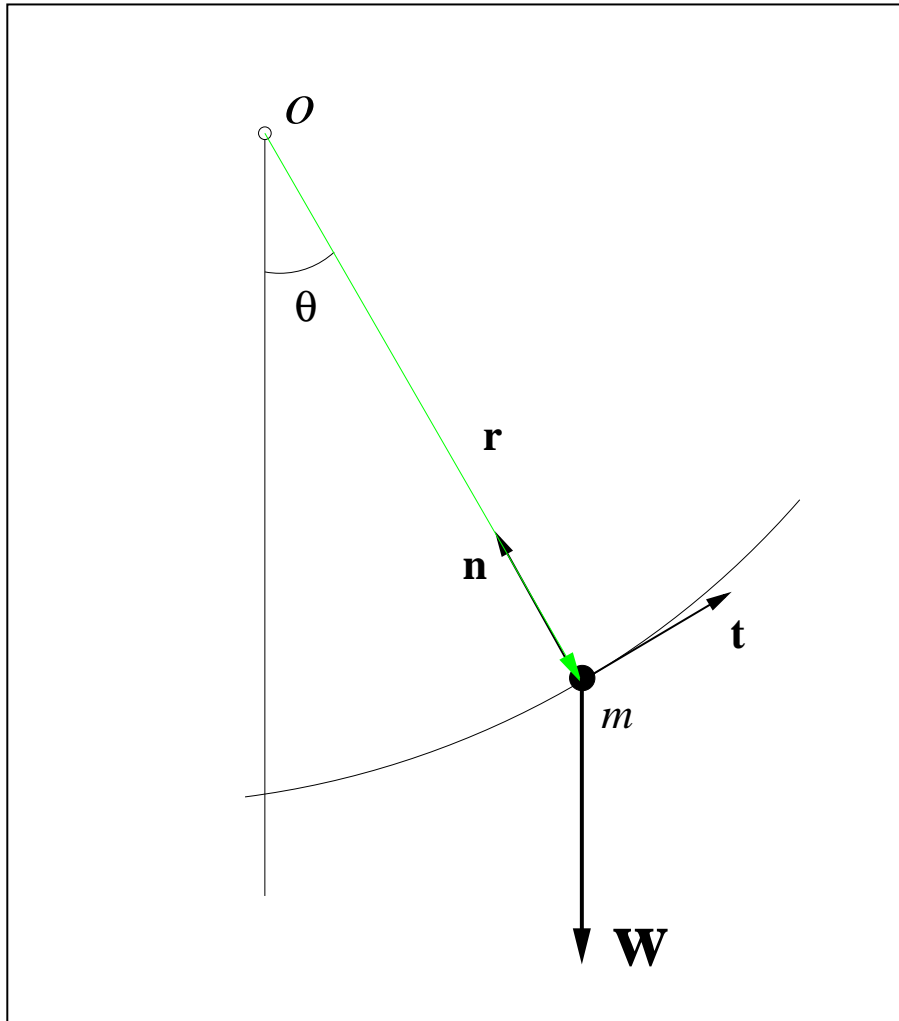


PHYS 210: Introduction to Computational Physics
Finite Difference Approximation (FDA)
The Nonlinear Pendulum

1. PHYSICAL & MATHEMATICAL FORMULATION



- Consider idealized pendulum:
 - Mass of bob, m
 - Infinitely rigid, massless pendulum arm of length L
 - No friction at pivot point O
 - Total mechanical energy (kinetic + potential) strictly conserved

1.1. Derivation of equation of motion

- Consider displacement vector, $\vec{r}(t)$ as shown in diagram
- $\vec{r}(t)$ makes an angle $\theta(t)$ with vertical
- Introduce normal-tangential coordinate systems with unit vectors \hat{n} and \hat{t} as shown
- Velocity, $\vec{v}(t)$, of bob given by

$$\vec{v}(t) = \frac{d\vec{r}}{dt} = v\hat{t}$$

where $v = |\vec{v}|$; i.e. velocity is purely tangential

- Acceleration, $\vec{a}(t)$ is

$$\vec{a}(t) = \frac{d^2\vec{r}}{dt^2} = \frac{d\vec{v}}{dt} = \frac{d}{dt}(v\hat{t}) = \frac{dv}{dt}\hat{t} + v\frac{d\hat{t}}{dt} = \frac{dv}{dt}\hat{t} + \frac{v^2}{L}\hat{n}$$

where we have used $|\vec{r}(t)| = L = \text{const.}$ as well as a standard result from kinematics, $d\hat{t}/dt = (v/L)\hat{n}$

- No motion in the normal direction, \hat{n} : consider only tangential motion
- Newton's second law

$$ma_t = F_t = -W \sin \theta = -mg \sin \theta \quad (\star)$$

where g is accn due to gravity

- Thus we have

$$a_t = -g \sin \theta$$

- Rewrite this as equation for $\theta(t)$:
- First recall

- *Angular velocity*, $\omega(t)$

$$\omega(t) = \frac{d\theta(t)}{dt}$$

- *Angular acceleration*, $\alpha(t)$

$$\alpha(t) = \frac{d\omega(t)}{dt} = \frac{d^2\theta(t)}{dt^2}$$

- Then

$$a_t(t) = L\alpha(t) = L\frac{d^2\theta}{dt^2}$$

- Substituting in (\star)

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L} \sin \theta \quad 0 \leq t \leq t_{\max}$$

- Need initial conditions

$$\begin{aligned} \theta(0) &= \theta_0 \\ \omega(0) &= \omega_0 \end{aligned}$$

where θ_0 and ω_0 are specified values.

Begin aside: Non-dimensionalization: Can choose system of units such that $g = 1$, $L = 1$, which makes the equation that we need to solve simpler

- Let's see how this would work for a specific set of initial units and length of rod: In particular, let's assume that we are working in *MKS* units so that $g = 9.8 \text{ m/s}^2$, and that $L = 4.9\text{m}$
- Then we first define a new unit of length that we will call a *rod* (not to be confused with the old Imperial unit having the same name!), so that

$$1 \text{ rod} \equiv 4.9 \text{ m}$$

- We then have

$$L = 1 \text{ rod}$$

- Now define a new unit of time, called the *tick*, so that

$$1 \text{ tick} \equiv \frac{1}{\sqrt{2}} \text{ s}$$

which implies

$$1 \text{ s} \equiv \sqrt{2} \text{ tick}$$

- Now we have

$$g = 9.8 \frac{\text{m}}{\text{s}^2} = \frac{9.8 \text{ m}}{\text{s}^2} = \frac{2 \text{ rod}}{\text{s}^2} = \frac{2 \text{ rod}}{(\sqrt{2} \text{ tick})^2} = \frac{2 \text{ rod}}{2 \text{ tick}^2} = 1 \frac{\text{rod}}{\text{tick}^2}$$

- Therefore, in our new set of units we have (suppressing the units themselves)

$$L = g = 1$$

End aside

- Adopting our new set of units, the (simplified) equation that we want to solve is

$$\frac{d^2\theta}{dt^2} = -\sin\theta \quad 0 \leq t \leq t_{\max} \tag{1}$$

with initial conditions

$$\theta(0) = \theta_0 \tag{2}$$

$$\omega(0) = \omega_0 \tag{3}$$

- **Note:** (1) is a *nonlinear* ordinary differential equation (ODE), since $\sin(\theta(t))$ is a nonlinear function of $\theta(t)$. Closed form solution is possible, but quite complex. Numerical solution no more difficult in principle/practice than linear case!

1.2 Linear limit

- Assume that angular displacement $\theta(t)$ is very small, $\theta(t) \ll 1$
- Then

$$\sin(\theta) \approx \theta$$

and (3) becomes

$$\frac{d^2\theta}{dt^2} = -\theta \quad 0 \leq t \leq t_{\max} \quad (4)$$

- which has the general solution

$$\theta(t) = A \sin(t + \delta)$$

where the constants A and δ are determined from the initial conditions (2) and (3).

- *Key fact:* In linear case, oscillation frequency $\Omega = \sqrt{g/L} = 1$ with our choice of units (i.e. $\theta(t) = A \sin(\Omega t + \delta)$ with $\Omega = 1$), is *independent* of amplitude, A of oscillation, or equivalently, independent of the initial conditions (2) and (3)
- *Not* the case for nonlinear pendulum!

2. SOLUTION VIA FINITE DIFFERENCE APPROXIMATION

2.1. Discretization: Step 1—Finite Difference Grid

- Continuum domain is

$$0 \leq t \leq t_{\max}$$

- Specify mesh via *level* parameter, ℓ , as discussed previously

$$n_t = 2^\ell + 1$$

$$\Delta t = \frac{t_{\max}}{n_t - 1} = 2^{-\ell} t_{\max}$$

$$t^n = (n - 1)\Delta t, \quad n = 1, 2, \dots, n_t$$

2.2. Discretization: Step 2—Derivation of FDAs

- Continuum equations \rightarrow discrete equations
- Usual FD notation

$$\theta^n \equiv \theta(t^n) \equiv \theta((n - 1)\Delta t)$$

- Have one derivative to replace, use $O(\Delta t^2)$ accurate approximation derived earlier in class

$$\left. \frac{d^2\theta}{dt^2} \right|_{t=t^n} \approx \frac{\theta^{n+1} - 2\theta^n + \theta^{n-1}}{\Delta t^2} \quad (5)$$

- **Note:** We view this formula as being applied (“centred”) at the grid point t^n ; thus the appropriate discretization of $\sin(\theta)$ is simply $\sin(\theta^n)$
- Substitute (5) in (1), get desired FDA

$$\frac{\theta^{n+1} - 2\theta^n + \theta^{n-1}}{\Delta t^2} = -\sin \theta^n \quad n + 1 = 3, 4, \dots, n_t \quad (6)$$

- We now regard this as an equation for θ^{n+1} , assuming that θ^n and θ^{n-1} are known

$$\theta^{n+1} = 2\theta^n - \theta^{n-1} - \Delta t^2 \sin \theta^n \quad n + 1 = 3, 4, \dots, n_t \quad (7)$$

- First discrete time at which we can use (6) is $t^{n+1} = t^3$
- Thus need values $\theta^1 = \theta(0)$ and $\theta^2 = \theta(\Delta t)$ to initialize scheme
- θ^1 is given by initial condition (2)

$$\theta^1 = \theta(0) = \theta_0$$

- Determining θ^2 is a bit more involved. State without proof that in order for overall solution to be $O(\Delta t^2)$, must determine $\theta^2 = \theta(\Delta t)$ up to and including terms of $O(\Delta t^2)$ (i.e. leading order error term in $\theta(\Delta t)$ must be $O(\Delta t^3)$)
- Proceed via Taylor series expansion, and use initial conditions (2) and (3)

$$\begin{aligned} \theta(\Delta t) &= \theta(0) + \Delta t \frac{d\theta}{dt}(0) + \frac{1}{2} \Delta t^2 \frac{d^2\theta}{dt^2}(0) + O(\Delta t^3) \\ &\approx \theta_0 + \Delta t \omega_0 + \frac{1}{2} \Delta t^2 \frac{d^2\theta}{dt^2} \end{aligned}$$

- Now use equation of motion (1) to eliminate $d^2\theta/dt^2$; i.e. $d^2\theta/dt^2 = -\sin\theta$, so we have

$$\theta(\Delta t) \approx \theta_0 + \Delta t \omega_0 - \frac{1}{2} \Delta t^2 \sin \theta_0$$

- Assembling results we have

$$\theta^{n+1} = 2\theta^n - \theta^{n-1} - \Delta t^2 \sin \theta^n \quad n + 1 = 3, 4, \dots, n_t \quad (8)$$

$$\theta^1 = \theta_0 \quad (9)$$

$$\theta^2 = \theta_0 + \Delta t \omega_0 - \frac{1}{2} \Delta t^2 \sin \theta_0 \quad (10)$$

- Equations (8)–(10) constitute our complete FDA (note that we have a total of n_t equations for the n_t unknowns $\theta^n, n = 1, 2, \dots, n_t$)

2.3. Convergence Analysis (EXTREMELY IMPORTANT!!)

- Want to examine behaviour of numerical solution as $\Delta t \rightarrow 0$
- *Assumption:* (following L.F. Richardson, 1909) Let $u_*(t)$ be the exact (continuum) solution of (1)–(3)
Then the error, $e(t^n)$, in the numerical solution, $u(t^n)$

$$e(t^n) \equiv u_*(t^n) - u(t^n)$$

takes the form

$$\lim_{\Delta t \rightarrow 0} e(t^n) = u_*(t^n) - u(t^n) = \Delta t^2 e_2(t^n) + O(\Delta t^4) \quad (11)$$

- **Note:** $e_2(t^n)$ is a *function*, not “random” values as would be the case if we were analyzing the error in experimental data!
- *Why should we expect (11) to hold?* Rather deep question, full answer beyond scope of this course—*but*, can be *verified* empirically
- **Note:** We expect second error term to be $O(\Delta t^4)$ due to the centred nature of the FDA for the second derivative that we are using (previously left as exercise for you)

2.3.1 Convergence Test (ALSO EXTREMELY IMPORTANT!!)

- *Draw sample mesh sequence*
- Define u_ℓ^n to be the soln computed at level ℓ with $\Delta t = \Delta t_\ell$
- Define $u_{\ell+1}^n$ to be the soln computed at level $\ell + 1$ with $\Delta t = \Delta t_{\ell+1} = \Delta t_\ell/2$
- Define $u_{\ell+2}^n$ to be the soln computed at level $\ell + 2$ with $\Delta t = \Delta t_{\ell+2} = \Delta t_{\ell+1}/2 = \Delta t_\ell/4$
- Then from (10) we have

$$\begin{aligned} u_\ell(t^n) &\approx u_*^n(t^n) - (\Delta t_\ell)^2 e_2(t^n) \\ u_{\ell+1}(t^n) &\approx u_*^n(t^n) - (\Delta t_{\ell+1})^2 e_2(t^n) \\ u_{\ell+2}(t^n) &\approx u_*^n(t^n) - (\Delta t_{\ell+2})^2 e_2(t^n) \end{aligned}$$

where t^n is the common set of discrete times t_ℓ^n (the times on the coarsest grid)

- Now consider subtracting solutions on adjacent levels; then

$$u_\ell(t^n) - u_{\ell+1}(t^n) \approx -\left((\Delta t_\ell)^2 - (\Delta t_{\ell+1})^2\right) e_2(t^n) = -\frac{3}{4}\Delta t_\ell^2 e_2(t^n)$$

$$u_{\ell+1}(t^n) - u_{\ell+2}(t^n) \approx -\left((\Delta t_{\ell+1})^2 - (\Delta t_{\ell+2})^2\right) e_2(t^n) = -\frac{3}{4}(\Delta t_{\ell+1})^2 e_2(t^n) = -\frac{3}{16}(\Delta t_\ell)^2 e_2(t^n)$$

- **Observe:**

1. Simply subtracting 2 solns computed on 2 different levels gives direct estimate of solution error (very general result!)

By assumption (equation (11)) we have

$$e(t^n) = \Delta t^2 e_2(t^n) + \dots$$

and we have just shown

$$u_\ell(t^n) - u_{\ell+1}(t^n) \approx \frac{3}{4}(\Delta t_\ell)^2 e_2(t^n)$$

so

$$-\frac{4}{3}\left(u_\ell(t^n) - u_{\ell+1}(t^n)\right) \approx e(t^n)$$

2. If we consider the ratio

$$\frac{u_\ell(t^n) - u_{\ell+1}(t^n)}{u_{\ell+1}(t^n) - u_{\ell+2}(t^n)}$$

then in the limit $\Delta t_\ell \rightarrow 0$, should get

$$\frac{-(3/4)(\Delta t_\ell)^2 e_2(t^n)}{-(3/16)(\Delta t_\ell)^2 e_2(t^n)} = 4$$

3. **More useful for labs/homeworks/projects:** If we scale (multiply)

$$\begin{aligned} u_\ell(t^n) - u_{\ell+1}(t^n) & \text{ by } 4^0 = 1 \\ u_{\ell+1}(t^n) - u_{\ell+2}(t^n) & \text{ by } 4^1 = 4 \\ u_{\ell+2}(t^n) - u_{\ell+3}(t^n) & \text{ by } 4^2 = 16 \end{aligned}$$

etc., and plot all the curves as fcn of t^n , curves should nearly coincide, and should become more coincident as $\Delta t \rightarrow 0$ (as was the case for the first order approximation of the first derivative example covered in the lab, where we rescaled the (known) errors by powers of 2)

4. Don't have to restrict convergence test to 3 levels, can use as many as possible, but *should always do 3-level test at a minimum!*
5. **IMPORTANT!** Don't have to know what the error is to do the convergence test (if we *did* know the error, what would be the point of doing the numerical calculation?)
 - Assume error has the form (11)
 - Do convergence test by running simulation with different grid spacings (levels), and subtract the results computed at successive levels, and rescale as above
 - If we *do* see near coincidence of the rescaled subtracted values, then we have confidence in our numerical solutions, and also have a good estimate of the error
6. **MORE IMPORTANT!**, if we do *not* observe convergence, then we *know* that there is *some* problem with our implementation, and that we need to do some debugging!

2.4. Energy Conservation

- For systems such as the nonlinear (linear) pendulum, where total (mechanical) energy is conserved, we can use conservation of energy as an additional check of the correctness and convergence of our numerical implementation
- For the nonlinear pendulum we have

$$\text{Kinetic energy} \equiv T(t) = \frac{1}{2}mv(t)^2 = \frac{1}{2}m(L\omega(t))^2$$

$$\text{Potential energy} \equiv V(t) = mgh(t)$$

where $h(t)$ is the vertical displacement of the bob/mass relative to its stable equilibrium position.

- Basic trigonometry tells us that $h(t) = L(1 - \cos \theta(t))$ so we have

$$V(t) = mgh(t) = mgL[1 - \cos \theta(t)]$$

- Thus we have

$$\text{Total energy} \equiv E(t) = T(t) + V(t) = \frac{1}{2}m(L\omega(t))^2 + mgL[1 - \cos \theta(t)]$$

- Now, in our units $g = L = 1$, and we will also take $m = 1$: can *always* do this via further choice of units (what would that choice be?), but in any case, since both terms are proportional to m , any particular choice of m is irrelevant to the central issue of how well the discrete solutions “conserves energy”
- Thus we have

$$E(t) = T(t) + V(t) = \frac{1}{2}\omega(t)^2 + [1 - \cos \theta(t)]$$

- In order to check for energy conservation, we can define the deviation in the total energy relative to the initial time

$$dE(t) \equiv E(t) - E(0)$$

- An obvious thing to do is to plot $dE(t)$ vs t to see whether the total energy “looks” conserved.
- However, a much better idea is to check the *convergence* of $dE(t)$ which, if our implementation is correct, should tend to 0 as $\Delta t \rightarrow 0$ like $O(\Delta t^2)$
- That is, we ensure that our calculations display “convergence to conservation”
- **IMPORTANT!** Note that the above formulae for the potential and total energies are **NOT** valid for the *linear* pendulum. We can get the correct formula by using the small angle approximation $\theta(t) \ll 1$ and keeping only the leading-order term.
- From Taylor series of $\cos \theta$ about $\theta = 0$ we have

$$\cos \theta = 1 - \frac{1}{2}\theta^2 + O(\theta^4) \approx 1 - \frac{1}{2}\theta^2$$

- So we have

$$E_{\text{linear}}(t) = T(t) + V(t) = \frac{1}{2}\omega(t)^2 + \frac{1}{2}\theta(t)^2$$