Exponential Time Differencing Explicit Runge-Kutta Methods

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We study ODEs of type

$$\frac{\mathrm{d}}{\mathrm{d}t}y(t) = Ly(t) + N(y(t), t), \tag{1}$$

where y may be a vector, L is a linear operator, and N is a nonlinear operator. If L has a wide range of eigenvalues, the above ODE is *stiff*. Exponential time differencing methods were designed to treat stiff ODEs.

1 Exponential Time Differencing (ETD) Methods

We make the same change of variable as we do in the Integrating Factor (IF) methods. We can rewrite Equation 1 as the following.

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\exp(-tL)y\right) = \exp(-tL)N(y, t) \tag{2}$$

Given a state $y_n := y(t_n)$, we can employ this change of variables at that time to move forward in time by h.

$$y_{n+1} = \exp(hL)\left(y_n + \int_0^h \exp(-\tau L)N(y(t_n + \tau), t_n + \tau)\mathrm{d}\tau\right) \tag{3}$$

This equation is exact. All ETD methods derive from approximating the integral.

1.1 Multi-step Explicit ETD methods

Some basic ETD methods work by approximating the nonlinear function in the integrand in Equation 3 using previous steps. Here, the task is to approximate $N(y, t) = N(y(t), t)$ only for values of t in $[t_n, t_n + h]$. A constant approximation of $N(y)$ by using $N(y_n))$ yields ETD1, and a linear approximation using $N(y_n)$ and $N(y_{n-1})$ yields ETD2.

$$\mathrm{ETD1} : N(y(t), t) \approx N(y_n)$$

$$\mathrm{ETD2} : N(y(t), t) \approx N(y_n) + \tau\frac{N(y_n) - N(y_{n-1})}{h}$$

We solve the integral exactly with these constant and linear approximations to get the full schemes, which are shown below.

$$\text{ETD1} : y_{n+1} = \exp(hL)y_n + N(y_n)\frac{\exp(hL)-1}{L}$$
$$\text{ETD2} : y_{n+1} = \exp(hL)y_n + N(y_n)\frac{(1+hL)\exp(hL)-2hL-1}{hL^2} + N(y_{n-1})\frac{-\exp hL + 1 + hL}{hL^2}$$

If L is a scalar linear operator, the above equations make sense, an if it is not, then 1's should be replaced by identity matrices.

1.2 Multi-stage methods: Runge-Kutta

Runge-Kutta methods with s-stages work by approximating the state, y, and its time-derivative, $\frac{\mathrm{d}}{\mathrm{d}t}y$, in various stages,$\{t_n + c_i h\}_{i=1}^s$, where $c_i \in [0, h]$ within a single time-step, h. Instead, ETD-RK methods only approximate the nonlinear function in the integrand of Equation 3 (instead of the whole RHS).

1.2.1 ETD-RK2

Consider Heun's second order scheme shown by Butcher tableau below.

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

This scheme has two stages which both approximate y_{n+1}

$$y_n = k_1 := y_n \tag{4}$$
$$y_{n+1} \approx k_2 := \exp(hL)y_n + N(y_n)\frac{\exp(hL)-1}{L} \quad \text{(same as ETD1)} \tag{5}$$
$$N(y,t) \approx N_{RK2}(k_1,k_2) := N(y_n,t_n) + \tau\frac{N(k_2)-N(k_1)}{h} \tag{6}$$

Integrating exactly with this linear approximation yields ETD-RK2.

$$y_{n+1} = k_2 + (N(k_2) - N(y_n))\frac{\exp(hL)-hL-1}{hL^2} \tag{7}$$

So the name of the game is to find approximations of the nonlinear term in the integrand. If we stick to polynomial approximations with interpolating nodes within a time-step, we can make the generalization that the resulting ETD-RK schemes all involve integrating $\exp(hL)\tau^i$.

Suppose that the RK scheme yields some polynomial approximant,

$$N(y) = N(y(t_n+\tau)) \approx N_{RK}(\tau) = p_0 + p_1\tau + \cdots p_s\tau^s.$$

Then the exact integral we must solve can now be separated by each term in the polynomial.

$$\int_0^h \exp(-\tau L)N(y(t_n+\tau), t_n+\tau)\mathrm{d}\tau \approx \sum_{i=0}^s p_i \int_0^h \exp(-\tau L)\tau^i \mathrm{d}\tau \tag{8}$$

Substituting this approximation into the general ETD scheme yields,

$$y_{n+1} = \exp(hL)\left(y_n + \sum_{i=0}^{s} p_i \int_0^h \exp(-\tau L)\tau^i \mathrm{d}\tau\right) \tag{9}$$

ϕ functions: Here we introduce a family of functions that deal with these sorts of integrals. We have $\phi_0(hL) := \exp hL$, and for $l \geq 1$,

$$\phi_l(hL) = \frac{\exp(hL)}{h^l(l-1)!}\int_0^h \exp(-\tau L)\tau^{l-1}\mathrm{d}\tau. \tag{10}$$

Let's define new coefficients q_l's, so that we can write the scheme in terms of the ϕ_l functions. The indexing is off, so think $l = i+1$. We have to require $q_l = (l-1)!h^l p_{l-1}$ for $l \geq 1$.

$$y_{n+1} = \exp(hL)y_n + \sum_{l=1}^{s+1} q_l \phi_l(hL) \tag{11}$$

ETDRK2 represented by ϕ functions: Equation 6 is simply a linear approximation with $p_0 = N(y_n)$ and $p_1 = \frac{N(k_2)-N(y_n)}{h}$. This gives us $s = 1$, $q_1 = hN(y_n)$, and $q_2 = h^2\frac{N(k_2)-N(y_n)}{h}$. Using this, we can construct a Butcher tableau like before.

$$\begin{array}{c|cc} 0 & 0 & \\ 1 & \phi_1(hL) & 0 \\ \hline & \phi_1(hL)-\phi_2(hL) & \phi_2(hL) \end{array} = \begin{array}{c|cc} 0 & 0 & \\ c_2 & a_{21} & 0 \\ \hline & b_1 & b_2 \end{array}$$

2 Tableau

How to interpret these ETD-RK tableaus as is implied in Equation 5.4 of [Minchev and Wright, 2005]:

$$\begin{aligned} k_1 &= y_n \\ k_i &= \exp(c_i hL)y_n + h\sum_{j=1}^{i-1} a_{ij}N(k_j) \\ y_{n+1} &= \exp(hL)y_n + h\sum_{j=1}^{s} b_j N(k_j) \end{aligned}$$

Furthermore, the a_{ij}'s and b_j's are defined via ϕ functions in the following way, (Equation 5.5 of [Minchev and Wright, 2005]), which was originally published in [Friedli, 1978].

$$\begin{aligned} a_{ij} &= \sum_{k=1}^{i-1} \alpha_{ijk}\phi_k(c_i hL) \\ b_i &= \sum_{k=1}^{s} \beta_{ik}\phi_k(hL) \end{aligned}$$

ETDRK3

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{2} & \frac{1}{2}\phi_1(\frac{h}{2}L) & & \\
1 & -\phi_1(hL) & 2\phi_1(hL) & \\
\hline
 & \phi_1(hL) - 3\phi_2(hL) + 4\phi_3(hL) & 4\phi_2(hL) - 8\phi_3(hL) & -\phi_2(hL) + 4\phi_3(hL)
\end{array}
$$

ETDRK4

$$
\begin{array}{c||c|c|c|c|}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\phi_1(\frac{h}{2}L) & & & \\
\frac{1}{2} & 0 & \frac{1}{2}\phi_1(\frac{h}{2}L) & & \\
1 & \frac{1}{2}\phi_1(\frac{h}{2}L)(\phi_0(\frac{h}{2}L) - 1) = \frac{h}{4}L[\phi_1(\frac{h}{2}L)]^2 & 0 & \phi_1(\frac{h}{2}L) & \\
\hline
 & \phi_1(hL) - 3\phi_2(hL) + 4\phi_3(hL) & 2\phi_2(hL) - 4\phi_3(hL) & 2\phi_2(hL) - 4\phi_3(hL) & -\phi_2(hL) + 4\phi_3(hL)
\end{array}
$$

ETDRK4-B :What's printed on (51) of [Krogstad, 2005].

$$
\begin{array}{c||c|c|c|c|}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\phi_1 & & & \\
\frac{1}{2} & \frac{1}{2}\phi_1 - \phi_2 & \phi_2 & & \\
1 & \phi_1 - 2\phi_2 & 0 & 2\phi_2 & \\
\hline
 & \phi_1 - 3\phi_2 + 4\phi_3 & 2\phi_2 - 4\phi_3 & 2\phi_2 - 4\phi_3 & -\phi_2 + 4\phi_3
\end{array}
$$

ETDRK4-B :What Ian's matlab code suggests.

$$
\begin{array}{c||c|c|c|c|}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\phi_1(\frac{h}{2}L) & & & \\
\frac{1}{2} & \frac{1}{2}\phi_1(\frac{h}{2}L) - \phi_2(\frac{h}{2}L) & \phi_2(\frac{h}{2}L) & & \\
1 & \phi_1(hL) - 2\phi_2(hL) & 0 & 2\phi_2(hL) & \\
\hline
 & \phi_1(hL) - 3\phi_2(hL) + 4\phi_3(hL) & 2\phi_2(hL) - 4\phi_3(hL) & 2\phi_2(hL) - 4\phi_3(hL) & -\phi_2(hL) + 4\phi_3(hL)
\end{array}
$$

References

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