Ordinary Differential EquationsODEs

Part 2

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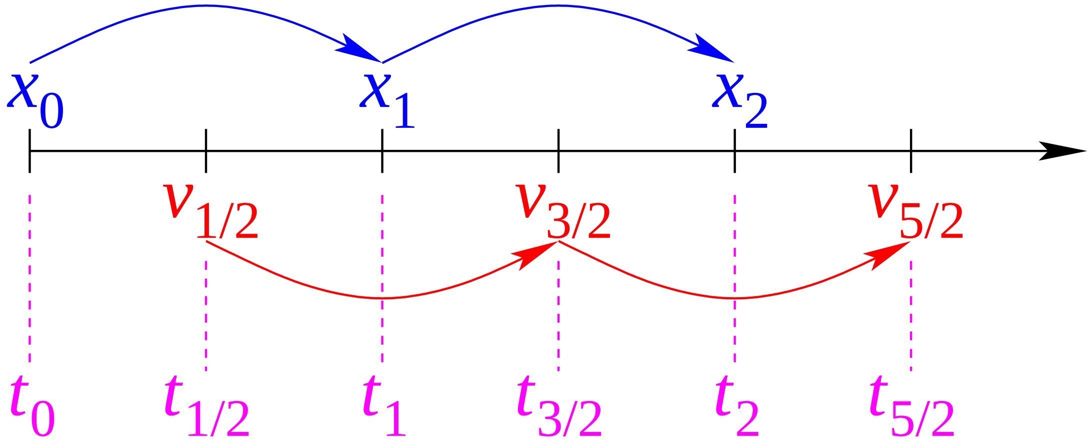
The Leapfrog Integrator

- Very useful for second-order DEs in which $d^2\mathbf{x}/dt^2 = \mathbf{f}(\mathbf{x})$, e.g., SHM, N-body, etc.
  - NOTE: Now dropping the prime ($'$) from $\mathbf{f}$...
- Suppose $\mathbf{x}$ is position, so $d^2\mathbf{x}/dt^2$ is acceleration.
- Procedure: define $\mathbf{v} = d\mathbf{x}/dt$ at the *midpoints* of the steps, i.e., velocities staggered wrt positions.
  - Set $\mathbf{v}_{n+1/2} = \mathbf{v}(t_n + \frac{1}{2}h)$.
  - Then advance $\mathbf{x}_n$ to $\mathbf{x}_{n+1}$ and $\mathbf{v}_{n+1/2}$ to $\mathbf{v}_{n+3/2}$:

$$
\begin{aligned}
\mathbf{x}_{n+1} &= \mathbf{x}_n + h\mathbf{v}_{n+1/2}, \\
\mathbf{v}_{n+3/2} &= \mathbf{v}_{n+1/2} + h\mathbf{f}(\mathbf{x}_{n+1}).
\end{aligned}
$$


x_0
x_1
x_2
$v_{1/2}$
$v_{3/2}$
$v_{5/2}$
t_0
$t_{1/2}$
t_1
$t_{3/2}$
t_2
$t_{5/2}$

- Complication: need to “jumpstart” and “resync”...

$$\begin{aligned}
\mathbf{v}_{n+1/2} &= \mathbf{v}_n + (h/2)\mathbf{f}(\mathbf{x}_n) && \text{[opening “kick”: Euler]} \\
\mathbf{x}_{n+1} &= \mathbf{x}_n + h\mathbf{v}_{n+1/2} && \text{[“drift”]} \\
\mathbf{v}_{n+1} &= \mathbf{v}_{n+1/2} + (h/2)\mathbf{f}(\mathbf{x}_{n+1}) && \text{[closing “kick”: resync]}
\end{aligned}$$

  - Note $\mathbf{v}_{n+3/2} = \mathbf{v}_{n+1} + (h/2)\mathbf{f}(\mathbf{x}_{n+1}) = \mathbf{v}_{n+1/2} + h\mathbf{f}(\mathbf{x}_{n+1})$.

- Also have "drift-kick-drift" (DKD) scheme.
- Like midpoint method, Leapfrog is second order:

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

but

$$\mathbf{v}(t+h/2) = \mathbf{v}(t) + (h/2)\mathbf{f}(t) + \mathcal{O}(h^2).$$

Therefore

$$\mathbf{x}(t+h) = \mathbf{x}(t) + h\mathbf{v}(t) + (h^2/2)\mathbf{f}(t) + \mathcal{O}(h^3).$$

  - This is formally equivalent to midpoint method.

- So why is Leapfrog so great?...
- Answer: Leapfrog is *time reversible*.
- Suppose we step back from $(t_{n+1}, \mathbf{x}_{n+1}, \mathbf{v}_{n+3/2})$ to $(t_n, \mathbf{x}_n, \mathbf{v}_{n+1/2})$. Applying the algorithm:

$$\begin{aligned} \mathbf{v}_{n+1/2} &= \mathbf{v}_{n+3/2} + (-h)\mathbf{f}(\mathbf{x}_{n+1}), \\ \mathbf{x}_n &= \mathbf{x}_{n+1} + (-h)\mathbf{v}_{n+1/2}. \end{aligned}$$

- These are precisely the steps (in reverse) that we took to advance the system in the first place!
- Hence if we Leapfrog forward in time, then reverse to $t = 0$, we're back to where we started, *precisely*.

- Leapfrog is time reversible because of the symmetric way in which it is defined, unlike the other schemes.
  - In Euler, forward and backward steps do not cancel since they use different derivatives at different times.
  - In Midpoint, the estimate of the derivative is based on an extrapolation from the left-hand side of the interval. On time reversal, the estimate would be based on the right-hand side, not the same.
  - Similarly, RK4 is not time reversible.
- Time reversibility is important because it guarantees conservation of energy, angular momentum, etc. (in many cases).
  - Suppose the integrator makes an error ε after one orbital period. Now reverse. Is the error $-\varepsilon$? No! The time-reversed orbit is a solution of the original ODE (with $\mathbf{v}$ replaced with $-\mathbf{v}$), so the energy error is still $+\varepsilon$. But we've returned to our starting point, so we know the final energy error is zero. Hence $\varepsilon = 0$!

- Leapfrog is only second order, but very stable.
- Leapfrog is an example of a class of "symplectic" integrators that conserve phase-space volume: exactly solves an approximate Hamiltonian system.

$$H = H_D + H_K + H_{\mathrm{err}} = \frac{1}{2}v^2 + V(\mathbf{r}) + H_{\mathrm{err}},$$

or $D(h/2)K(h)D(h/2)$, with $H_{\mathrm{err}} \sim \mathcal{O}(h^3)$. You can also construct the usual kick-drift-kick scheme, $K(h/2)D(h)K(h/2)$, because the Hamiltonian is separable.

Adaptive Stepsize Control

- Up to now, have assumed stepsize h is constant.
- Clearly prefer choosing h small when $|\mathbf{f}'|$ is large, and h large when $|\mathbf{f}'|$ is small. (We've reintroduced the prime ($'$) notation, just to be confusing...)
- The tradeoff is extra trial steps to determine optimum h, but may achieve factor of 10 to 100 increase in stepsize, so it's often worth it.
- *NRiC* provides a routine `odeint()` for RK4 with adapative stepsize control. Complicated to use!