Notes on Dynamic Optimization

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1 Initial Value Problems

The general form of a first order initial value problem (IVP) for ordinary differential equation (ODE) systems can be stated as follows:

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

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

Different notation for differentiation:

Gottfried Leibniz	$\frac{\mathrm{d}z^{\mathrm{n}}}{\mathrm{d}t^{\mathrm{n}}}$
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.

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 Basic First Order Approaches

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

1.1.1 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

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

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

This is an explicit formula

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

Truncation error is obtained by inserting the analytical solution z(t) into the numerical method and dividing by the step size:

$$T_n = \frac{z_{n+1} - z_n}{h} - f(t_n, z(t_n))$$

, and $f(t_n, z(t_n)) = z'(t_n)$.

1.1.2 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:

This is an implicit formula

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

1.1.3 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:

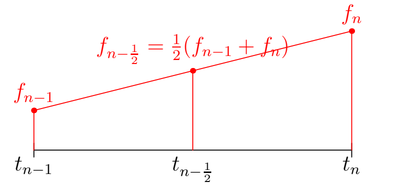
$$\frac{z_n - z_{n-1}}{h_n} = z'_{n-\frac{1}{2}} + \mathcal{O}(h_n^2) \tag{11}$$

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

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

Derivative at the middle point

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



1.2 Stability and Stiffness

1.2.1 Stability

Stability can be interpreted as the integration solution $z_{n=1,..,N}$ should not instigate substantial changes with small changes in the initial condition z_0. This transaltes to the careful choice of the step size h_n in the Euler and Trapezoidal methods. A linear test fucntion is often introudced for stability analysis:

$$z' = \lambda z, \qquad z(0) = z_0 \tag{13}$$

with the exact solution:

$$z(t) = z_0 e^{\lambda t} \tag{14}$$

We should be careful when using the term stability: it could refer to the stability of the prolem or the numerical method, and we exam the latter in this section.

For nonlinear systems, consider the derivative (Jocobian in case of mutiple states) $\lambda = \frac{\mathrm{d}f}{\mathrm{d}z}$.

More rigourous definition on stability is given in Chapter 2 of Ascher and Petzold [1]

Depending on the different values of the real part of λ, we have

$\mathrm{Re}(\lambda) \leq 0$	Stable	May oscillate ($\mathrm{Re}(\lambda) = 0$ and $\lambda \neq 0$)
$\mathrm{Re}(\lambda) < 0$	Asymptotically Stable	Exponential decay
$\mathrm{Re}(\lambda) > 0$	Unstable	Exponential growth

Take the forward Euler method as an example, we substitute the recursive formula (7) to Eq.(14):

$$z_n = z_0(1 + h\lambda)^n \tag{15}$$

Here we assume a uniform step size h

The solution is stable if

$$|1 + h\lambda| \leq 1 \tag{16}$$

This describes the region of absolute stability. Similar results can be derived for the backward Euler and the Trapezoidal methods:

Decay of $|z_n|$ requires $\left|\frac{z_n}{z_{n-1}}\right| \leq 1$

If a method is absolutely stable for all $\mathrm{Re}(\lambda) \leq 0$, then it is A-stable, where h is no longer limtied by stability conditions.

$$\frac{1}{|1 - h\lambda|} \leq 1, \qquad \text{(Backward Euler)} \tag{17a}$$

$$\left|\frac{1 + h\lambda/2}{1 - h\lambda/2}\right| \leq 1, \qquad \text{(Trapezoidal Rule)} \tag{17b}$$

1.2.2 Stiffness

The term stiffness is also used broadly to capture differential equations systems that:

- contain widely varying time scales, i.e., some components of the solution decay much more rapidly than others.
- have numerical integration step size dictated by stability requirements rather than by accuracy requirements.
- cannot be solved by explicit methods, or only extremely slowly.

1.3 Runge-Kutta Methods

Runge-Kutta methods aim to achieve higher accuracy by using intermediate evaluation points between t_n and t_{n+1}. If s intermediate points are used, we call this a s-stage Runge-Kutta formula:

$$z_{n+1} = z_n + h\sum_{i=1}^{s} b_i k_i \tag{18a}$$

$$k_i = f\left(t_n + c_i h, z_n + h\sum_{j=1}^{i-1} a_{ij}k_j\right) \tag{18b}$$

$$c_1 = 0, \qquad c_i = \sum_{j=1}^{i-1} a_{ij}. \tag{18c}$$

Here, a_{ij} is the Runge-Kutta matrix, b_i is the weights, and c_i is the nodes. A short hand notation for the coefficients is known as the Buthcer tableau:

$$\begin{array}{c|ccccc}
c_1 & & & & & \\
c_2 & a_{21} & & & & \\
c_3 & a_{31} & a_{32} & & & \\
\vdots & \vdots & & \ddots & & \\
c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & \\
\hline
 & b_1 & b_2 & \cdots & b_{s-1} & b_s
\end{array}$$

This is the explicit Runge-Kutta methed family, and it reduces to the forward Euler method when $i = 1$

Derivation of 2-stage Runge-Kutta formula

$$\begin{aligned}
z_{n+1} &= z_n + hf\left(b_1k_1 + b_2k_2\right)\\
k_1 &= f\left(t_n, y_n\right)\\
k_2 &= f\left(t_n + c_2h, z_n + ha_{21}k_1\right)
\end{aligned}$$

We have $c_2 = a_{21}$ from Eq. (18c). The other coefficients are chosen to maximize the numerical accuracy by looking at the local truncation error. Consider Taylor series to z_{n+1}:

$$\begin{aligned}
z_{n+1} &= z(t_{n+1}) = z\left(t_n + h\right)\\
z_{n+1} &= z_n + z'_n h + \frac{1}{2}z''_n h^2 + \mathcal{O}(h^2)\\
z_{n+1} &= z_n + hf_n + \frac{1}{2}h^2\left(f_t + ff_z\right)_n + \mathcal{O}(h^2)
\end{aligned}$$

Consider Taylor series to k_1 and k_2:

$$\begin{aligned}
k_1 &= f_n\\
k_2 &= f_n + h\left(c_2f_t + a_{21}ff_z\right)_n + \mathcal{O}(h^2)\\
z_{n+1} &= z_n + (b_1 + b_2)hf_n\\
&\quad + b_2h^2\left(c_2f_t + a_{21}ff_z\right)_n + \mathcal{O}(h^2)
\end{aligned}$$

Compare the two expressions, we have $b_1 + b_2 = 1$ and $b_2c_2 = b_2a_{21} = \frac{1}{2}$

One of the most popular numerical approaches for IVPs is the classic four-stage Runge-Kutta method:

$$z_{n+1} = z_n + \frac{1}{6}h\left(k_1 + 2k_2 + 2k_3 + k_4\right) \tag{19a}$$

$$k_1 = f\left(t_n, z_n\right) \tag{19b}$$

$$k_2 = f\left(t_n + \frac{1}{2}h, z_n + \frac{1}{2}hk_1\right) \tag{19c}$$

$$k_3 = f\left(t_n + \frac{1}{2}h, z_n + \frac{1}{2}hk_2\right) \tag{19d}$$

$$k_4 = f\left(t_n + h, z_n + hk_3\right) \tag{19e}$$

TODO implicit Runge-Kutta

1.4 Multi-step Approaches

2 Bundary Value Problems

References

[1] Uri M.Ascher and Linda R.Petzold. *Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations*. 1998.