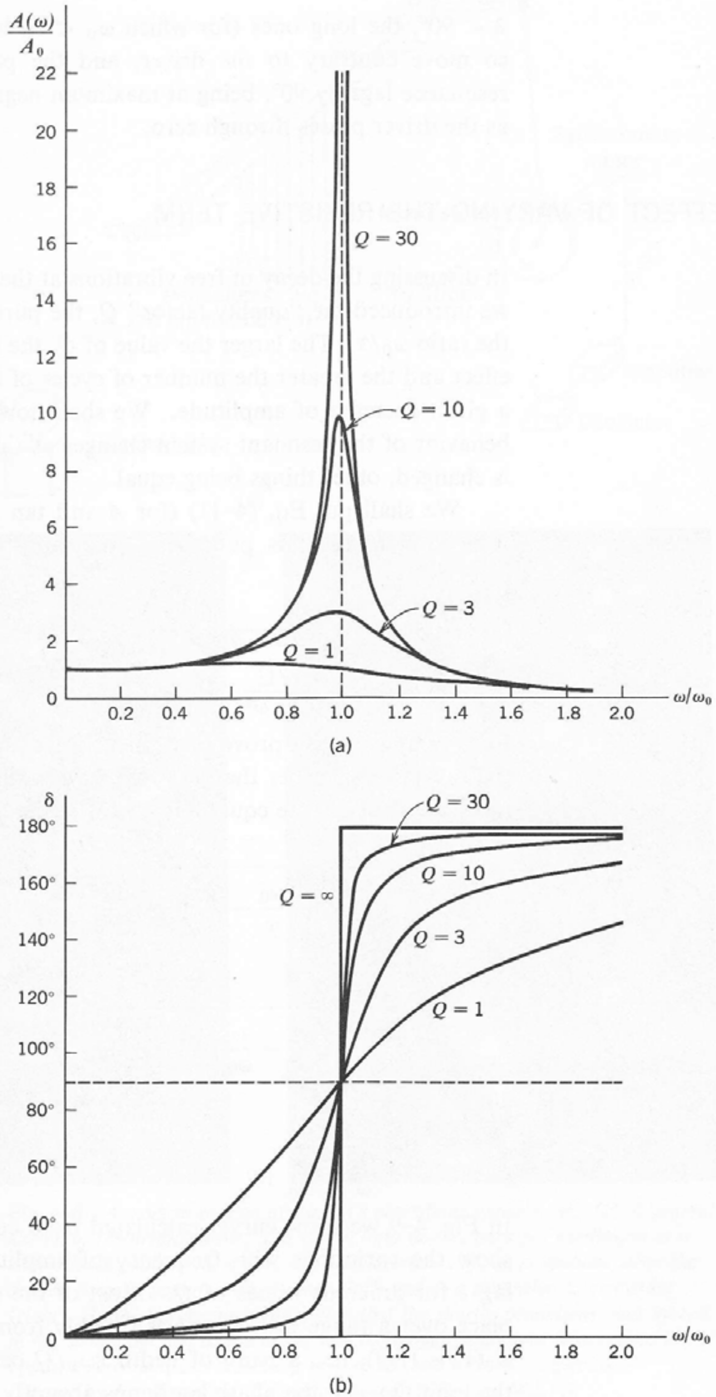


Fig. 4–9 (a) Amplitude as function of driving frequency for different values of Q, assuming driving force of constant magnitude but variable frequency. (b) Phase difference δ as function of driving frequency for different values of Q.

Steady-state frequency response

Consider the sinusoidally "driven" case:

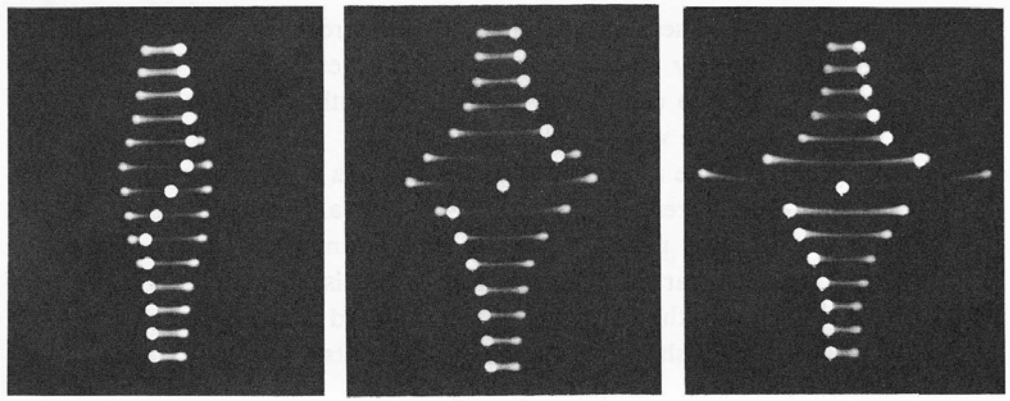
$$\ddot{x} + \gamma\dot{x} + \omega_o^2 x = \frac{F_o}{m} e^{i\omega t}$$

$$Q = \omega_o / \gamma$$

Q is the 'quality factor'

- The "system" stores energy, and more of it when driven near the natural frequency
- Less damping (i.e., higher Q) means more energy stored

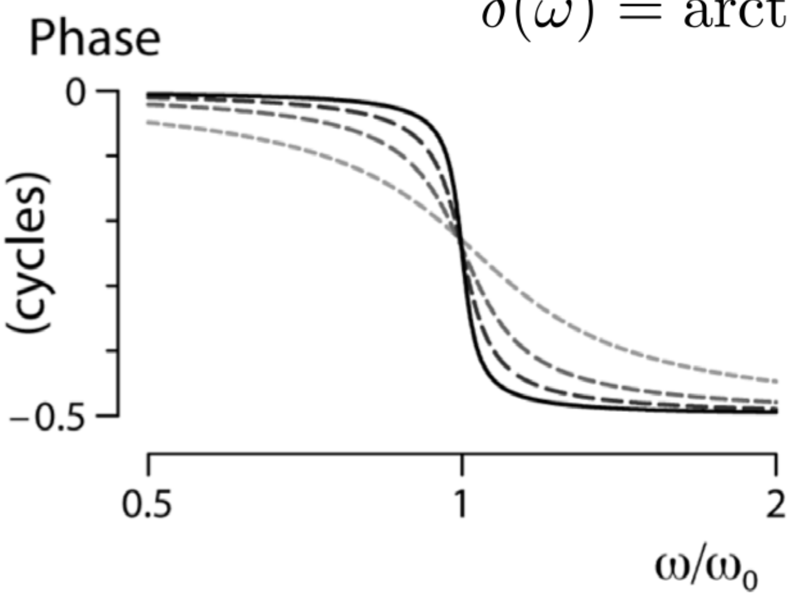
French (1971)



$$\ddot{x} + \gamma\dot{x} + \omega_o^2 x = \frac{F_o}{m}e^{i\omega t}$$

$$\delta(\omega) = \arctan\left(\frac{\gamma\omega}{\omega^2 - \omega_o^2}\right)$$

$N \equiv f_0$ * phase slope
(group delay)

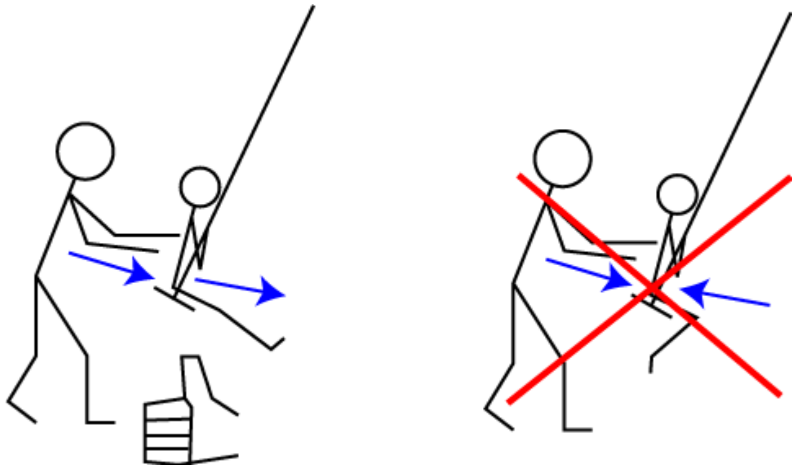


$\boxed{N \propto 1/\gamma}$

$\Rightarrow$ Characterizing phase slope near resonance provides measure of damping

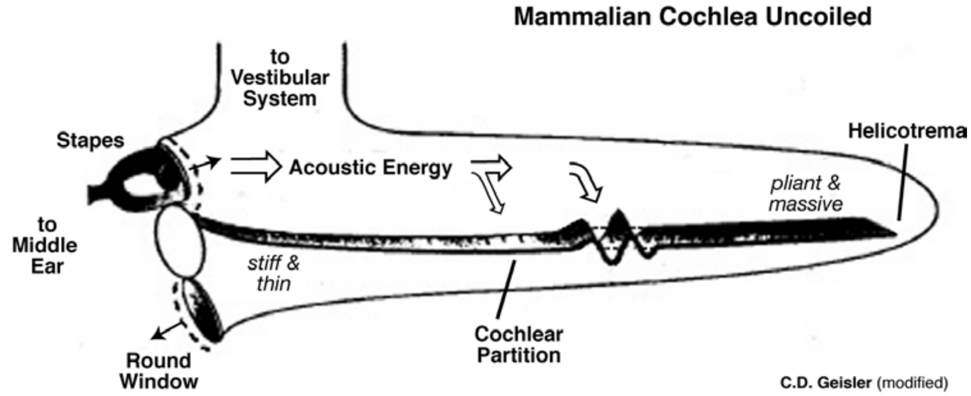
See “appendix” of these slides re some basic theory more fully fleshed out….
(this theory will be helpful/relevant well beyond this lecture, as we will return to this often as we explore different computational topics)

Resonance - Examples



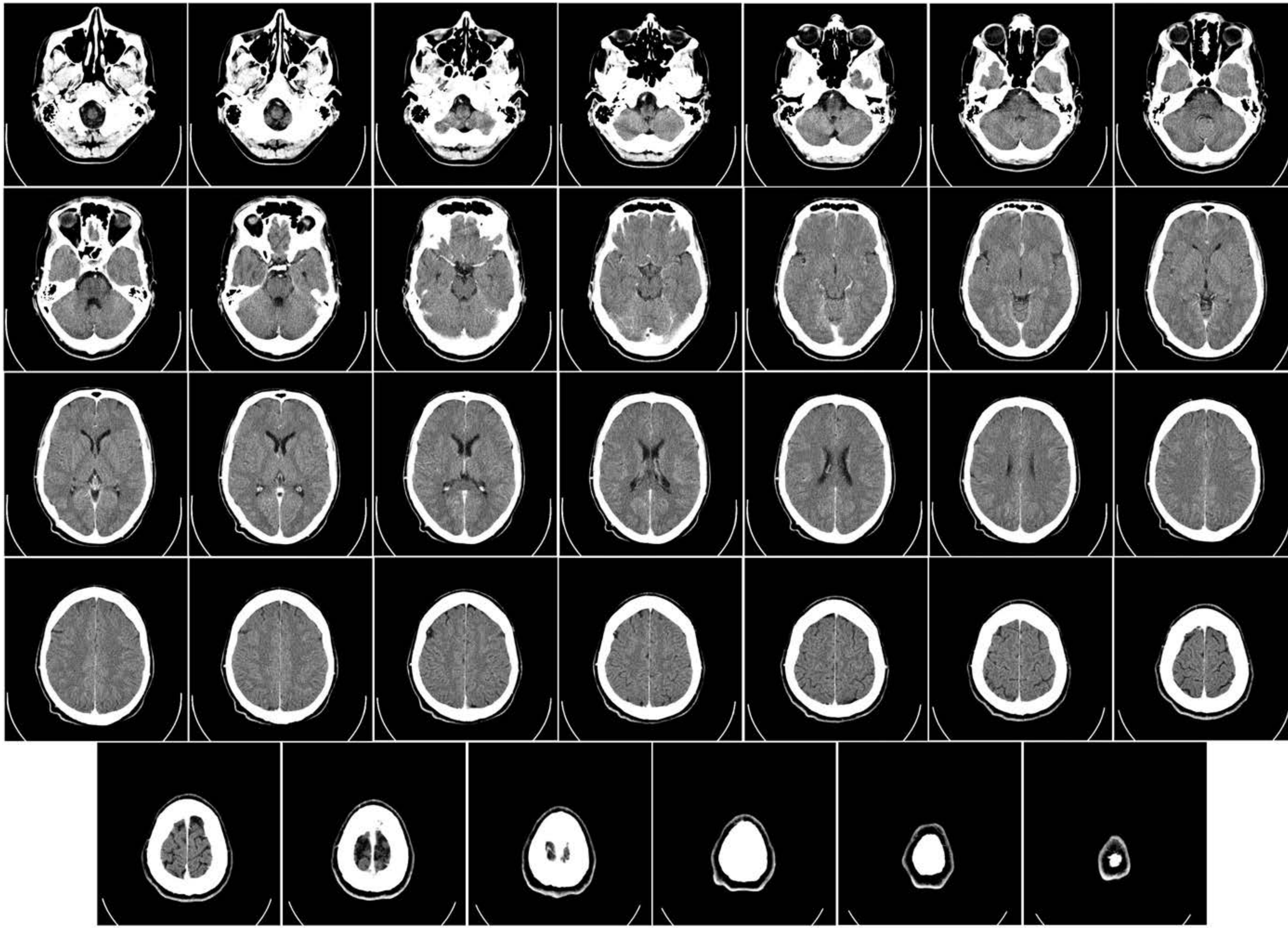
http://physics.stackexchange.com/questions/159728/forced-oscillations-resonance

"Tonotopy" of the inner ear



Slightly different type of "resonance"...

MRI



Wikipedia

Wikipedia

Practical example: MEMS (**M**icro**e**lectro**m**echanical **s**ystems)

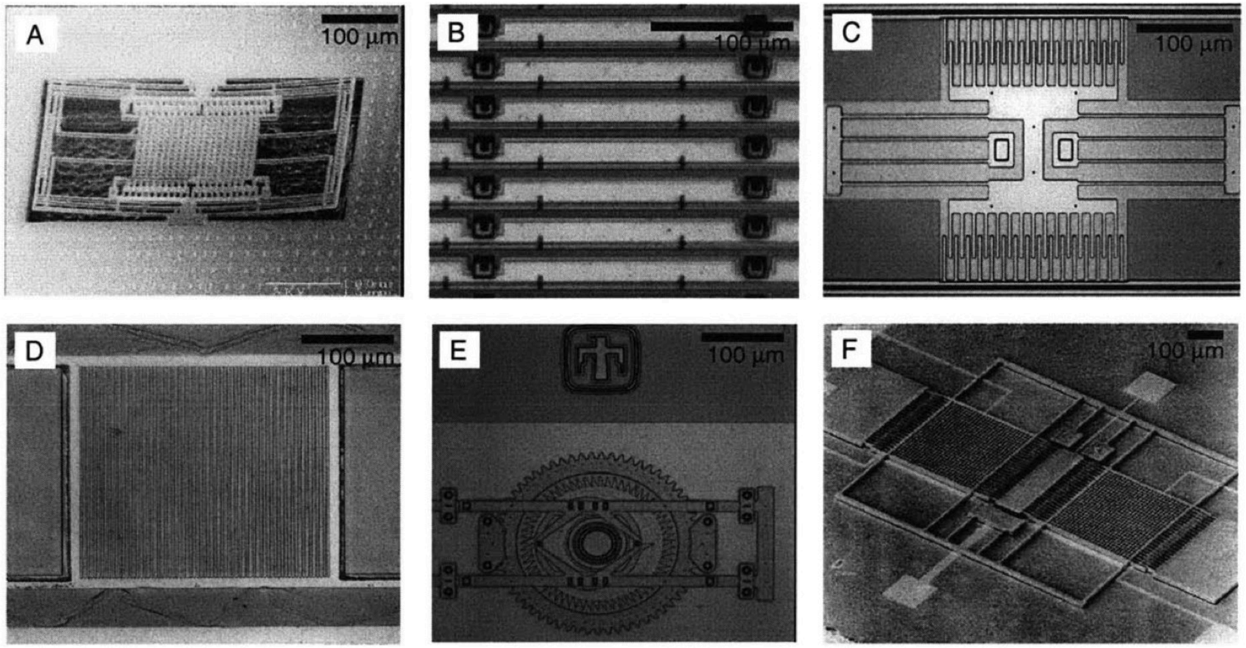
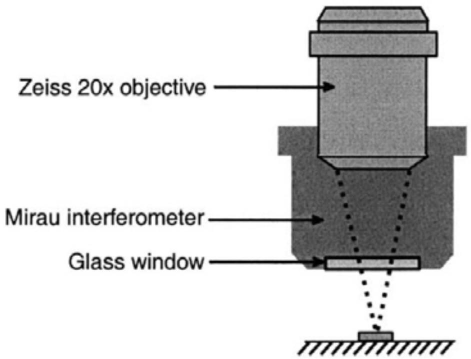


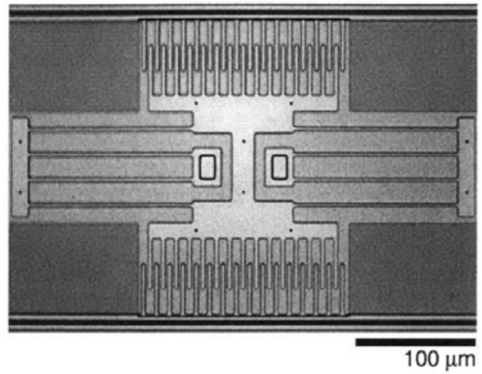
Figure 1-1: Microelecromechanical systems encompassing a wide variety of applications and a broad spectrum of fabrication processes: (A) SEM image of CMOS MEMS (Fedder et al., 1996) multiple degree-of-freedom microresonator fabricated at Carnegie Mellon University, (B) Optical micrograph of surface micromachined polysilicon diffraction gratings fabricated at the State University of New York at Albany, (C) Optical micrograph of surface micromachined lateral resonator fabricated using Cronos MUMPs, (D) Optical micrograph of platinum diffraction gratings fabricated at the Massashusetts Institute of Technology, (E) Optical micrograph of indexing motor fabricated using Sandia SUMMiT4 fabrication process, and (F) SEM image of Draper Laboratory tuning fork gyroscope (SEM picture courtesy Charles Stark Draper Laboratory, Cambridge MA).

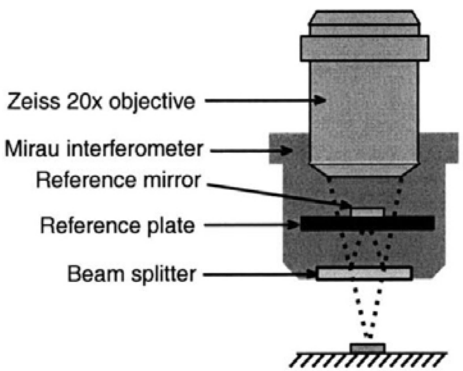
$\Rightarrow$ Resonant behavior

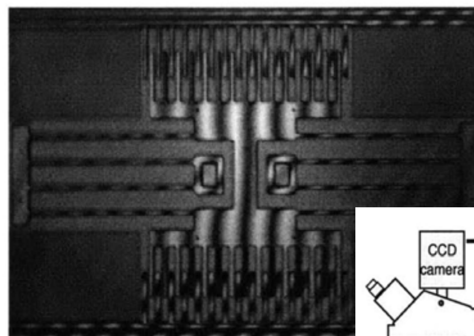
http://dspace.mit.edu/handle/1721.1/87312#files-area

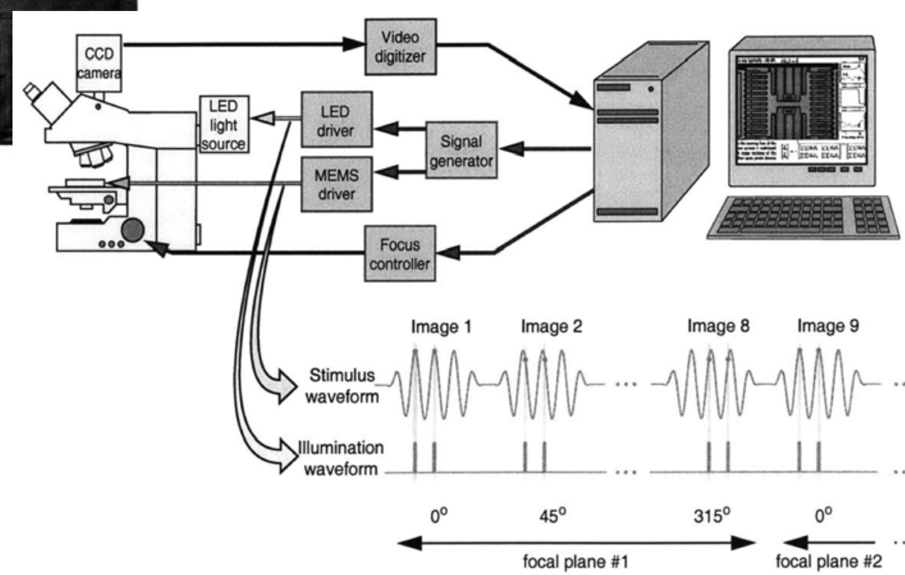
Practical example: MEMS (**M**icro**e**lectro**m**echanical **s**ystems)











$\Rightarrow$ Stroboscopic imaging allows dynamics to be characterized

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Practical example: MEMS (**M**icro**e**lectro**m**echanical **s**ystems)

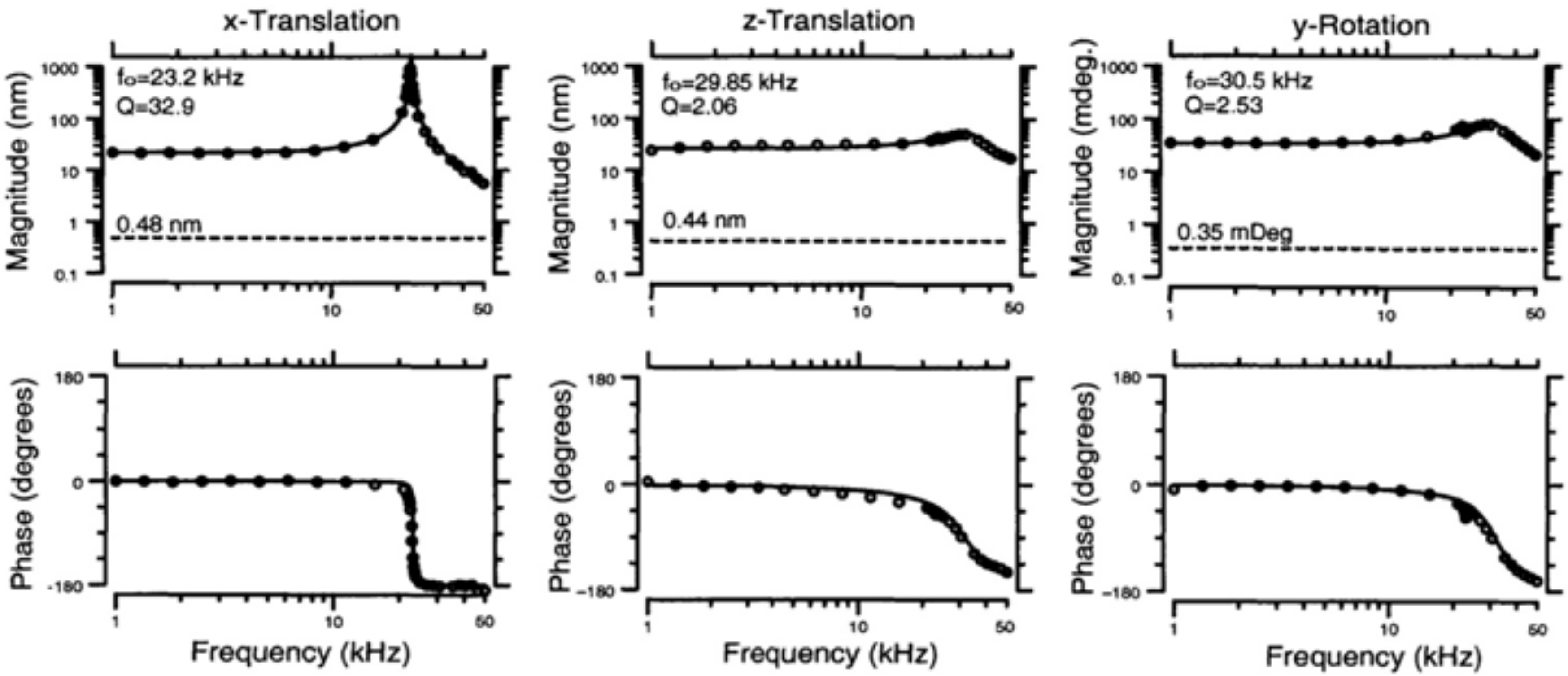

Figure 4-5: Magnitude and phase of frequency response for translation along x (left panel), translation along z (center panel), and rotation about y (right panel)

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Practical example: MEMS (**M**icro**e**lectro**m**echanical **s**ystems)

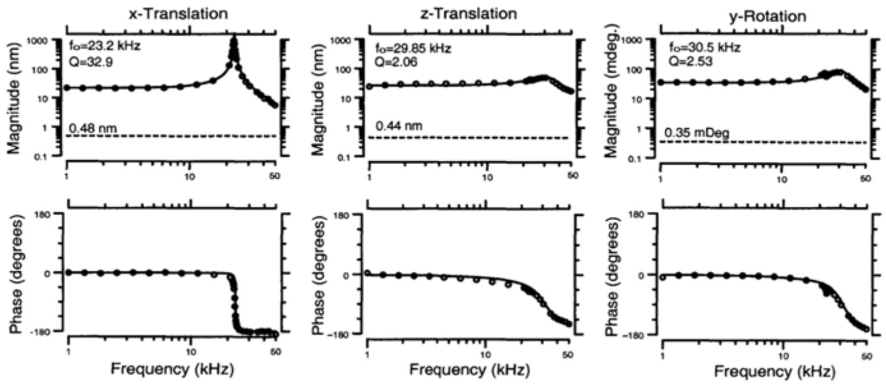
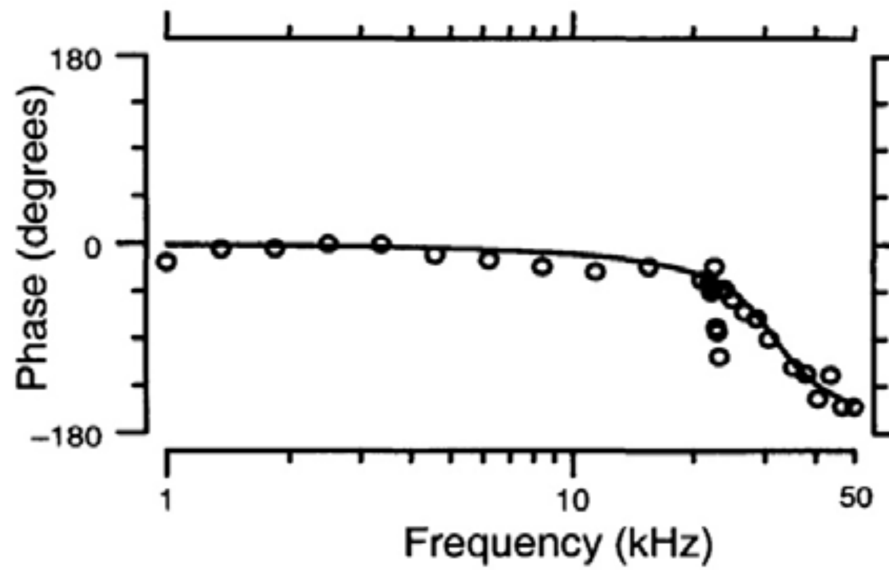


Figure 4-5: Magnitude and phase of frequency response for translation along x (left panel), translation along z (center panel), and rotation about y (right panel)

$\Rightarrow$ Characterizing phase slope near resonance provides measure of damping



Question: Can we effectively quantify the amount of damping in the MEMs device from these data?

http://dspace.mit.edu/handle/1721.1/87312#files-area

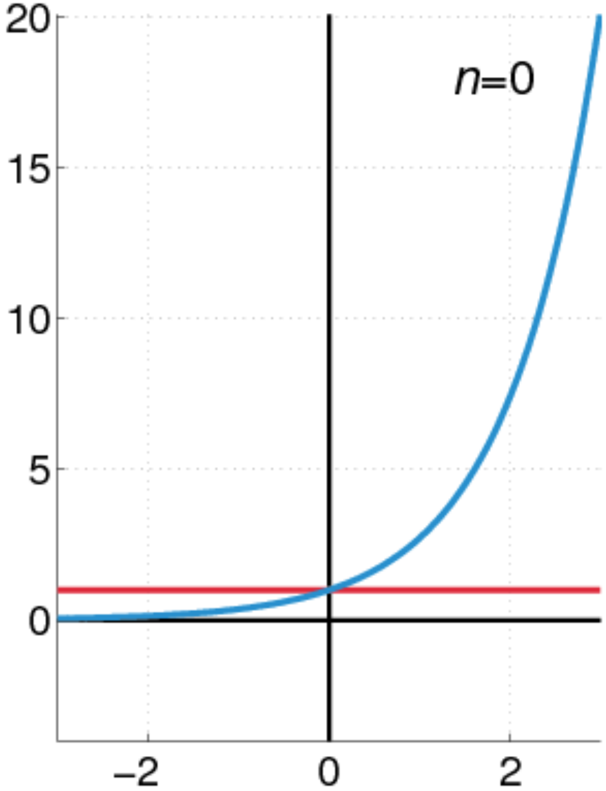
Numerical differentiation: Basics

Derivative (by definition)

$$\frac{df(t)}{dt} = \lim_{\Delta t \to 0} \frac{f(t+\Delta t) - f(t)}{\Delta t}. \tag{4.1.1}$$

Taylor series (by definition)

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \dots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \dots.$$



→ Think of a Taylor series as a means to 'transform' a (continuously differentiable) function into an infinite series of polynomials. Put more generally, you are specifying an alternative way of describing things.

The exponential function e^x (in blue), and the sum of the first n+1 terms of its Taylor series at 0 (in red).

Kutz (2013)
https://en.wikipedia.org/wiki/Taylor_series

Numerical differentiation: Basics

Derivative (by definition)

$$\frac{df(t)}{dt} = \lim_{\Delta t \to 0} \frac{f(t+\Delta t) - f(t)}{\Delta t}. \qquad (4.1.1)$$

Simple approximation of the first derivative

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Taylor series expansion about x

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi)$$

Note: This equality is not strictly true!

Note: We are making some assumptions about $f(x)$ (e.g., differentiability, continuity)

"Forward difference"

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi)$$

Note: Only including lowest order terms from Taylor series (quadratic captures the "error" or the truncation term)

Kutz (2013)
http://www2.math.umd.edu/~dlevy/classes/amsc466/lecture-notes/differentiation-chap.pdf

Numerical differentiation: Basics

"Forward difference"

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi)$$

Can also go the "other way"...

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

"Backward difference"

... or better yet, both ways(!)

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

"Centered difference"

Let's firm up this last step a bit and see what implications arise....

Consider two nearby time steps:

$$f(t+\Delta t) = f(t) + \Delta t \frac{df(t)}{dt} + \frac{\Delta t^2}{2!}\frac{d^2 f(t)}{dt^2} + \frac{\Delta t^3}{3!}\frac{d^3 f(c_1)}{dt^3} \tag{4.1.2a}$$

$$f(t-\Delta t) = f(t) - \Delta t \frac{df(t)}{dt} + \frac{\Delta t^2}{2!}\frac{d^2 f(t)}{dt^2} - \frac{\Delta t^3}{3!}\frac{d^3 f(c_2)}{dt^3} \tag{4.1.2b}$$

Difference between them is:

$$f(t+\Delta t) - f(t-\Delta t) = 2\Delta t \frac{df(t)}{dt} + \frac{\Delta t^3}{3!}\left(\frac{d^3 f(c_1)}{dt^3} + \frac{d^3 f(c_2)}{dt^3}\right). \tag{4.1.3}$$

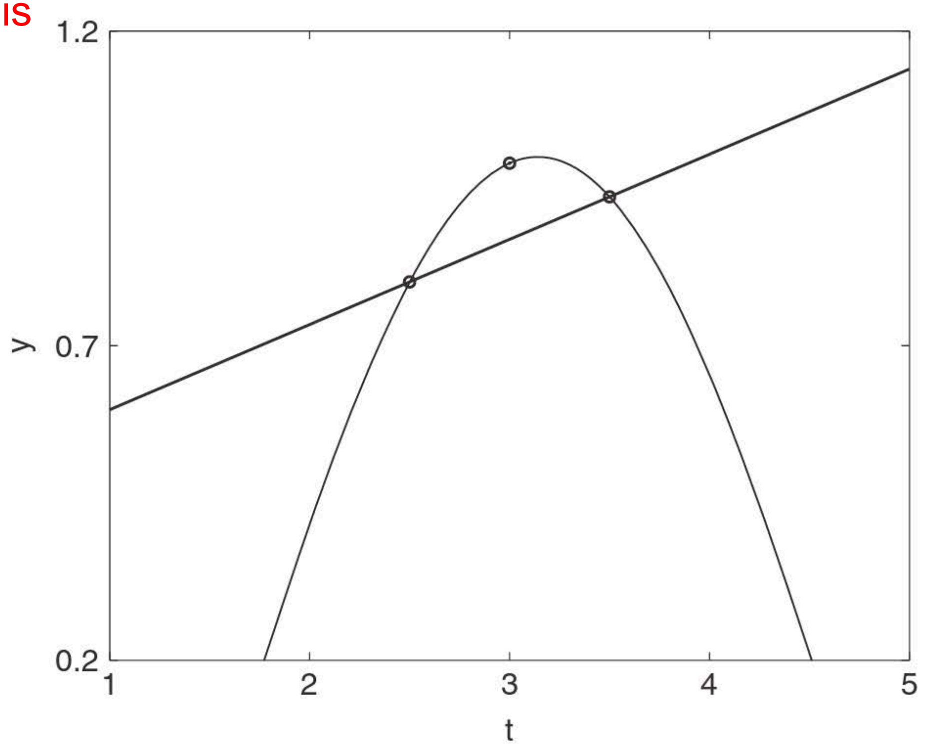
Kutz (2013)
http://www2.math.umd.edu/~dlevy/classes/amsc466/lecture-notes/differentiation-chap.pdf

Numerical differentiation: Basics

$$\frac{df(t)}{dt} = \frac{f(t+\Delta t) - f(t-\Delta t)}{2\Delta t} - \frac{\Delta t^2}{6}\frac{d^3 f(c)}{dt^3}$$

Since time step is small, higher terms become relatively small (but not necessarily negligible!)

Note: This equality is not strictly true!



Note: When using cenetered differences, the quadratic error term subtracted out!

Figure 4.1: Graphical representation of the second-order accurate method for calculating the derivative with finite differences. The slope is simply rise over run where the nearest neighbors are used to determine both quantities. The specific function considered is $y = -\cos(t)$ with the derivative being calculated at $t = 3$ with $\Delta t = 0.5$.

Kutz (2013)

Back to our resonator: $$\delta(\omega) = \arctan\left(\frac{\gamma\omega}{\omega^2 - \omega_o^2}\right)$$

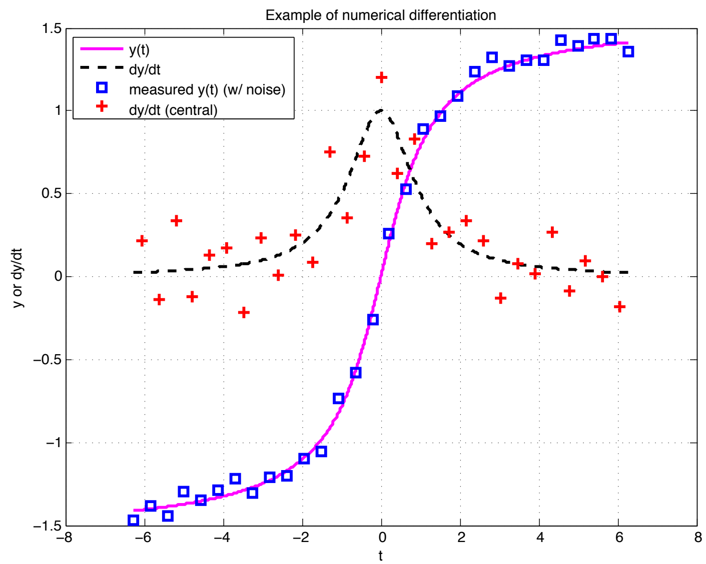
For simplicity, consider: $$\delta(\omega) = \arctan(\omega)$$

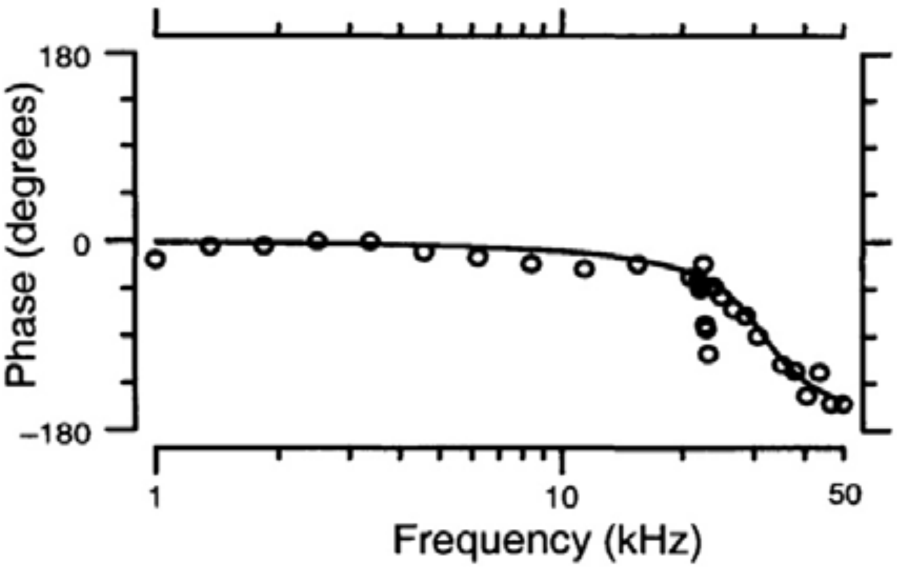
$$\frac{d\delta}{d\omega} = \frac{1}{1+\omega^2}$$

<u>Goal(s)</u>:

- Numerically estimate the derivative for this function using 'differences'
- Examine how different factors influence such an estimate (e.g., noise)

Numerical differentiation: Error





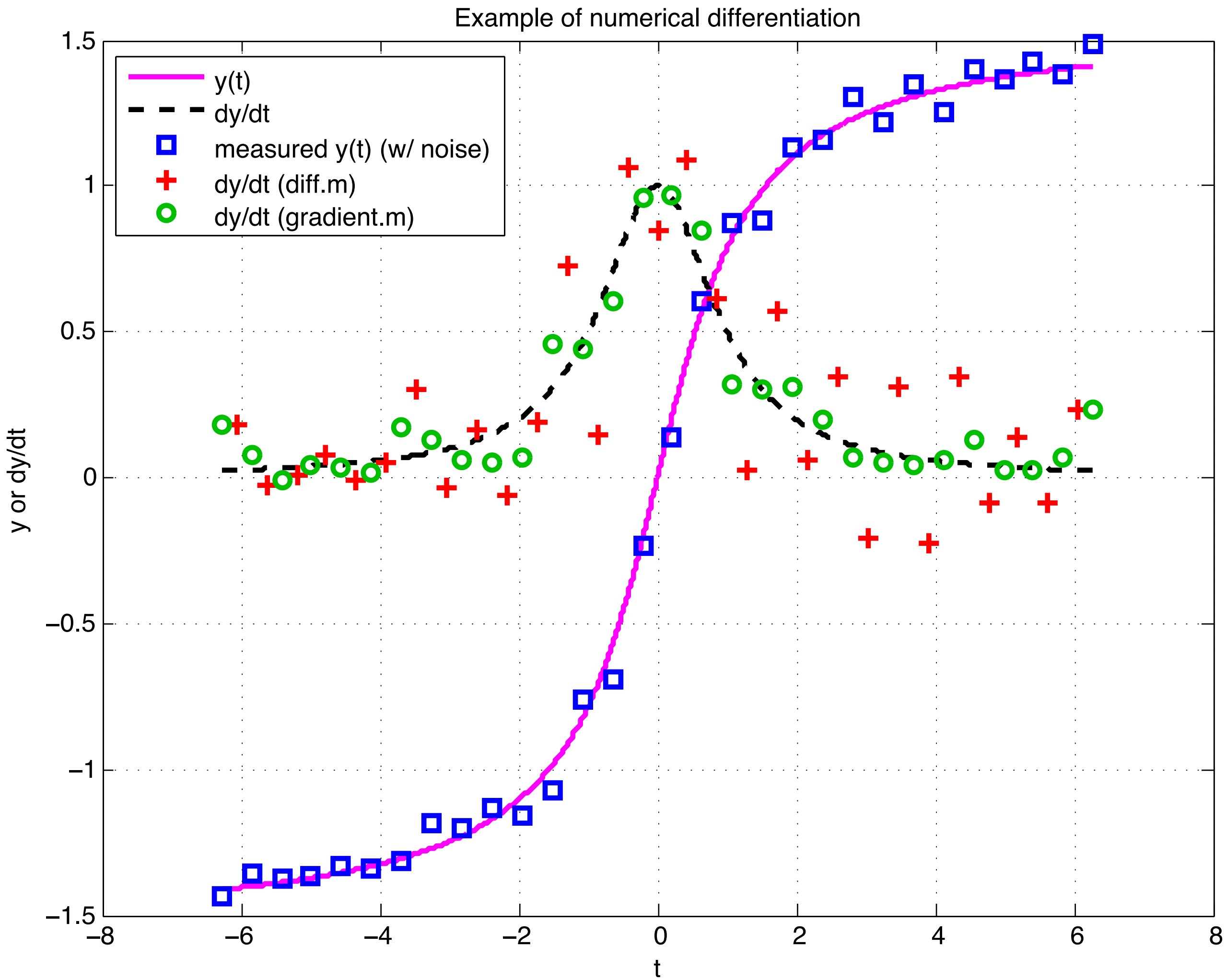
$\Rightarrow$ Very sensitive to measurement error!!

As we will see, your intuition is likely reversed:

- Analytically, differentiation is ‘easy’ and integration is hard
- Numerically, the converse is true (differentiation = hard, integration = easy)

French (1971)

Numerical differentiation: Error




```
slope= gradient(y,t);
plot(t,slope,'go')
```

⇒ Improvement when using 'centered differences' (via gradient.m)

⇒ Be careful! Decreasing step size can ultimately lead to increased error

('rounding error'; see text)

French (1971)

Post-class exercises

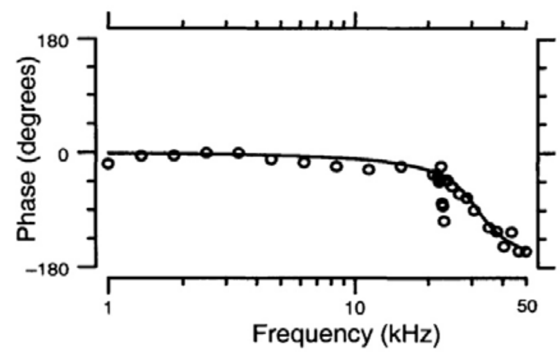
- Determine what diff.m and gradient.m do, and what is different between them

- Derive an expression for the derivative of the phase for the HO and modify EXdiff1.m appropriately

$$\delta(\omega) = \arctan\left(\frac{\gamma\omega}{\omega^2 - \omega_o^2}\right)$$

- Develop a means to quantify the 'error' associated with the derivative estimate

- What is the 'line' included in this plot?



Useful online reference:
http://ef.engr.utk.edu/ef230-2011-01/modules/matlab-integration/

Appendix: Theoretical background on linear harmonic oscillators (HOs)

Note:
Mathematically, this deals w/ 2nd order ODEs and complex numbers. 2030 students should feel reasonably comfortable with such. Physically, this is a foundational problem that you will see again and again and again and..... (i.e., now is a good time to learn it!0

Classic demonstration: pendula on a bob

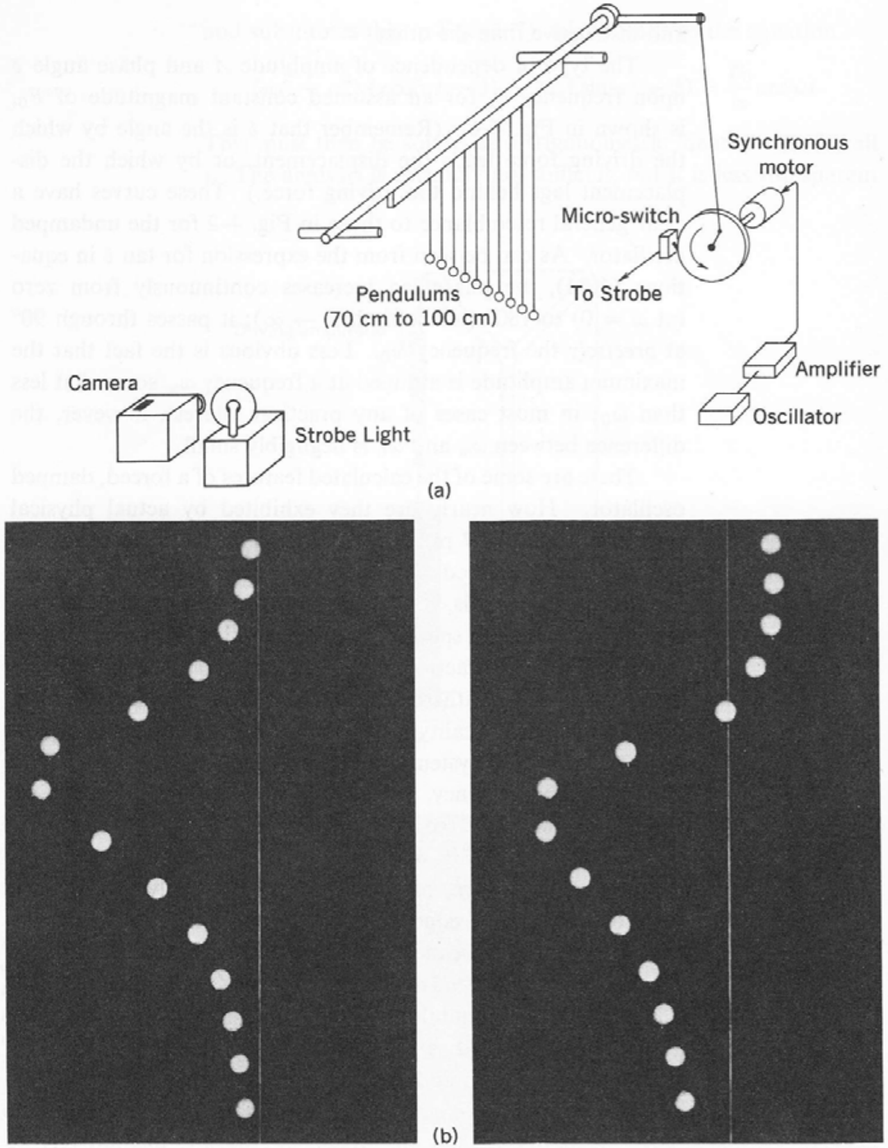


Fig. 4–8 A modern version of Barton's pendulums experiment. (a) A general sketch of the arrangement. The strobe light flashes once per oscillation at a controllable point in the cycle. (b) Displacements of the pendulums when the driving force is passing through zero (left) and at a somewhat later instant (right). In the latter photograph, note that the shorter pendulums have moved in the same direction as the driver and the longer pendulums have moved in the opposite direction, corresponding to $\delta < 90°$ and $\delta > 90°$ respectively. (Photos by Jon Rosenfeld, Education Research Center, M.I.T.).

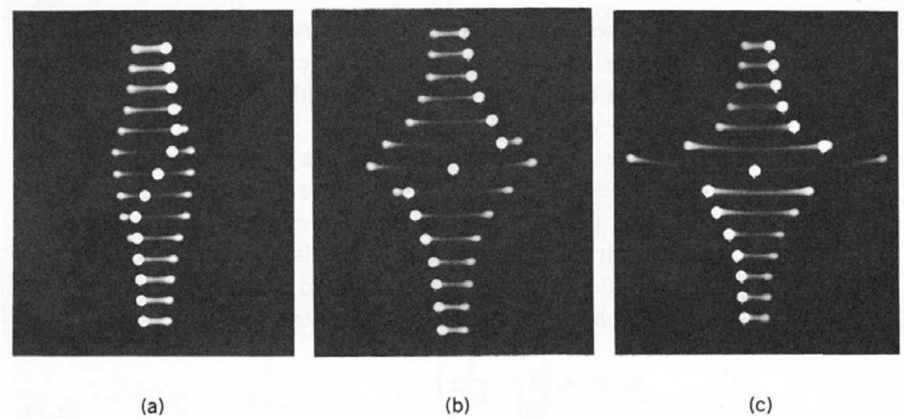
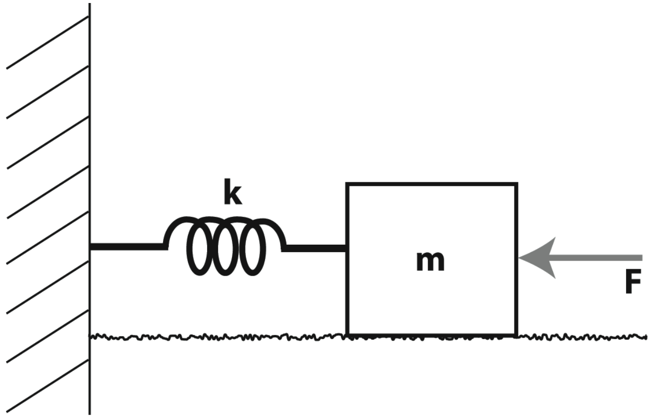


Fig. 4–10 Time exposure photograph of Barton's pendulums (cf. Fig. 4–8) showing resonance properties. The pendulum bobs were light styrofoam spheres (from PSSC Electrostatics Kit). (a) Pendulum bobs unloaded and therefore heavily damped, showing little selective resonance. (b) Each pendulum bob lightly loaded (with one thumbtack) giving moderate damping and more selective resonance. (c) Each pendulum bob heavily loaded (one thumbtack + one small washer) giving small damping and fairly high Q. (Photos by Jon Rosenfeld, Education Research Center, M.I.T.) In each case an instantaneous flash photograph is superimposed in order to display the phase relationships among the driven pendulums.

French (1971)

Case 1: Undamped, Undriven



$$F = ma = m\ddot{x} = -kx$$

Newton's Second Law
Hooke's Law

$$\ddot{x} + \frac{k}{m}x = 0$$

Second order ordinary differential equation
(no need worrying about how to "solve", yet...)

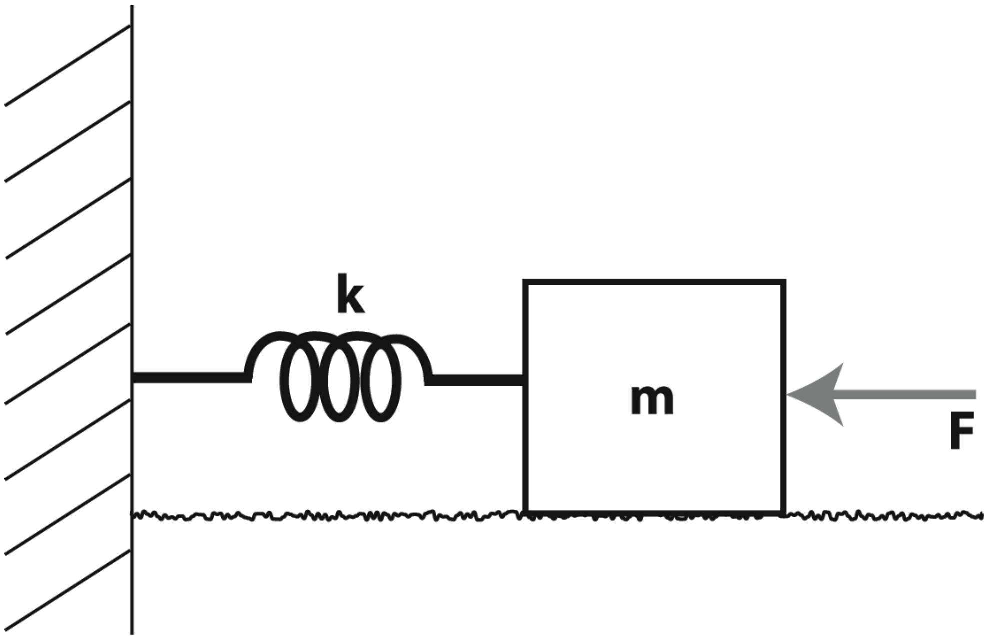
$$x(t) = A\cos\left(\omega_o t + \phi\right)$$

$\Rightarrow$ Solution is oscillatory!

$$\omega_o = \sqrt{k/m}$$

System has a *natural* frequency

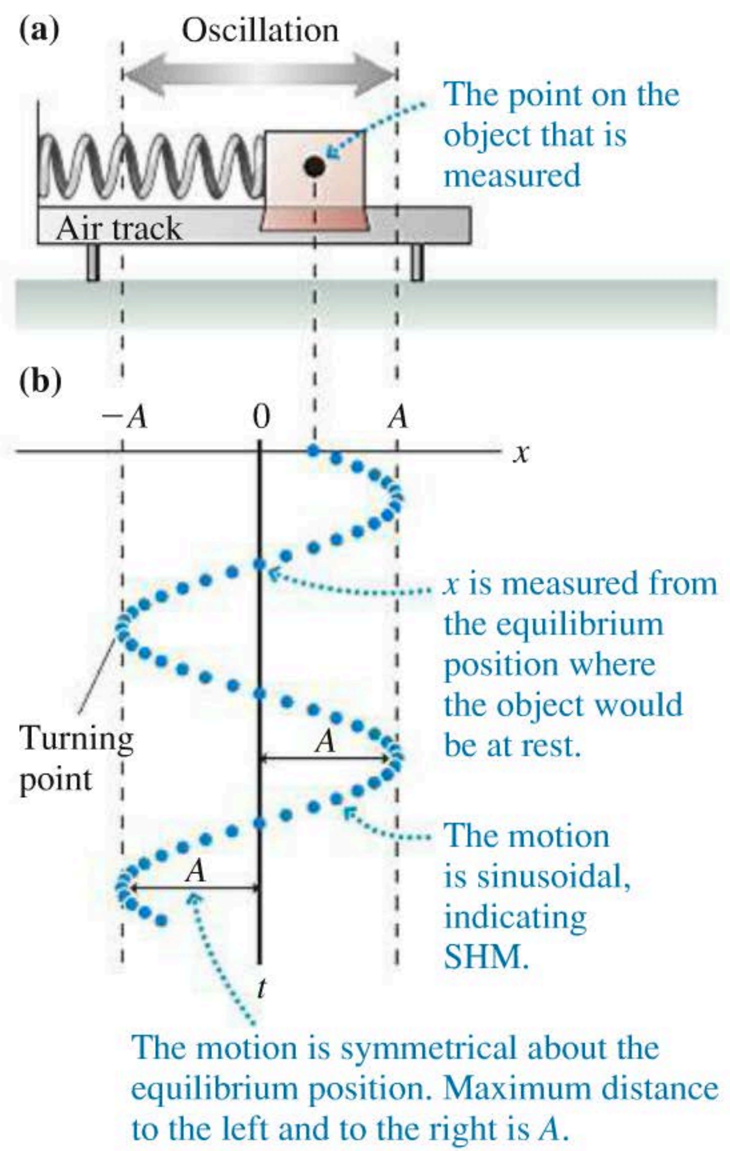
Harmonic oscillator



$$x(t) = A\cos(\omega_o t + \phi)$$

$$\omega_o = \sqrt{k/m} \qquad f = \frac{1}{T}$$

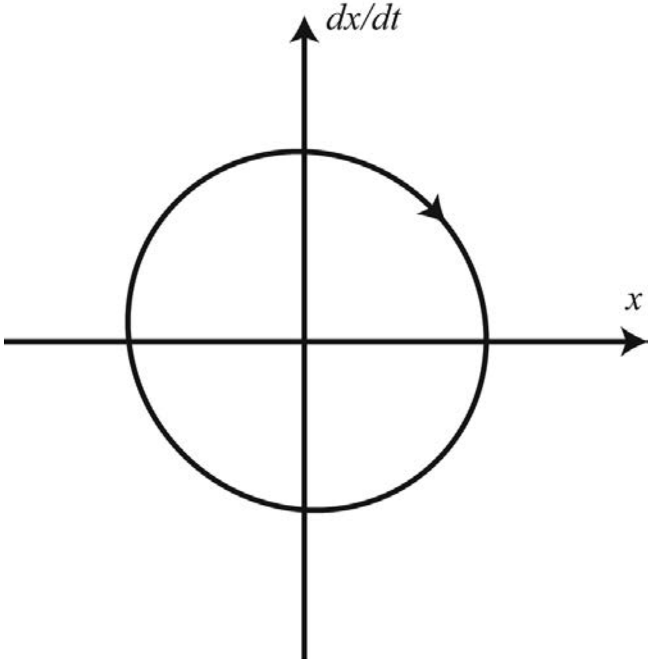
A prototype simple-harmonic-motion experiment.



Case 1: Undamped, Undriven (cont.)

Consider the system's energy:

$$E = T + U = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2$$



phase plane portrait

- Two means to *store* energy: mass and spring

- Oscillation results as energy transfers back and forth between these two *modes* (i.e., system is considered second-order)

Case 2: Undamped, Driven

$$\ddot{x} + \frac{k}{m}x = F_o \cos \omega t$$

Sinusoidal driving force at frequency ω

Assumption: Ignore onset behavior and that system oscillates at frequency ω

$$x(t) = B\cos(\omega t + \alpha)$$

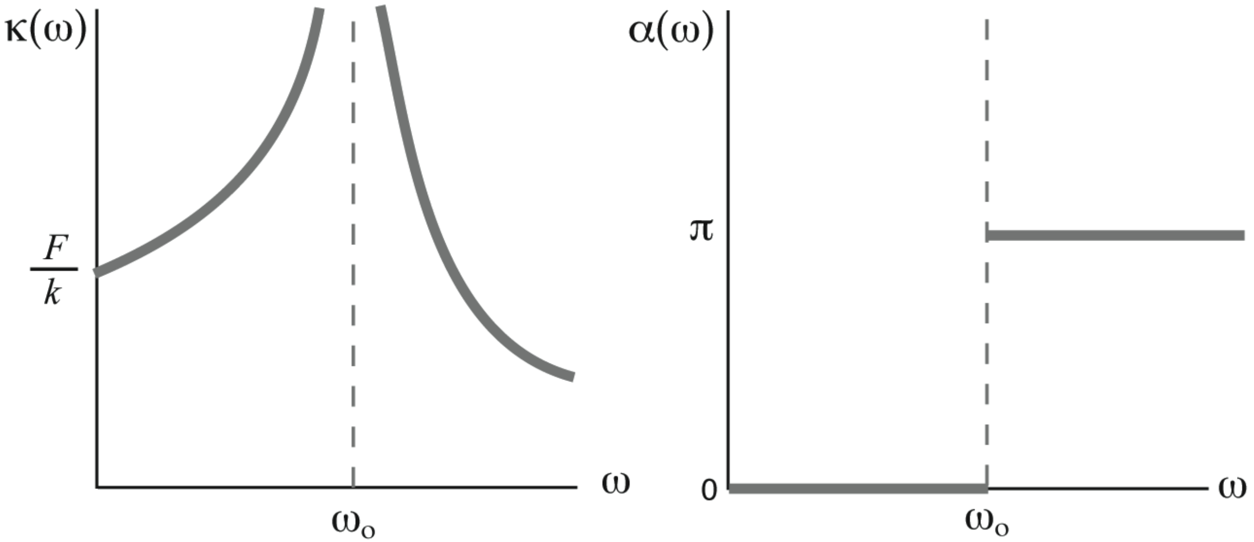
Assumed form of solution

$$-m\omega^2 B\cos\omega t + kB\cos\omega t = F_o\cos\omega t$$

$$\boxed{x(t) = \frac{F_o/m}{\omega_o^2 - \omega^2}\cos(\omega t + \alpha)}$$

Case 2: Undamped, Driven (cont.)

$$x(t) = \frac{F_o/m}{\omega_o^2 - \omega^2} \cos(\omega t + \alpha) = \kappa(\omega) \cos(\omega t + \alpha)$$



Two Important Concepts Demonstrated Here:

- *Resonance* when system is driven at natural frequency

- Phase shift of 1/2 cycle about resonant frequency

Case 3: Damped, Undriven

$$m\ddot{x} + b\dot{x} + kx = 0$$

Purely sinusoidal solution
no longer works!

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

Change variables

Assumption: Form of solution is a
complex exponential

$$x(t) = Ae^{i(\omega t + \delta)}$$

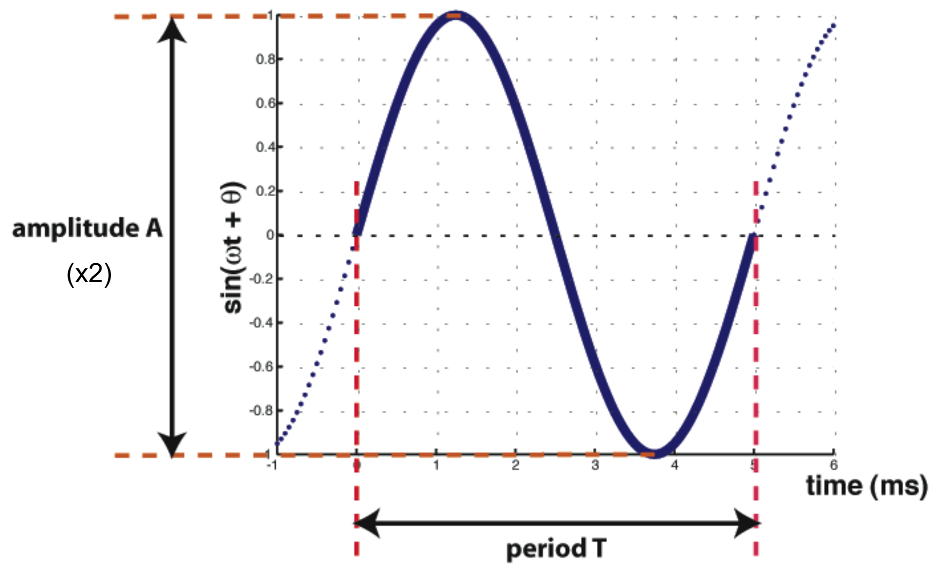
Trigonometry review ⇒ Sinusoids

Sinusoid has 3 basic properties:

i. Amplitude - height

ii. Frequency = 1/T [Hz]

iii. Phase - tells you where the peak is (needs a reference)

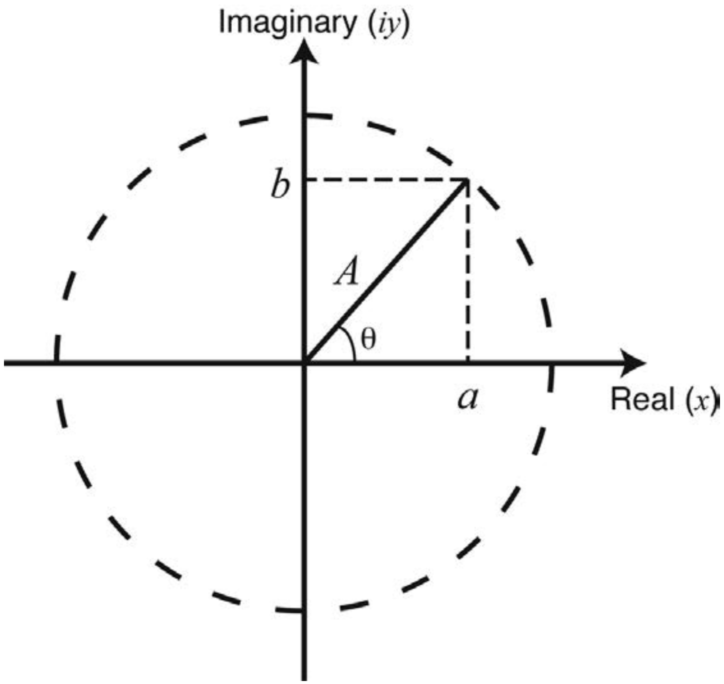


⇒ Phase reveals timing information

Case 3: Damped, Undriven (cont.)

Motivation for complex solution:

$$a + ib = Ae^{i\theta}$$
$$= A(\cos\theta + i\sin\theta)$$



Cartesian Form

$$a = A\cos(\theta)$$
$$b = A\sin(\theta)$$

$\Leftrightarrow$

Polar Form

$$A = \sqrt{a^2 + b^2}$$
$$\theta = \tan^{-1}\left(\frac{b}{a}\right)$$

$\Rightarrow$ Complex solution contains both magnitude and phase information

Case 3: Damped, Undriven

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

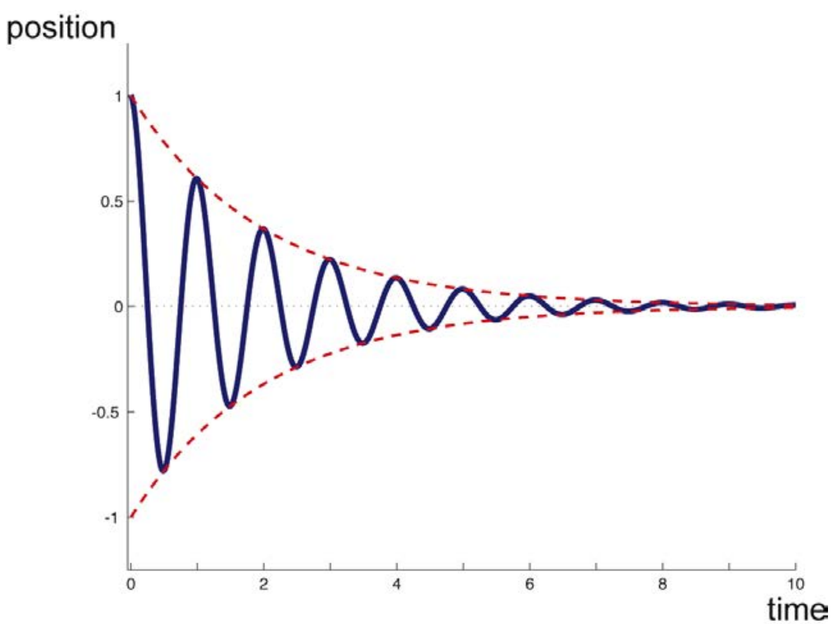
$$x(t) = A e^{i(\omega t + \delta)}$$

$$\boxed{x(t) = A e^{-\gamma t/2} \; e^{i(\omega t + \alpha)}}$$

$$\omega^2 = \omega_o^2 - \frac{\gamma^2}{4}$$

(slightly lower frequency of oscillation due to damping)

[A and α are constants of integration, depending upon initial conditions]



$\Rightarrow$ Damping causes energy loss from system

Case 4: Damped, Driven

$$\ddot{x} + \gamma\dot{x} + \omega_o^2 x = \frac{F_o}{m}e^{i\omega t}$$

Sinusoidal driving force at frequency ω

Assumption: Ignore onset behavior and that system oscillates at frequency ω

$$x(t) = Ae^{-i(\omega t+\delta)}$$

Assumed form of solution

$$\boxed{A(\omega) = \frac{F_o/m}{[(\omega_o^2 - \omega^2)^2 + (\gamma\omega)^2]^{1/2}}}$$

(magnitude)

$$\boxed{\delta(\omega) = \arctan\left(\frac{\gamma\omega}{\omega^2 - \omega_o^2}\right)}$$

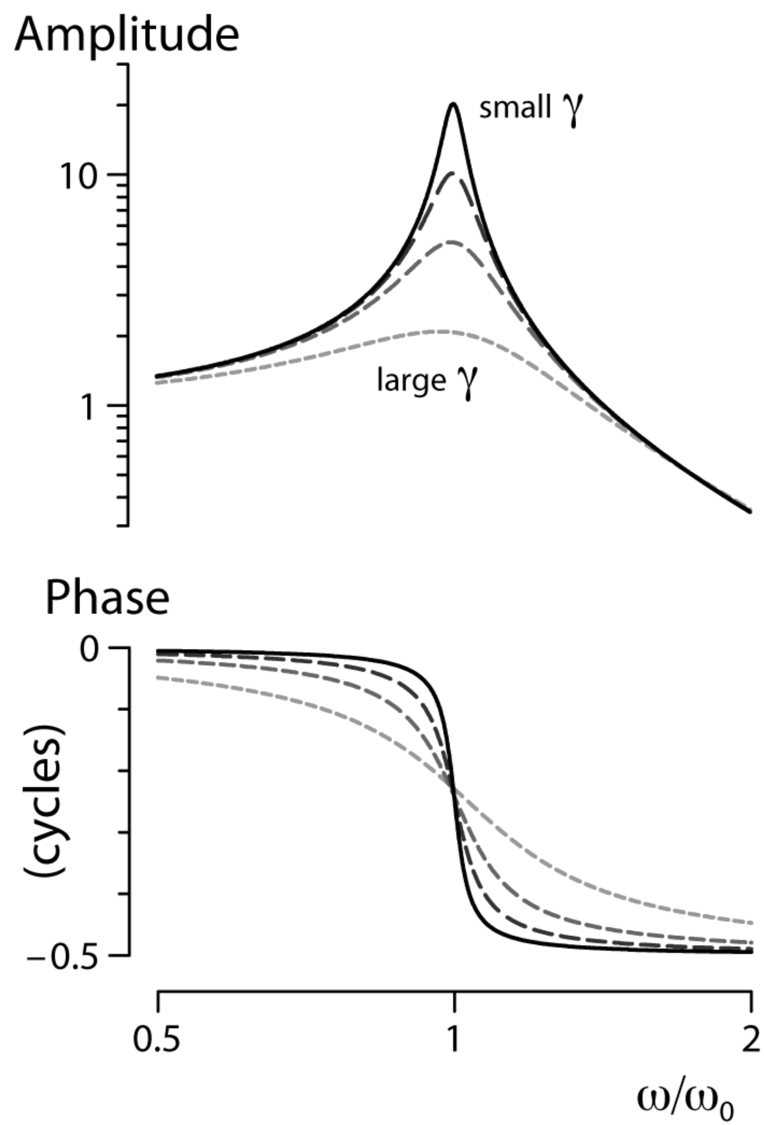
(phase)

Case 4: Damped, Driven (cont.)

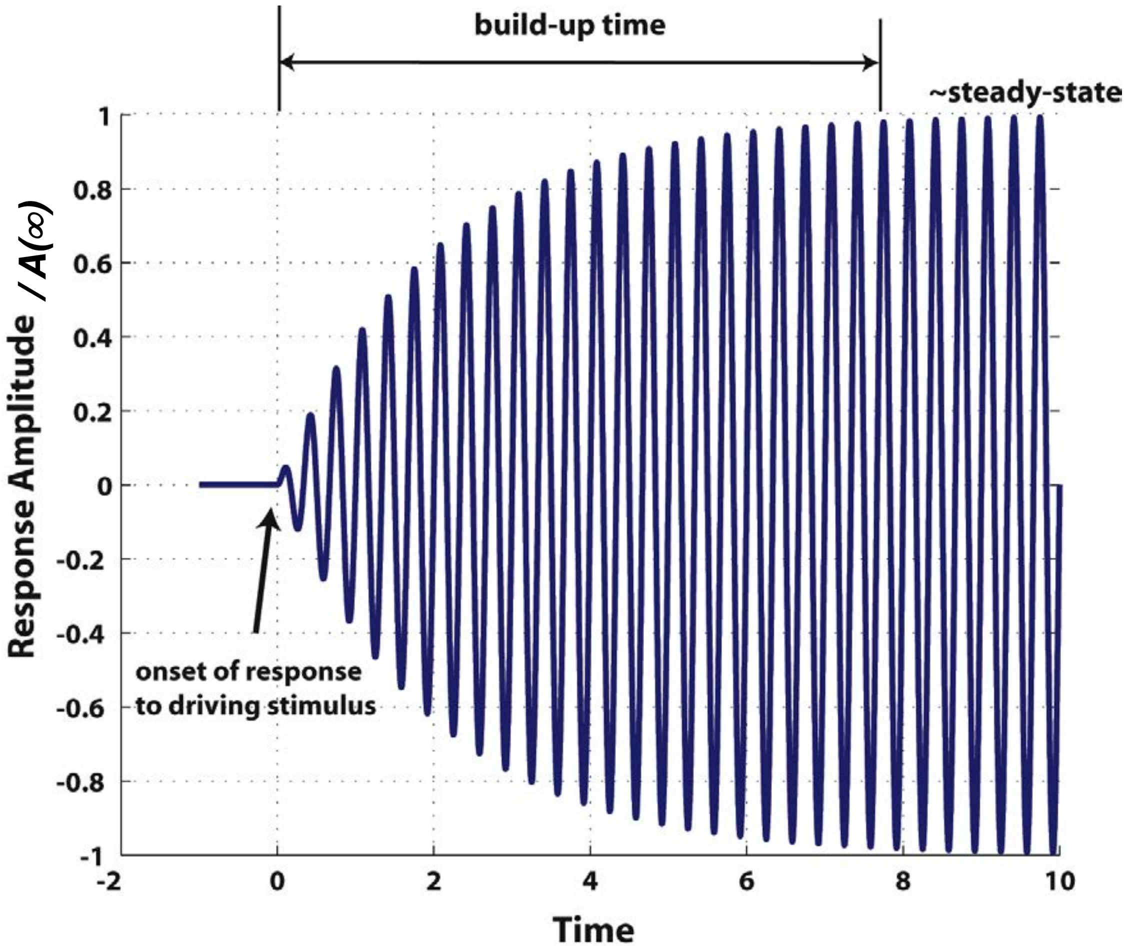
$$A(\omega) = \frac{F_o/m}{[(\omega_o^2 - \omega^2)^2 + (\gamma\omega)^2]^{1/2}}$$

$$\delta(\omega) = \arctan\left(\frac{\gamma\omega}{\omega^2 - \omega_o^2}\right)$$

⇒ Second-order oscillator behaves as
as *band-pass filter*



Basic Idea: Tuned Responses Take Time



Second Order System
(resonant frequency ω_o)

$\Rightarrow$ **External driving force at frequency ω**

$$x(t) = A(\infty)\,[1 - e^{(-t/\tau)}]$$

$$\boxed{\tau = 1/\gamma = Q / \omega_o}$$

Steady-state frequency response

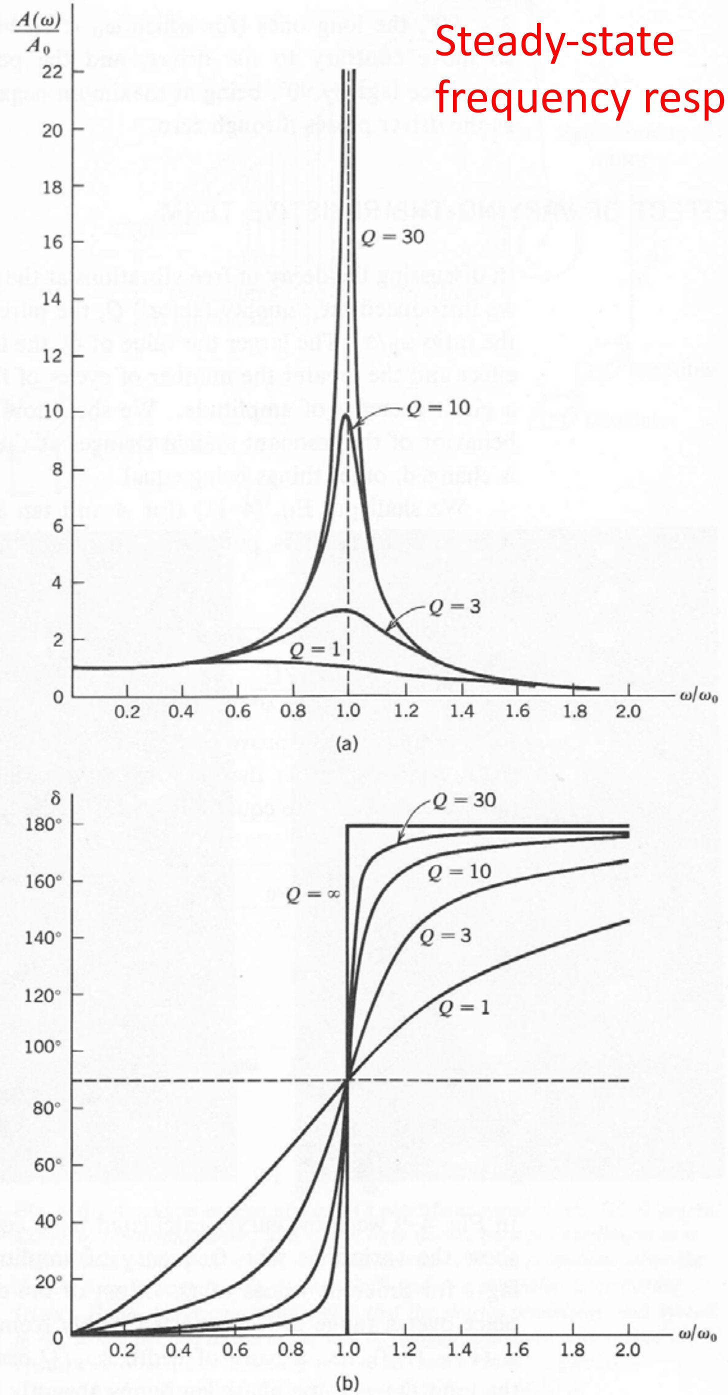


Fig. 4–9 (a) Amplitude as function of driving frequency for different values of Q, assuming driving force of constant magnitude but variable frequency. (b) Phase difference δ as function of driving frequency for different values of Q.

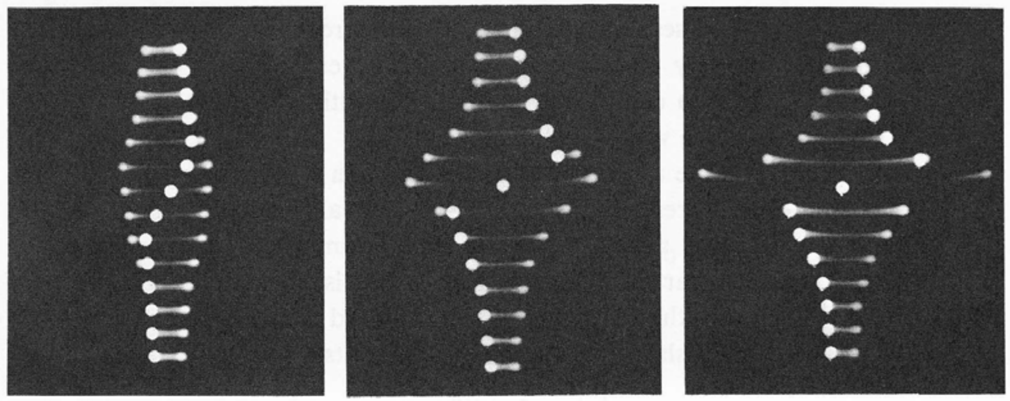
Q is the 'quality factor'

$$\ddot{x} + \gamma \dot{x} + \omega_o^2 x = \frac{F_o}{m} e^{i\omega t}$$

$$Q = \omega_o / \gamma$$

→ Phase information tells us something about the damping

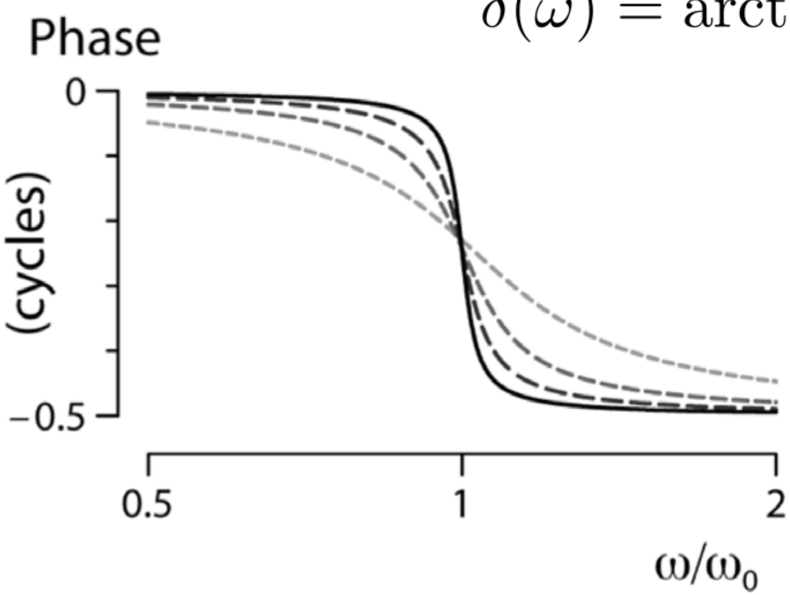
French (1971)



$$\ddot{x} + \gamma\dot{x} + \omega_o^2 x = \frac{F_o}{m} e^{i\omega t}$$

$$\delta(\omega) = \arctan\left(\frac{\gamma\omega}{\omega^2 - \omega_o^2}\right)$$

$N \equiv f_0$ * phase slope
(group delay)



$\boxed{N \propto 1/\gamma}$

⇒ Characterizing phase slope near resonance provides measure of damping

Ex.

A load of mass m lies on a perfectly smooth plane, being pulled in opposite directions by springs 1 and 2, whose coefficients of elasticity are k_1 and k_2 respectively (Fig. 60). If the load be forced out of its state of equilibrium (by being drawn aside), it will begin to oscillate with period T. Will the period of oscillation be altered if the same springs be fastened not at points A_1 and A_2, but at B_1 and B_2? Assume that the springs are subject to Hooke's law for all strains.

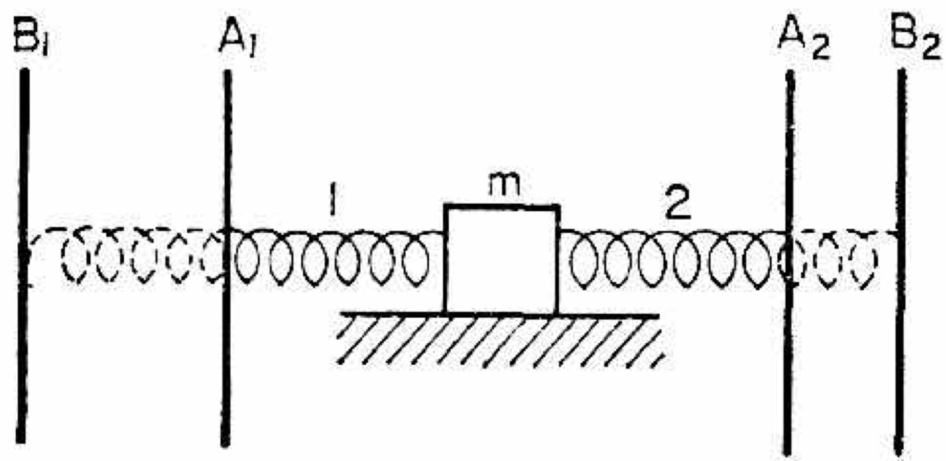


FIG. 60

Shaskol'Skaya & El'Tsin (1963)