Notes on Numerical Optimization Methods

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October 30, 2015

1 Initial Value Problems

The general form of a first order initial value problem (IVP) can be stated as follows[1]:

$$\frac{\mathrm{d}z}{\mathrm{d}t} = f(t, z), \qquad t \in [0, t_f]; \tag{1a}$$

$$z(0) = z_0. \tag{1b}$$

[1] Different notation for differentiation

Gottfried Leibniz	$\frac{\mathrm{dz^n}}{\mathrm{dt^n}}$
Joseph Louis Lagrange	$z'(t), z''(t), ..z^{(n)}(t)$
Isaac Newton	$\dot{z}, \ddot{z}, ..$

The dependent variable z is a vector of m components. The independent variable t is a scalar within the specified range from 0 to t_f.If t does not appear explicitly in the governing equation $f(\cdot)$, the system is called *autonomous*. Otherwise, the system is *nonautomonous*. The initial state of the system is given by a known parameter vector z_0.

1.1 Numerical Solution Methods

Numberical solution approaches deal with finite dimensional representations of Eq.(1) after discritizing the equations in the continuous interval. For that, a mesh is introduced with a sequence of $N + 1$ distant points:

$$0 = t_0 < t_1 < \cdots < t_{n-1} < t_n < \cdots < t_N = t_f \tag{2}$$

and the length of the n^{th} step is denoted by:

$$h_n = t_n - t_{n-1}, \qquad n = 1, 2, \ldots, N. \tag{3}$$

It's generally helpful to use Taylor's expansion to derive numerical solution procedures to Eq.(1a). Consider a Taylor series at $t = t_{n-1}$:

$$z(t_n) = z(t_{n-1}+h_n) = z(t_{n-1})+h_n z'(t_{n-1})+\frac{h_n^2}{2}z''(t_{n-1})+\ldots+\frac{h_n^p}{k!}z^{(p)}(t_{n-1})+\ldots, \tag{4}$$

which is often trucated up to the second order:

$x = \mathcal{O}(h^p)$ means $\exists C > 0$ such that $|x| \leqslant Ch^p$.

$$z(t_n) = z(t_{n-1}) + h_n z'(t_{n-1}) + \frac{h_n^2}{2} z''(t_{n-1}) + \mathcal{O}(h_n^2) \tag{5}$$

1.1.1 First Order Approaches

Three well known basic approaches for IVPs are the forward Euler, backward Euler, and Trapezoidal methods.

Forward Euler If the expansion in Eq.(4) is only up to the first order, we have

We note $z(t_n)$ as z_n for short

$$z_n \approx z_{n-1} + h_n z'_{n-1}, \qquad , n = 1, 2, \dots, N. \tag{6}$$

Evaluate the derivative $z'_{n-1} = f(t_{n-1}, z_{n-1})$ and use the first order approaxiation, and the forward Euler formula[2] is

[2] This is an explicit formula

$$z_n = z_{n-1} + h_n f(t_{n-1}, z_{n-1}), \qquad , n = 1, 2, \dots, N. \tag{7}$$

Backward Euler The backward Euler formula is also derived from Taylor series of centered at $t = t_n$:

$$z(t_n) = z(t_{n+1} - h_{n+1}) = z(t_{n+1}) - h_{n+1} z'(t_n) + \frac{h_{n+1}^2}{2} z''(t_n) + \mathcal{O}(h_{n+1}^2) \tag{8}$$

Similar to the previous procedure, we obtain the backward Euler formula[3]:

[3] This is an implicit formula

$$z_{n+1} = z_n + h_{n+1} f(t_n, z_n) \tag{9}$$

Trapezoidal Method The Trapezoidal rule is developed by Taylor expansion centered at $t_{n-\frac{1}{2}} = t_{n-1} + \frac{h_n}{2}$:

$$z(t_n) = z(t_{n-\frac{1}{2}} + \frac{h_n}{2}) = z(t_{n-\frac{1}{2}}) + \frac{h_n}{2} z'(t_{n-\frac{1}{2}}) + \frac{h_n^2}{2 \cdot 2^2} z''(t_{n-\frac{1}{2}}) + \mathcal{O}(h_n^2) \tag{10a}$$

$$z(t_{n-1}) = z(t_{n-\frac{1}{2}} - \frac{h_n}{2}) = z(t_{n-\frac{1}{2}}) - \frac{h_n}{2} z'(t_{n-\frac{1}{2}}) + \frac{h_n^2}{2 \cdot 2^2} z''(t_{n-\frac{1}{2}}) + \mathcal{O}(h_n^2) \tag{10b}$$

Substract Eq.(10b) with Eq.(10a) and devide by the step size h_n:

$$\frac{z_n - z_{n-1}}{h_n} = z'_{n-\frac{1}{2}} + \mathcal{O}(h_n^2) \tag{11}$$

Evaluating the derivatie at the middle point and rearranging the above equation leads to

Derivative at the middle point $z'_{n-\frac{1}{2}} = \frac{1}{2}\left(f(t_{n-1}, z_{n-1}) + f(t_n, z_n)\right)$

$$z_n = z_{n-1} + \frac{h_n}{2}\left(f(t_{n-1}, z_{n-1}) + f(t_n, z_n)\right) \tag{12}$$