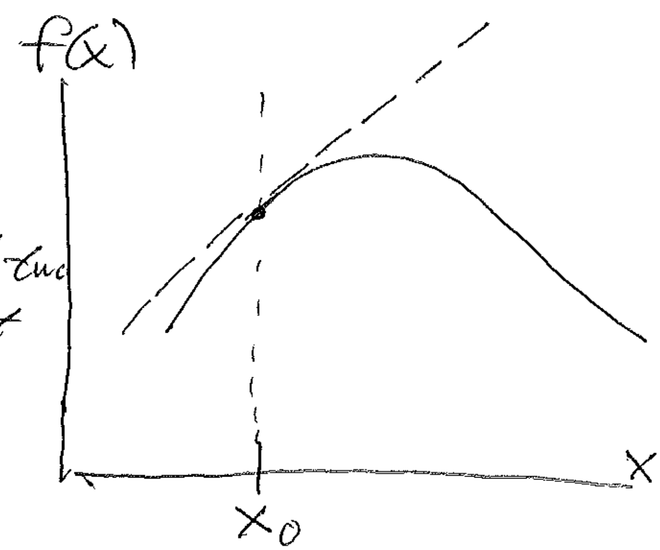
Taylor Series

Suppose you have a function, $f(x)$, that is defined in some region around the point $x = x_0$. Then, $f(x)$ can be expanded in a Taylor series

1) $$f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{1}{2} f''(x_0)(x-x_0)^2 + \frac{1}{3!} f'''(x_0)(x-x_0)^3 + \ldots$$

Here, $f'(x_0) = \left.\frac{df}{dx}\right|_{x=x_0}$. Oftentimes, one only needs to keep the first two terms, i.e., the constant and linear terms. Then



2) $$f(x) \simeq f(x_0) + f'(x_0)(x-x_0)$$

This is equivalent to approximating the function as a straight line in the vicinity of x_0, as shown in the diagram.

Forward Euler Method

Now, consider an ordinary differential equation (ODE) of the form

$$3) \quad \frac{dx}{dt} = F(x,t) \qquad x(t_0) = x_0$$

This is an ODE, rather than a partial differential equation (PDE), because it involves only a single independent variable, t. If the function $x(t)$ depended on another variable as well, e.g. $x(t,s)$, and if derivatives were taken with respect to both t and s, then we would have a PDE.

Eq. (3) is called a first-order ODE because only a first derivative, $\frac{dx}{dt} = x'(t)$, is involved. If we had a term in $\frac{d^2x}{dt^2}$, then we would have a second-order ODE. Eq. (3) is sometimes called an "initial value problem," because it starts from an initial value x_0 at $t=t_0$.

Now, the simplest way to integrate (i.e. solve) eq. (3) is called the forward Euler method. We start by expanding $x(t)$ in a Taylor series around the point t_0:

$$4) \quad x(t) \cong x_0 + \left.\frac{dx}{dt}\right|_{t=t_0} (t-t_0) + \ldots$$

where we have kept only the linear term of the expansion. Let's assume that we want to time-step our solution along with a fixed time step, Δt. Graphically

Then, letting $t_1 - t_0 = \Delta t$, and recalling from eq. (3) that $\frac{dx}{dt} = F(x,t)$, we can write

5) $x_1 \simeq x_0 + F(x_0, t_0)\,\Delta t$

One then simply repeats this process at the next time step, and so forth. Generalizing, we can write

$$\boxed{6)\quad x_{n+1} \simeq x_n + F(x_n, t_n)\,\Delta t}$$

This is the forward Euler method.

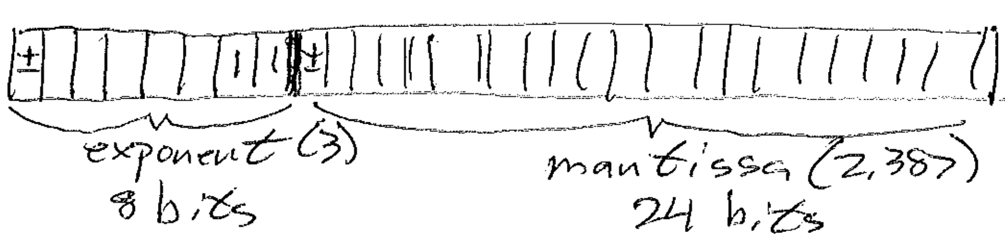
Errors in Integration (Accuracy)

There are two sources of error when integrating (solving) differential equations numerically. The first is called <u>truncation error</u>. We get this because we have neglected terms in the Taylor series expansion. For forward Euler, we've neglected everything beyond the linear term, i.e.

$$7)\quad x_{n+1} = x_n + \frac{dx}{dt}\Big|_{t=t_n}\Delta t + \underbrace{\frac{1}{2}\frac{d^2x}{dt^2}\Big|_{t=t_n}(\Delta t)^2}_{O(\Delta t)^2 \ \text{(neglected}}$$

The first neglected term is of order $(\Delta t)^2$, so we say the error is $O(\Delta t)^2$.

The second source of error is called <u>roundoff error</u>. It arises because the computer can only store numbers to a certain accuracy. For 32-bit machines operating in single precision, that accuracy is about 1 part in 10^7. One can see this by considering a "floating point" (real) number of the form $2{,}387 \times 10^3$. This is stored in the computer in the following way:



The accuracy is determined by the number of bits in the mantissa. One bit is needed for a $\pm$ sign, so this leaves 23 bits for the number. There are thus $2^{23} \cong 10^7$ possibilities, as each bit must be either 1 or 0. If you are working in double precision, or if you have a 64-bit machine (which nearly all computers are these days), then you have twice this accuracy, or about 1 part in 10^{14}.

Balancing errors

For a given numerical method, then, there will be some optimal time step, Δt, at which you get the best accuracy. If Δt is ~~smaller~~ larger than this, then truncation error dominates. If Δt is too small, then roundoff error dominates.

Note that the accuracy of forward Euler increases proportionately to Δt. One makes an error of $O(\Delta t)^2$ at each step. But if one is integrating, say, from $t=0$ to 1, then the number of steps is $N = 1/\Delta t$. Thus, the accumulated error at the end of the integration is:

$$\text{Error} \propto O(\Delta t)^2 \cdot \underbrace{\left(\frac{1}{\Delta t}\right)}_{N} \propto \Delta t$$

Thus, FE is called a "first-order" method.

Runge-Kutta methods.

Put these in the same notation as Euler's method.

1) Second-order method:

Let

$$\Delta X_1 = F(X_n, t_n)\,\Delta t$$
$$X_{n+1/2} = X_n + \tfrac{1}{2}\Delta X_1$$
$$t_{n+1/2} = t_n + \tfrac{1}{2}\Delta t$$
$$\Delta X_2 = F(X_{n+1/2}, t_{n+1/2})$$
$$X_{n+1} = X_n + \Delta X_2 + O(\Delta t^3)$$

2) 4^{th}-order method

$$\Delta X_1 = F(X_n, t_n)\,\Delta t$$
$$X_1 = X_n + \tfrac{1}{2}\Delta X_1$$
$$t_{n+1/2} = t_n + \tfrac{1}{2}\Delta t$$
$$\Delta X_2 = F(X_1, t_{n+1/2})\,\Delta t$$
$$X_2 = X_n + \tfrac{1}{2}\Delta X_2$$
$$\Delta X_3 = F(X_2, t_{n+1/2})\,\Delta t$$
$$X_3 = X_n + \tfrac{1}{2}\Delta X_3$$
$$t_{n+1} = t_n + \Delta t$$
$$\Delta X_4 = F(X_3, t_{n+1})\,\Delta t$$

$$X_{n+1} = X_n + \frac{\Delta X_1}{6} + \frac{\Delta X_2}{3} + \frac{\Delta X_3}{3} + \frac{\Delta X_4}{6} + O(\Delta t^5)$$

Types of errors:

1) Truncation error

2) Roundoff error

Now, talk about stability $\Rightarrow$ implicit methods

Forward Euler: Stability

Recall that the method comes from a Taylor series expansion:

$$\frac{dx}{dt} = F(x_n, t_n) \qquad x(t_0) = x_0$$

$$x_{n+1} \tilde{=} x_n + F(x_n, t_n)\Delta t + \underbrace{\frac{1}{2}F'(x_n, t_n)(\Delta t)^2}_{\text{error}}$$

Now, consider the exponential function:

$$\frac{dx}{dt} = \lambda x(t) \qquad x(t_0) = x_0$$

This has the analytic solution:

$$x(t) = x_0 e^{\lambda t} \qquad \begin{array}{l} F(x_n) = \lambda x_n \\ F'(x_n) = \lambda^2 x_n \end{array}$$

so

$$x_{n+1} = x_n + \lambda x_n \Delta t + \frac{1}{2}\lambda^2 x_n (\Delta t)^2$$

$$= x_n \left(1 + \lambda\Delta t + \underbrace{\frac{1}{2}(\lambda\Delta t)^2}_{\text{error}}\right)$$

We ran into trouble if the error term is larger than the first-order term, i.e. if

$$\frac{1}{2}(\lambda\Delta t) > 1$$

or

$$\Delta t > \frac{2}{\lambda}$$

So, the requirement for stability is just the opposite of this:

$$\boxed{\Delta t < \frac{2}{\lambda}}$$

Now, consider a decaying exponential:

$$x(t) = x_0 e^{-\lambda t}$$

$$F'(x_n) = -\lambda x_n$$
$$F'(x_n) = \lambda^2 x_n$$

$$x_{n+1} = x_n - \lambda x_n \Delta t + \frac{1}{2}\lambda^2 x_n (\Delta t)^2$$

$$= x_n\left(1 - \lambda \cancel{x_n} \Delta t + \frac{1}{2}(\lambda \Delta t)^2\right)$$

We still run into trouble if

$$\frac{1}{2}(\cancel{\Delta}\lambda\Delta t) > 1$$

or

$$\boxed{\Delta t > \frac{2}{\lambda}}$$