Runge-Kutta Methods

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Notation

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Let $h = t_{n+1} - t_n$ be the step size.

Finally, let $x_i' = \left.\frac{dx}{dt}\right|_{t=t_i}$, $x_i'' = \left.\frac{d^2x}{dt^2}\right|_{t=t_i}$ and so on.

Forward Euler Method

Taylor's Series:

$$x_{n+1} = x_n + hx'_n + \frac{h^2}{2!}x''_n + \frac{h^3}{3!}x'''_n + \dots \tag{1}$$

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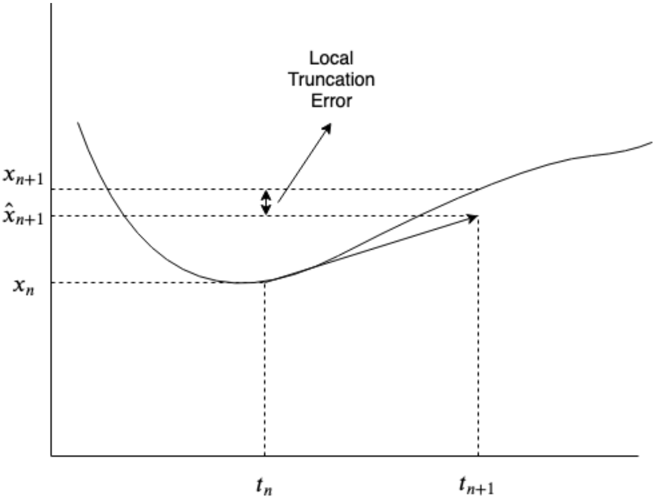
Local truncation error is $\mathcal{O}(h^2)$.

Visualizing the Forward Euler Method



Second Order Runge-Kutta Method

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Using Chain Rule

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Substituting this above gives

$$x_{n+1} \approx x_n + hf(x_n,t_n) + \frac{h^2}{2!}\left[\frac{\partial f(x_n,t_n)}{\partial t} + \frac{\partial f(x_n,t_n)}{\partial x}f(x_n,t_n)\right]. \tag{5}$$

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$$t_k = t_n + \alpha h \tag{6}$$

for some α and

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$$x_k = x_n + \beta h f(x_n, t_n) \tag{7}$$

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Goal: Develop method with error $\mathcal{O}(h^3)$ without computing derivatives of $f(x,t)$

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Also define

$$\begin{aligned} k_1 &= hf(x_n, t_n), \\ k_2 &= hf(x_k, t_k). \end{aligned} \tag{8}$$

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Want to use k_1 and k_2 to get x_{n+1}

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Note that

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Error is $\mathcal{O}(h^3)$

Second Order Runge-Kutta Method

Substitute and rearrange:

$$x_{n+1} \approx x_n + (a+b)hf(x_n, t_n) + \frac{h^2}{2!}\left[b\beta f(x_n, t_n)\frac{\partial f(x_n, t_n)}{\partial x} + b\alpha\frac{\partial f(x_n, t_n)}{\partial t}\right]$$

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Compare coefficients

$$\begin{aligned} a + b &= 1, \\ b\beta &= 1, \\ b\alpha &= 1. \end{aligned}$$

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Infinite number of possible solutions.

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$$\begin{aligned} k_1 &= hf(x_n, t_n), \\ k_2 &= hf(x_n + hk_1, t_n + h), \\ x_{n+1} &= x_n + \frac{1}{2}(k_1 + k_2). \end{aligned}$$

Fourth Order Runge-Kutta

$$
\begin{aligned}
k_1 &= hf(x_n, t_n), \\
k_2 &= hf(x_n + k_1/2, t_n + h/2), \\
k_3 &= hf(x_n + k_2/2, t_n + h/2), \\
k_4 &= hf(x_n + k_3, t_n + h), \\
x_{n+1} &= \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4).
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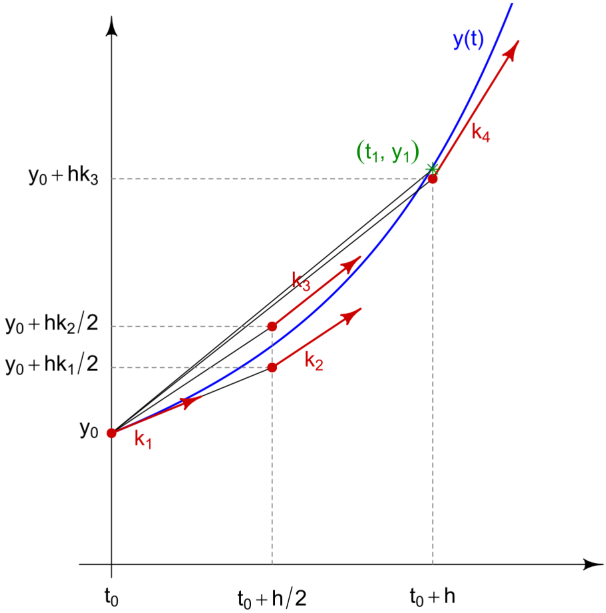
Error is $\mathcal{O}(h^5)$

Visualizing the Fourth Order Runge-Kutta Method



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Are stable for all values of h.

However, we can not express x_{n+1} in terms other than itself.

Backward Euler Method

Let us expand x_n using the Taylor's Series as follows

$$x(t_n) = x(t_{n+1} - h) = x_{n+1} - hx'_{n+1} - \frac{h^2}{2!}x'_{n+1} + \dots \tag{10}$$

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Considering only the first two terms on the right hand side above and rearranging gives

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Error however is still $\mathcal{O}(h^2)$.

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For q-stage implicit Runge-Kutta

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k_j is approximating $\frac{dx}{dt}$ at $t + c_j h$.

First argument to f is approximation of $x(t + c_j h)$ using all k's.

Alternative Formulation

Approximate x_{n+1} via

$$x_{n+1} = x_n + h \sum_{i=1}^{q} b_i f(x^{n+c_i}, t^{n+c_i}) \tag{15}$$

where $t^{n+c_i} = t_n + c_i h$ and

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$$x^{n+c_i} = x_n + h \sum_{j=1}^{q} a_{ij} f(x^{n+c_j}, t^{n+c_j}) \tag{16}$$

approximates $x(t_n + c_i h)$

A Deep Learning Application

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Rearrange previous two equations:

$$x_n = x_{n+1} - h \sum_{i=1}^{q} b_i f(x^{n+c_i}) \tag{17}$$

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Ask a neural net to predict

$$[x^{n+c_1}, \ldots, x^{n+c_q}, x_{n+1}]. \tag{19}$$

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Enforce

$$\mathcal{L} = \sum_{j=1}^{q+1} ||\hat{x}_{n,j} - x_n||^2. \tag{20}$$