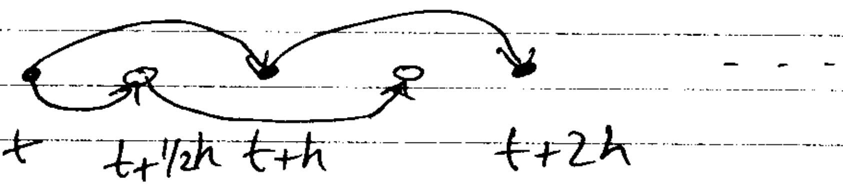
Lecture 18

Recall leap-frog method



Equations were

(*)
$$x(t+h) = x(t) + h\, f\big(x(t+\tfrac{1}{2}h),\, t+\tfrac{1}{2}h\big)$$
$$x(t+\tfrac{3}{2}h) = x(t+\tfrac{1}{2}h) + h\, f\big(x(t+h),\, t+h\big)$$

The method is time reversal symmetric

Substitute $h \to -h$ & get

$$x(t-h) = x(t) - h\, f\big(x(t-\tfrac{1}{2}h),\, t-\tfrac{1}{2}h\big)$$
$$x(t-\tfrac{3}{2}h) = x(t-\tfrac{1}{2}h) - h\, f\big(x(t-h),\, t-h\big)$$

Now time shift $t \to t+\tfrac{3}{2}h$ & get

$$x(t+\tfrac{1}{2}h) = x(t+\tfrac{3}{2}h) - h\,f(x(t+h), t+h)$$

$$x(t) = x(t+h) - h\,f(x(t+\tfrac{1}{2}h), t+\tfrac{1}{2}h)$$

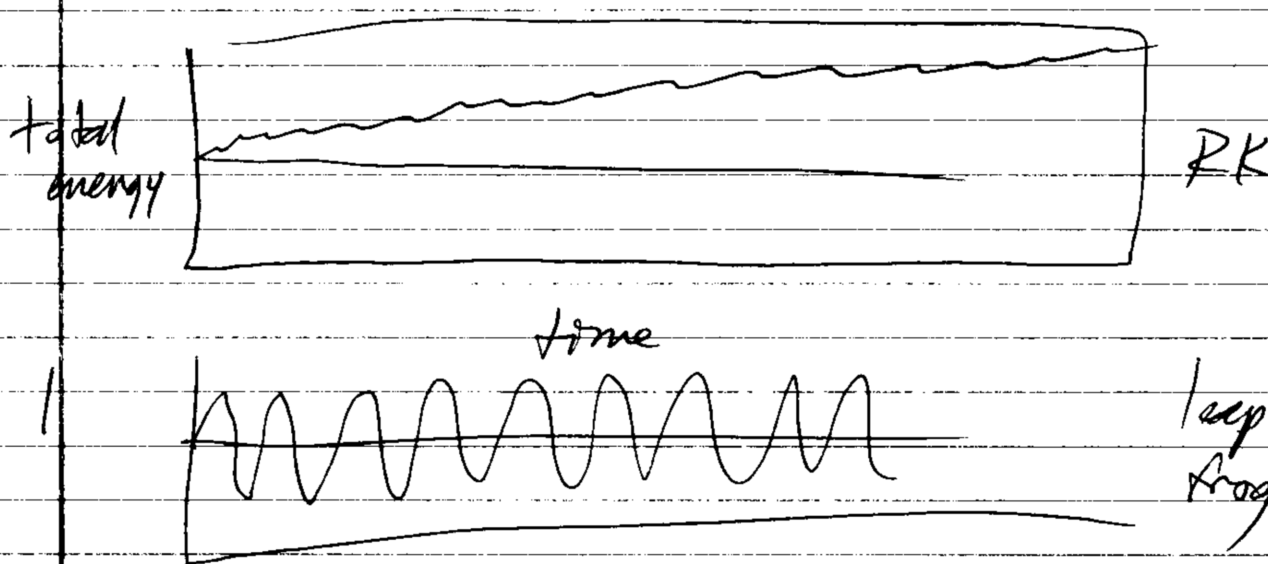
Compare to (*) & we see that the equations are the same, but run backwards

This is not true of Runge-Kutta (can do the same calculation & you won't have the time reversal symmetry)

Why is the time reversal symmetry important? One reason is conservation of energy.

When using Runge-Kutta for nonlinear pendulum, the total energy fluctuates & drifts over time

For the leap-frog method,
the total energy fluctuates but
there is no drift



So leap frog method is useful
for solving energy conserving
physical systems over long periods
of time.

Verlet method

variation of leap frog

Suppose equations of motion take the form $\frac{d^2x}{dt^2} = f(x,t)$

e.g., $F = ma$

can convert to

$$\frac{dx}{dt} = v \qquad \frac{dv}{dt} = f(x,t)$$

could directly apply leap frog method to vector $\underline{r} = (x, v)$

w/ $$\frac{d\underline{r}}{dt} = \underline{f}(\underline{r}, t)$$

But let's instead ~~write~~ out the leap frog method in full

$$x(t+h) = x(t) + h\, v(t + \tfrac{1}{2}h) \qquad \text{(1st eq.)}$$

$$v(t + \tfrac{3}{2}h) = v(t + \tfrac{1}{2}h) + h\, f(x(t+h), t+h)$$

We can derive a full solution using these ~~two~~ equations alone. The vector method requires double the work, but have we only calculate x @ $t+kh$ & v @ $t+(\frac{1}{2}+k)h$

- works for diff eq's w/ special form

$$\underbrace{\frac{dx}{dt} = v}_{\text{doesn't depend on } x} \qquad \underbrace{\frac{dv}{dt} = f(x,t)}_{\text{doesn't depend on } v}$$

- Potential issue: What if we want to calculate quantity that depends on x & v, like ~~total~~ energy?

we only have x @ $t+kh$ & v @ $t+(k+\frac{1}{2})h$

Supposing that we did know $v(t+h)$ then we could calculate ~~[illegible]~~ $v(t+\frac{1}{2}h)$ by going backwards w/ the Euler method giving

$$v(t+\tfrac{1}{2}h) = v(t+h) - \tfrac{1}{2}h\, f(x(t+h), t+h)$$

then rearrange as

$$v(t+h) = v(t+\tfrac{1}{2}h) + \tfrac{1}{2}h\, f(x(t+h), t+h)$$

So the full <u>Verlet</u> method is

$$x(t+h) = x(t) + h\, v(t+\tfrac{1}{2}h)$$

$$k = h\, f(x(t+h), t+h)$$

$$v(t+h) = v(t+\tfrac{1}{2}h) + \tfrac{1}{2}k$$

$$v(t+\tfrac{3}{2}h) = v(t+\tfrac{1}{2}h) + k$$

put "bars" underneath to get vector quantities ...

Modified midpoint method

Another advantage of leap frog method is that the total error is an even function of the step size h (due to time reversal symmetry)

$\Rightarrow$ expansion of error in power series of h has only even terms & no odd terms.

We can see this in more detail:

A single step of leap frog method is accurate to order h^2 & has error to order h^3

Write error as $\varepsilon(h)$ w/ first term proportional to h^3.

What do the other terms look like?

Take a small step forward w/ leap frog method.

Gives the solution plus $\varepsilon(h)$ (error)

Now go backwards, i.e., step size is $-h$

Due to time symmetry, the <u>change</u> in the solution is the reverse of the forward change

$\Rightarrow$ backward error is the negative of the forward error, i.e.,

$$\varepsilon(-h) = -\varepsilon(h)$$

$\Rightarrow$ $\varepsilon(h)$ is an odd function & has only odd powers in Taylor expansion.

For overall error, we compute error on a single step times the # of steps.

So if the time interval of interest is Δ, then # of steps is Δ/h $\Rightarrow$

total error is $\varepsilon(h) \cdot \frac{\Delta}{h}$

i.e., an even function of error. w/ first term proportional to h^2.

Slight catch: For the 1st step of leap frog, we take a 1/2 step using Euler method & introduce an error of order h^2 (as is case w/ Euler method)

However, Euler method higher order terms are not even. So the total error has even & odd powers.

Can solve this problem using the modified midpoint method.

Suppose we want to solve starting @ t & ending @ $t+H$ where H is not small.

use n steps of size $h = H/n$

can write leap frog as

$$x_0 = x(t)$$
$$y_1 = x_0 + \tfrac{1}{2} h f(x_0, t)$$

& then

$$x_1 = x_0 + h f(y_1, t + \tfrac{1}{2}h)$$
$$y_2 = y_1 + h f(x_1, t+h)$$
$$x_2 = x_1 + h f(y_2, t + \tfrac{3}{2}h)$$

etc. general form is

$$y_{m+1} = y_m + h f(x_m, t+mh)$$
$$x_{m+1} = x_m + h f(y_{m+1}, t + (m+\tfrac{1}{2})h)$$

last 2 points are

$$y_n = x(t+H-\tfrac{1}{2}h)$$

$$x_n = x(t+H)$$

usually would take x_n as solution but we can also estimate $x(t+H)$ using Euler method as

$$x(t+H) = y_n + \tfrac{1}{2}h\, f(x_n, t+H)$$

can take the average of the two estimates for $x(t+H)$ to be the estimate:

$$x(t+H) = \frac{1}{2}\left[x_n + y_n + \frac{1}{2}h\, f(x_n, t+H)\right]$$

Can show that doing so cancels out the odd order error terms introduced in the 1st step of Euler method (need to track errors carefully to see this) contains only even-order error terms. Remember how this was useful for Romberg integration? This will be useful for a similar method for solving diff. eq's

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Bulirsch - Stoer Method

reminiscent of Romberg integration

Suppose we wish to solve

$$\frac{dx}{dt} = f(x,t)$$

from t to $t+H$

Begin by using a single step of size H & use modified midpoint method

Let $h_1 = H$

gives an estimate of $x(t+H)$,

call it $R_{1,1}$.

Now go back to time t,

divide interval into 2 steps of

size $h_2 = \frac{1}{2}H$. Gives

another estimate of $x(t+H)$,

call it $R_{2,1}$

Since total error of modified

midpoint method is an even function

of step size, we have that

$$x(t+H) = R_{2,1} + c_1 h_2^2 + O(h_2^4)$$

where c_1 is some constant

Also consider that

$$x(t+H) = R_{1,1} + c_1 h_1^2 + O(h_1^4)$$
$$= R_{1,1} + 4c_1 h_2^2 + O(h_2^4)$$

using $h_1 = 2h_2$

Then since both of these are equal to $x(t+H)$, equate them ~~+ neglect h.o.t.~~ to get

$$c_1 h_2^2 = \frac{1}{3}(R_{2,1} - R_{1,1}) + O(h_2^4)$$

Substitute into the above to get

$$x(t+H) = R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1}) + O(h_2^4)$$

- method has error of order h_2^4
- call the new estimate

$$R_{2,2} = R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1})$$

can continue w/ this idea

- increase # of steps to 3
  so that $h_3 = \frac{H}{3}$
- solve from t to $t+H$ to get
  estimate $R_{3,1}$

calculate estimate

$$R_{3,2} = R_{3,1} + \frac{4}{5}(R_{3,1} - R_{2,1})$$

(reasoning same as before)

we can then write

$$x(t+H) = R_{3,2} + c_2 h_3^4 + O(h_3^6)$$

w/ c_2 a constant

From before we have that

$$x(t+H) = R_{2,2} + c_2 h_2^4 + O(h_2^6)$$

$$= R_{2,2} + \frac{81}{16} c_2 h_3^4 + O(h_2^6)$$

using $h_2 = 3/2\, h_3$

Equating & rearranging gives

$$c_2 h_3^4 = \frac{16}{65}\left(R_{3,2} - R_{2,2}\right)$$

substituting back in gives

$$x(t+H) = R_{3,3} + O(h_3^6)$$

where $R_{3,3} = R_{3,2} + \frac{16}{65}\left(R_{3,2} - R_{2,2}\right)$

result is accurate to order h_3^6

w/ just 3 steps.

Power is the cancellation of higher order errors on successive steps along w/ modified midpoint method having only even-order terms.

can continue this process iteratively

& estimate is

$$x(t+H) = R_{n,m+1} + O(h_n^{2m+2})$$

w/ $m < n$ +

$$R_{n,m+1} = R_{n,m} + \frac{R_{n,m} - R_{n-1,m}}{[n/(n-1)]^{2m} - 1}$$

diagram similar to that for Romberg integration

$$\begin{array}{llllllll}
n=1 & R_{1,1} & & & & & & \\
 & & \searrow & & & & & \\
n=2 & R_{2,1} & \rightarrow & R_{2,2} & & & & \\
 & & \searrow & & \searrow & & & \\
n=3 & R_{3,1} & \rightarrow & R_{3,2} & \rightarrow & R_{3,3} & & \\
 & & \searrow & & \searrow & & \searrow & \\
n=4 & \underbrace{R_{4,1}}_{\text{modified midpoint method}} & \rightarrow & \underbrace{R_{4,2} \rightarrow R_{4,3} \rightarrow R_{4,4}}_{\text{Richardson extrapolation}} & & & &
\end{array}$$

also get estimate of error as

$$\frac{R_{n,m} - R_{n-1,m}}{[n/(n-1)]^{2m} - 1}$$

Limitations :

1) answer only accurate for $x(t+H)$

2) method only converges quickly if the power series expansion of $x(t+H)$ converges quickly.

can overcome these problems by dividing interval into smaller ones & apply ~~Burlisch~~ Bulirsch - Stoer to each one.