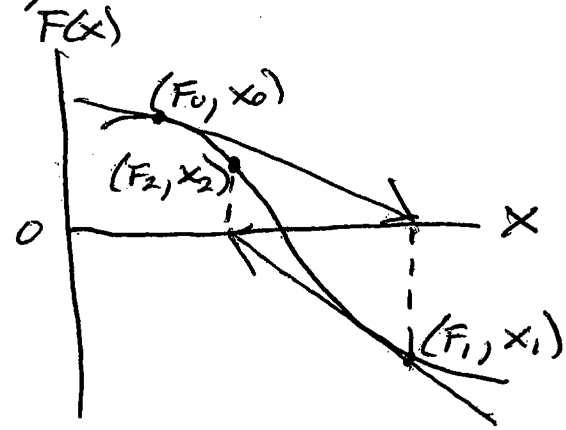
Newton's method in 1-D

Suppose we want to solve an equation

(1) $$F(x) = 0$$



Let x_0 represent your initial guess. Now expand $F(x)$ in a Taylor series around point x_0:

(2) $$F(x) \simeq F(x_0) + \left.\frac{dF}{dx}\right|_{x=x_0} (x - x_0) + \ldots$$

Set $F(x) = 0$. Then

(3) $$x - x_0 = -F(x_0)/F'(x_0)$$

or

(4) $$\boxed{x = x_0 - F(x_0)/F'(x_0)}$$

Repeat until procedure converges

Extension to many dimensions

Now, let's suppose we have a vector function $\vec{F}$ with vector arguments $\vec{x}$. Want to solve

(5) $$\vec{F}(\vec{x}) = 0$$

[illegible] $\vec{x} = \Delta \vec{r}$)

$$\frac{d\vec{F}}{d\vec{X}} = \begin{pmatrix} \frac{\partial F_1}{\partial x_1} & \frac{\partial F_1}{\partial x_2} & \cdots & \frac{\partial F_1}{\partial x_N} \\ \frac{\partial F_2}{\partial x_1} & & & \\ \vdots & & & \\ \frac{\partial F_N}{\partial x_1} & \cdots & \cdots & \frac{\partial F_N}{\partial x_N} \end{pmatrix} \equiv J$$

(Jacobian matrix)

Expand $\vec{F}$ around pt. $\vec{X}_0$:

$$(6) \quad \vec{F}(\vec{X}) = \vec{F}(\vec{X}_0) + \underbrace{\left.\frac{d\vec{F}}{d\vec{X}}\right|_{\vec{X}=\vec{X}_0}}_{J} \underbrace{(\vec{X}-\vec{X}_0)}_{\vec{\Delta X}} + \ldots$$

Setting $\vec{F}(\vec{X}) = 0$ gives

$$\boxed{(7) \quad J\vec{\Delta X} = -\vec{F}(\vec{X}_0)}$$

This is a matrix equation that can be solved numerically for $\vec{\Delta X}$. Then

$$(8) \quad \vec{X} = \vec{X}_0 + \vec{\Delta X}$$

In general, then, the iterative method is

$$(9) \quad J\vec{\Delta X} = -\vec{F}(\vec{X}_n)$$

$$(10) \quad \vec{X}_{n+1} = \vec{X}_n + \vec{\Delta X}$$

Forward & Reverse Euler Method

Consider an ordinary differential equation (ODE) of the form:

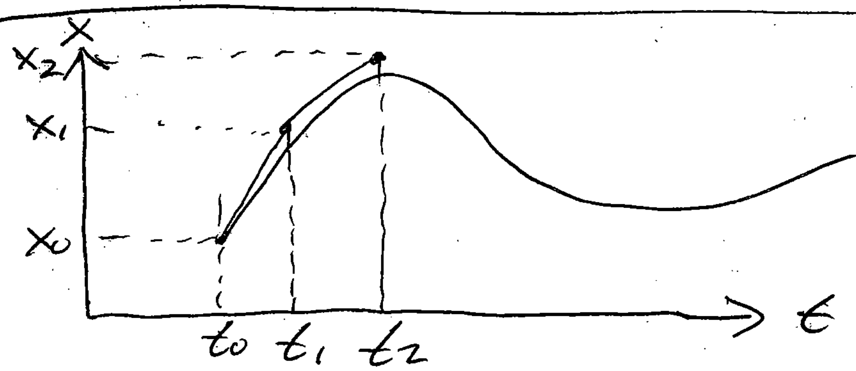
1) $$\frac{dx}{dt} = F(x,t) \qquad x(t_0) = x_0$$

This is an initial value problem, Can find an approximate solution at time t_1 by expanding $x(t)$ in a Taylor series. Let $x_1 \equiv x(t_1)$. Then

2) $$x_1 \simeq x_0 + \left.\frac{dx}{dt}\right|_{t=t_0} \underbrace{(t_1 - t_0)}_{\Delta t}$$
$$= x_0 + F(x_0, t_0)\,\Delta t$$

Can generalize this to the forward Euler method:

3) $$\boxed{x_{n+1} = x_n + F(x_n, t_n)\,\Delta t}$$



In N dimensions, we can generalize this to:

4) $$\frac{d\vec{x}}{dt} = \vec{F}(\vec{x},t) \equiv \vec{F}(\vec{x})$$

where I will suppress the t-dependence for convenience. (It's still there, though!) The generalization of forward Euler is straigtforward:

5) $$\boxed{\vec{x}_{n+1} = \vec{x}_n + \vec{F}(\vec{x}_n)\Delta t}$$

(Now do Runge-Kutta)

For stiff equations, we need an implicit method. The simplest of these is the reverse Euler method:

6) $$\vec{x}_{n+1} = \vec{x}_n + \vec{F}(\vec{x}_{n+1})\Delta t$$

We get $\vec{F}(\vec{x}_{n+1})$ by expanding $\vec{F}$ in a Taylor series:

7) $$\vec{F}(\vec{x}_{n+1}) \simeq \vec{F}(\vec{x}_n) + \underbrace{\left.\frac{d\vec{F}}{d\vec{x}}\right|_{\vec{x}=\vec{x}_n}}_{J} \underbrace{(\vec{x}_{n+1} - \vec{x}_n)}_{\Delta\vec{x}} + \ldots$$

where J is the Jacobian matrix. From eq. (6) above, we can write:

8) $$\Delta\vec{x} = \vec{F}(\vec{x}_{n+1})\Delta t$$

and then, using (7) to replace $\vec{F}(\vec{x}_{n+1})$, we have:

9) $\vec{\Delta x} \cong \left[\vec{F}(\vec{x}_n) + J \vec{\Delta x} \right] \Delta t$

Now, we have a $\vec{\Delta x}$ on both sides of the equation. So, use the relation:

10) $\vec{\Delta x} = I \vec{\Delta x}$

where I is the identity matrix

$$I = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & \ddots \; 1 \end{pmatrix}$$

Then, we can write (9) as:

11) $(I - J\Delta t) \vec{\Delta x} = \vec{F}(\vec{x}_n) \Delta t$

or, dividing through by Δt:

$$\boxed{12) \quad \left(\frac{1}{\Delta t} I - J\right) \vec{\Delta x} = \vec{F}(\vec{x}_n)}$$

This, along with the formula: $\vec{\Delta x} = \vec{x}_{n+1} - \vec{x}_n$, is the prescription for reverse Euler. Note that as $\Delta t \to \infty$, eq. (12) reduces to

$$J\overrightarrow{\Delta x} = -\vec{F}(\vec{x}_n)$$

which is Newton's method for algebraic equations.

Crank-Nicholson

Now, suppose we use the expression

$$\vec{x}_{n+1} = \vec{x}_n + \left[\theta\vec{F}(\vec{x}_{n+1}) + (1-\theta)\vec{F}(\vec{x}_n)\right]\Delta t$$

Then

$$\overrightarrow{\Delta x} = \left\{\theta\left[\vec{F}(\vec{x}_n) + J\overrightarrow{\Delta x}\right] + (1-\theta)\vec{F}(\vec{x}_n)\right\}\Delta t$$

$$= \left[\vec{F}(\vec{x}_n) + \theta J\overrightarrow{\Delta x}\right]\Delta t$$

Solving for $\overrightarrow{\Delta x}$ yields:

$$\boxed{\left(\frac{1}{\Delta t}I - \theta J\right)\overrightarrow{\Delta x} = \vec{F}(\vec{x}_n)}$$

Crank-Nicholson corresponds to $\theta = \frac{1}{2}$, i.e. centered differencing in time. This gives you 2nd-order time accuracy, as opposed to 1st-order accuracy for forward or reverse Euler.