i) Adaptive step

·) We want to estimate the error we make with RK4, by taking a step h. RK4 makes an error $O(h^5)$. Therefore if x_1 is the solution estimated with step h and $x(t+h)$ is the true value, we have

$$x(t+h) = x_1 + ch^5 \quad , \text{ where } c \text{ is some constant}$$

·) Let us now take a step $2h$. Assume that x_2 is our solution:

$$x(t+2h) = x_2 + c(2h)^5 = x_2 + 32ch^5 \quad (\gamma)$$

·) Let us move from h to $2h$, by taking two consecutive h steps. Since the error is ch^5 at each step, we get:

$$x(t+2h) = x_1 + 2ch^5 \quad (\star)$$

·) Therefore, combining (γ) and $(\star)$:

$$\begin{cases} x(t+2h) = x_2 + 32ch^5 \\ x(t+2h) = x_1 + 2ch^5 \end{cases} \Rightarrow (x_1 - x_2) = 30ch^5$$

·) Note that $\varepsilon = ch^5$, where ε is the error we make with RK4, when we take a step h. Hence we can compute ε a

$$\boxed{\varepsilon = \frac{1}{30}(x_1 - x_2)}$$

.) Assume we have a target tolerance $\delta =$ error per unit time

Then the accepted error per step is $\delta h'$, if the step is h'!

For step h', the error is $\varepsilon' = c h'^5$. Hence

$$\varepsilon' = c h'^5 = c h'^5 \frac{c h^5}{c h^5} = c h^5 \left(\frac{h'^5}{h^5} \right)$$

We saw before that $c h^5 = \varepsilon = \frac{1}{30}(x_1 - x_2)$. Therefore

$$\varepsilon' = \frac{1}{30}(x_1 - x_2)\left(\frac{h'}{h}\right)^5$$

We want ε' to ~~be~~ satisfy the target tolerance. Hence:

$$\varepsilon' = \frac{1}{30}(x_1 - x_2)\left(\frac{h'}{h}\right)^5 = h'\delta$$

Solve for h':

$$\boxed{h' = h\left(\frac{30\, h\, \delta}{|x_1 - x_2|}\right)^{\frac{1}{4}} = h \rho^{\frac{1}{4}}, \qquad \text{where } \rho \equiv \frac{30\, h\, \delta}{|x_1 - x_2|}}$$

.) Adaptive step algorithm:

1) Get $x + 2h$ by incrementing twice by single step h. Call this solution x_1

2) Get $x + 2h$ by incrementing once by step $2h$. Call

this solution x_2.

3) Use x_1 and x_2 to compute $\rho = \dfrac{30 h \delta}{|x_1 - x_2|}$, where δ is the input target accuracy

4) If $\rho < 1$ we are not meeting the accuracy requirement. Update the step to $h' = h \rho^{\frac{1}{4}}$ and try again

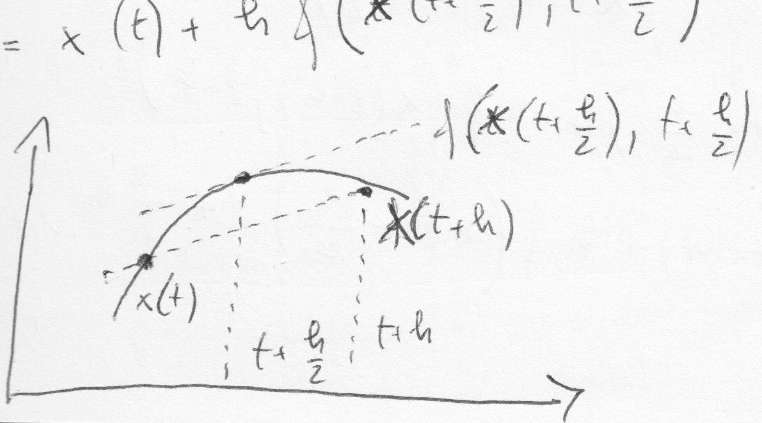
5) If $\rho > 1$ we are doing better than the accuracy requirement. Take the step, moving to $t+2h$ with solution x_1. Then, use $h' = h\rho^{\frac{1}{4}}$ for your next step and repeat.

.) Note that you use x_2 <u>only</u> to estimate the error and compute ρ. When you accept the solution, you always use x_1.

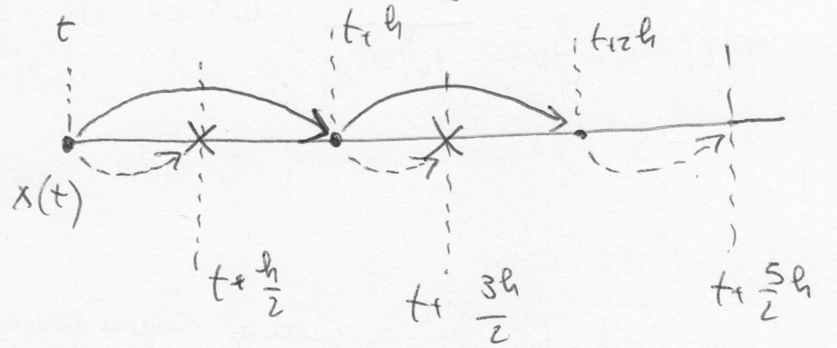
ii) <u>Leapfrog method</u>

.) In the midpoint method, we approximate $x(t+\frac{h}{2})$ with the Euler and use $f(x(t+\frac{h}{2}), t+\frac{h}{2})$ to evaluate the slope:

$$\begin{cases} x(t+\frac{h}{2}) = \frac{h}{2} f(x,t) + x(t) \\ x(t+h) = x(t) + h f\left(x(t+\frac{h}{2}), t+\frac{h}{2}\right) \end{cases}$$

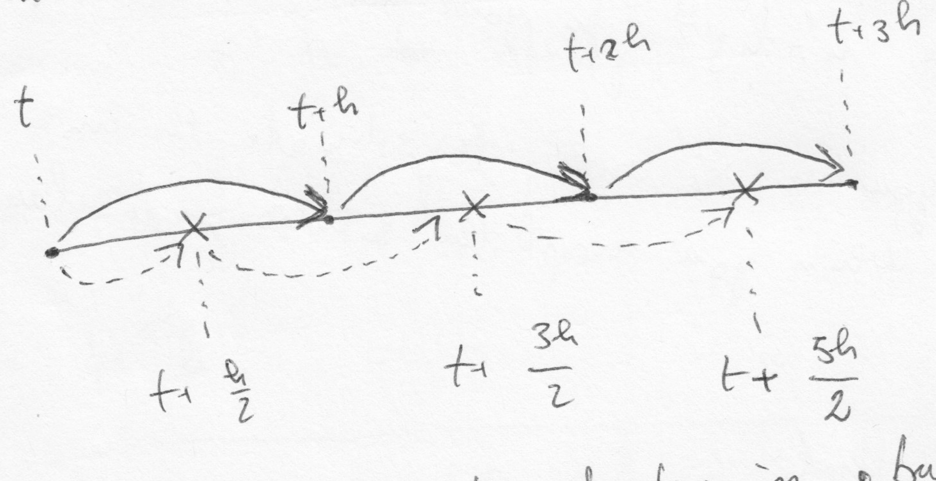


We can schematize graphically as



I use Euler with $\dashrightarrow$ to get slope in X. Then I use the slope in X to approximate the solution in $\bullet$

•) The leapfrog method uses a different approach, we can represent it with the following scheme:



We still evaluate the function in $\bullet$ but after the first step, we evaluate the slope at mid-point x, using the previous mid-point x. In formulae:

1) $x\left(t+\frac{h}{2}\right) = x(t) + \frac{h}{2} f\left(x(t), t\right)$

2) $x(t+h) = x(t) + h f\left(x\left(t+\frac{h}{2}\right), t+\frac{h}{2}\right)$

3) $x\left(t+\frac{3h}{2}\right) = x\left(t+\frac{h}{2}\right) + h f\left(x(t+h), t+h\right)$

4) $x(t+2h) = x(t+h) + h f\left(x\left(t+\frac{3h}{2}\right), t+\frac{3}{2}h\right)$,

and so on.

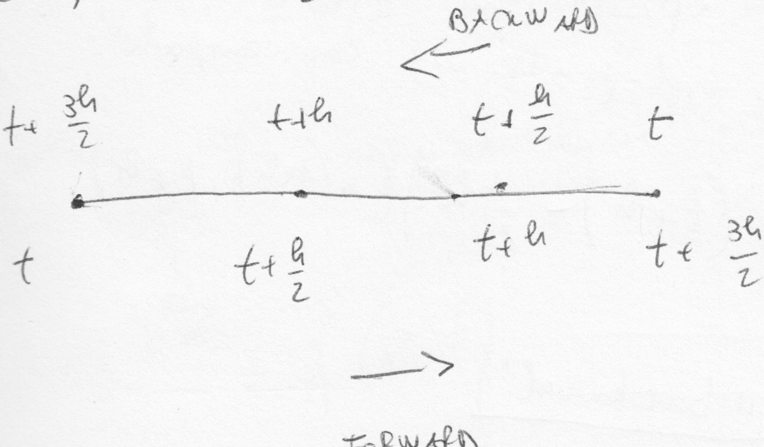
•) The leapfrog method gives an error $O(h^3)$, because it is a mid-point method. Therefore it is less accurate than RK4.

It's useful property is that it is <u>time-reversal symmetric</u>.
This makes it <u>energy conserving</u>, if we compute the ~~energ~~ the mechanical energy of ~~peri~~ physical systems with the periodic motion, at the end of each period.

•) To verify it is time reversal symmetric, take steps 2) and 3) in the leapfrog formulae in the previous page, and <u>replace</u> $\boxed{h \mapsto -h}$, to get

$$2R)\quad x(t-h) = x(t) - h\, f\left(x\left(t-\frac{h}{2}\right),\, t-\frac{h}{2}\right)$$

$$3R)\quad x\left(t-\frac{3h}{2}\right) = x\left(t-\frac{h}{2}\right) - h\, f\left(x(t-h),\, t-h\right)$$



Now, since we move backward (see graph above), we replace $\boxed{t \to t+\frac{3h}{2}}$, and get

$$2R)\quad x\left(t+\frac{h}{2}\right) = x\left(t+\frac{3h}{2}\right) - h\, f\left(x(t+h),\, t+h\right)$$

$$3R)\quad x(t) = x(t+h) - h\, f\left(x\left(t+\frac{h}{2}\right),\, t+\frac{h}{2}\right)$$

$\Downarrow$

Comparing these with 2) and 3) in the previous page shows that we are reproducing the same values in the same points.

•) Let us consider a classical equation of motion

$$\frac{d^2x}{dt^2} = f(x,t)$$

We write this as a system of 1st ordinary DE:

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

In this case, the leapfrog method becomes:

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

This is known as the <u>Verlet method</u>. It gives velocities in the mid-points and $x(t)$ in the endpoints. If we want also velocities at the end-points we can compute:

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

$$\downarrow$$

<u>Euler "backward"</u>

which gives:

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

Putting everything together:

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

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

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

4) $v(t+h) = v(t+\frac{h}{2}) + \frac{k}{2}$

5) $v\left(t+\frac{3h}{2}\right) = v\left(t+\frac{h}{2}\right) + k$

1) to 5) give the complete Verlet method to integrate equations of motion

∘) For systems of equations, Verlet can be written as:

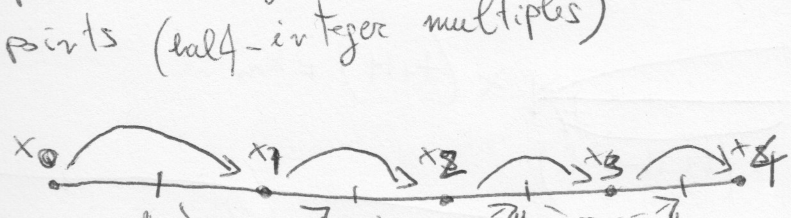
$$\begin{cases} \vec{v}\left(t+\frac{h}{2}\right) = \vec{v}(t) + \frac{h}{2}\vec{f}\left(\vec{r}(t), t\right) \\ \vec{r}\,(t+h) = \vec{r}(t) + h\,\vec{v}\left(t+\frac{h}{2}\right) \\ \vec{k} = h\,\vec{f}\,\left(\vec{r}(t+h), t+h\right) \\ \vec{v}\,(t+h) = \vec{v}\left(t+\frac{h}{2}\right) + \frac{\vec{k}}{2} \\ \vec{v}\left(t+\frac{3}{2}h\right) = \vec{v}\left(t+\frac{h}{2}\right) + \vec{k} \end{cases},$$

where the original equation of motion is written as:

$$\frac{d^2\vec{r}}{dt^2} = \vec{f}\left(\vec{r}, t\right)$$

iii) Modified mid-point method

Consider leapfrog method and call x_i the solutions at the "end-points" (integer multiples of h) and y_i the solutions at the mid-points (half-integer multiples)



We can write leapfrog as:

$x_0 = x(t)$

$y_1 = x_0 + \frac{h}{2} f(x_0, t)$

$x_1 = x_0 + h f(y_1, t + \frac{h}{2})$

$y_2 = y_1 + h f(x_1, t+h)$

$x_2 = x_1 + h f(y_2, t + \frac{3h}{2})$

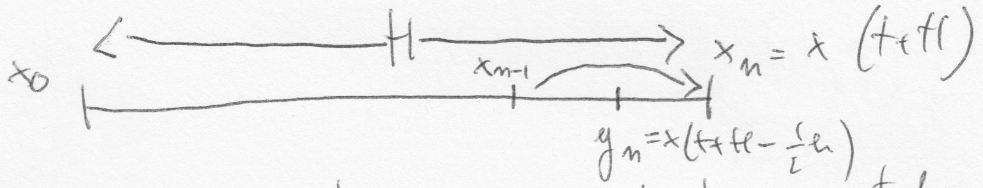
$\vdots$

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

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

This is just leapfrog, written in a slightly different way.

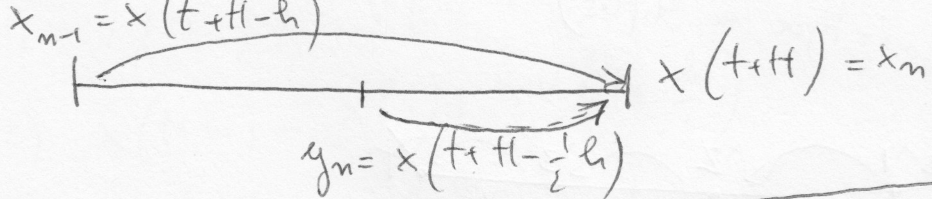
•) Call $x_n = x(t+H)$ the last point (see figure):



Then the last y_n is going to be computed in $y_n = x(t+H-\frac{1}{2}h)$

•) We can however compute $x(t+H)$ also in another way.

See figure:



In leapfrog we have $\boxed{x(t+H) = x_n = x_{n-1} + h f(y_n, t+H-\frac{h}{2})}$

Consider now a "backward" Euler step to go to y_n, from x_n

$$y_n = x_n - \frac{h}{2} f(x_n, t+H)$$

Use it to solve for x_n (Same as in Verlet method):

$$\boxed{x_n = y_n + \frac{h}{2} f(x_n, t+H)}$$

Therefore: $\begin{cases} x_n = x_{n-1} + h f\left(y_n, t+H - \frac{h}{2}\right) & \text{"standard leapfrog"} \\ x_n = y_n + \frac{h}{2} f(x_n, t+H) & \text{"half-step from } y_n\text{"} \end{cases}$

Let's estimate $x(t+H)$ as an average between these two:

$$\boxed{x(t+H) = \frac{1}{2}\Big[\underset{\substack{\downarrow \\ \text{standard} \\ \text{leapfrog}}}{x_n} + y_n + \frac{h}{2} f(x_n, t+H) \Big]}$$

The leapfrog method, modified to include this last formula to evaluate $x(t+H)$, is called the modified mid-point method.

The reason to use it is that it was shown that modified ~~leapfrog~~ mid-point give an error that contains only even powers of the step h:

$$\varepsilon_{\text{modified MP}} = c_1 h^2 + c_2 h^4 + c_3 h^6 + \cdots$$

This is the starting point for the Bulirsch-Stoer method

iv) Bulirsch - Stoer method

·) Consider the equation $\frac{dx}{dt} = f(x,t)$. Want to solve over the interval $[t, t+H]$.

·) Use modified midpoint method and just one step $t \to t+H$. This is a very rough estimate of $x(t+H)$. Call it $R_{1,1}$

·) Now split the interval in two: $h_1 = H$, $h_2 = \frac{H}{2}$. Get a second estimate of $x(t+H)$ and call it $R_{2,1}$. Using the mid-point method, the error will contain only even power of h:

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

Before we had

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

We know that $h_1 = 2h_2$, therefore:

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

Take the difference $2) - 1)$:

$$0 = R_{1,1} - R_{2,1} + 3c_1 h_2^2 + O(h^4)$$

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

Now use this last expression and put it in place of the $c_1 h_2^2$ term on the rhs in 1), to get

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

Combining $R_{1,1}$ and $R_{2,1}$ we have now an error $O(h^4)$! This is the same procedure as we did for Romberg. It is called Richardson extrapolation. As for Romberg, we can iterate recursively, deriving the formulae

$$
\begin{cases}
R_{n,m+1} = R_{n,m} + \dfrac{R_{n,m} - R_{n-1,m}}{\left(\dfrac{n}{n-1}\right)^{2m} - 1} \\[2ex]
x(t+H) = R_{n,m+1} + O\left(h_n^{2m+2}\right)
\end{cases}
$$

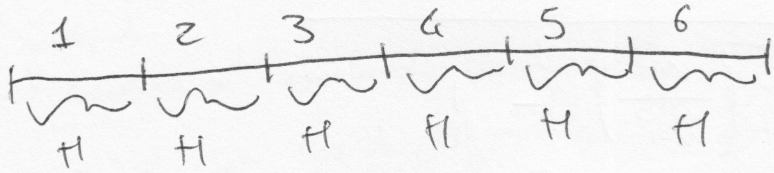
$$
\begin{array}{llllll}
n=1: & R_{1,1} & & & & \\
 & & \searrow & & & \\
n=2: & R_{2,1} & \rightarrow & R_{2,2} & & \\
 & & \searrow & & \searrow & \\
n=3: & R_{3,1} & \rightarrow & R_{3,2} & \rightarrow & R_{3,3} \\
 & & \searrow & & \searrow & & \searrow \\
n=4: & R_{4,1} & \rightarrow & \underbrace{R_{4,2} \;\rightarrow\; R_{4,3} \;\rightarrow\; R_{4,4}}_{\text{Richardson extrapolation.}} \\
\vdots & \downarrow & & & & \\
 & \text{Modified mid-point} & & & &
\end{array}
$$

•) Note: the B-S method works as long as the expansion for the error in powers of h converges fast. Hence you want H to be not too large. Ideally, you would like to converge in maximum 8 steps. Therefore, you want to divide the starting [a, b] interval in which you integrate your equation, in many substeps and use B-S separately in each of them.

Algorithm →

a) Divide your interval in N sub-interval of length H:

$$H = \frac{b-a}{N} \quad (N = \text{number of sub-intervals})$$



(N=6 in this example)

b) Start with interval 1 and apply B-S to get $R_{1,1}$

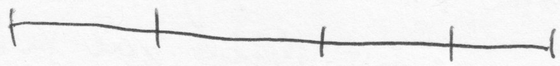
c) Now set $n=2$ and compute $R_{2,1}$ and $R_{2,2}$. At the end, compute the error which, for row n is given by:

$$\varepsilon_{n,m} = \frac{R_{n,m} - R_{n-1,m}}{\left(\frac{n}{n-1}\right)^{2m} - 1}$$

d) Compare this error with the target tolerance $H\delta$. If the error is smaller, accept the solution for your current interval and move to the next. Otherwise, go back to c) and increment n by 1.

•) You can also implement adaptive steps in this way:

a) Choose an initial N. E.g.: N = 4



b) Go through the B-S algorithm on the various intervals. If, in a given interval, you converge within 8 rows of the Richardson extrapolation scheme, accept and move on. If you <u>don't</u> converge to the desired precision, then <u>stop</u>, subdivide the "problematic interval in 2, and repeat B-S separately in each subinterval