Exponential Integrators for ODEs

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In our discussion of IMEX (implicit-explicit) schemes we considered ODEs of the form (these often arise when discretizing PDEs with the "method of lines"):

$$u'(t) = \underbrace{A\,u(t)}_{\substack{\text{stiff linear} \\ \text{with } A \text{ constant} \\ \text{(e.g. diffusion)}}} + \underbrace{B(u(t))}_{\substack{\text{non-stiff} \\ \text{but non-linear} \\ \text{(e.g. advection)}}}$$

If $B \equiv 0$ then $u' = Au \Rightarrow$

$$u_A(t) = e^{At} u(0)$$

Requires action of matrix exponential

For small normal A, use eigenvalue or SVD decomposition:

$$A = U \Sigma V^* \Rightarrow$$

$$\exp(A) = U \exp(\Sigma) V^*$$

scalar exponential of singular values

Trivial for diagonal A!

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If A is large but sparse, can use Krylov / Lanczos / Arnoldi to compute $\exp(At)u$.

<u>An example</u>

Pseudo spectral discretization in space for KdV (homeworks 2 & 4)

$$\frac{d\hat{\varphi}}{dt} = \underbrace{ik^3 \boxed{\cdot}\, \hat{\varphi}} - \underbrace{3ik \boxed{\cdot}\, \mathcal{F}\left(\left(\mathcal{F}^{-1}\hat{\varphi}\right)^2\right)}$$

$$= A\hat{\varphi} + B(\hat{\varphi})$$

$$A = \mathrm{Diag}(ik^3) \quad \text{(easy!)}$$

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For more general stiff ODEs, Rosenbrock methods simply **linearize** the ODE around the current solution. Take the general autonomous ODE:

$$u' = f(u(t))$$

$$u' = \left.\left(\frac{\partial f}{\partial u}\right)^n (u - u^n) + f^n \right\} \text{linear part}$$

$$+ f(u) - \left[\left(\frac{\partial f}{\partial u}\right)^n (u - u^n) + f^n\right]$$

(add and subtract)

$$\Rightarrow \quad u' = A^n u + B^n(u)$$

$$A^n = \left.\frac{\partial f}{\partial u}\right|_{u=u^n}$$

Jacobian

$$B^n(u) = f(u) - \left(\frac{\partial f}{\partial u}\right)^n u$$

This is an <u>exact</u> splitting into stiff and (hopefully!) non-stiff terms. Note that

$$\frac{\partial B}{\partial u}(u^n) = \left.\frac{\partial f}{\partial u}\right|_{u^n} - A^n = 0$$

which means $B(u)$ is almost constant during the time step!

$$u' = Au + B(u) = f(u)$$

Variation-of-constants / Duhamel's methods + Picard iteration give:

$$u^{n+1} = \left(e^{A^n \Delta t}\right) u^n + \underbrace{\int_{t^n}^{t^{n+1}} e^{A^n (t_{n+1} - \tau)} B^n(u(\tau))\, d\tau}$$

Exact!

Approximate integral using a quadrature rule as for RK/multistep

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If $A \equiv 0$, $\exp(A\Delta t) = \text{Identity}$, we want to get explicit RK.

If $B \equiv 0$, we want to get exact solution $\exp(A\Delta t)\cdot u(t)$.

For example, for RK1 (forward Euler), approximate/extrapolate:

$$B^n(u(\tau)) \simeq B^n(u^n)$$

and use

$$\int_{t_n}^{t_{n+1}} \exp(A^n(t_{n+1}-\tau))\,d\tau = A_n^{-1}\left(e^{A_n \Delta t} - I\right)$$

to get

$$u^{n+1} = e^{A_n \Delta t} + A_n^{-1}\left(e^{A_n \Delta t} - I\right) B_n(u^n)$$

Exponential Euler scheme:

$$u^{n+1} = u^n + (A^n)^{-1}\left(e^{A_n \Delta t} - I\right) \underbrace{f(u^n)}_{\text{r.h.s.}}$$

If $\|A_n\|_2 \Delta t \ll 1$, then

$$u^{n+1} \approx u^n + \Delta t \, f(u^n)$$

which is the usual forward Euler, with <u>bad</u> stability properties.

Local truncation error (LTE):

$$\sigma^n = \left(\frac{u(t_{n+1}) - u(t_n)}{\Delta t}\right) - \frac{1}{\Delta t}(A^n)^{-1}\left(e^{A_n \Delta t} - I\right)\underset{\text{from ODE}}{u'(t_n)}$$

$$= \frac{\Delta t}{2}\left(\frac{\partial f}{\partial u}(u(t_n)) - A_n\right) u'(t_n) + O(\Delta t^2)$$

$\Rightarrow$ {
second-order accurate if $A_n = \left(\frac{\partial f}{\partial u}\right)^n$ (Rosenbrock)

first-order in general (but much better than standard Euler for stiff ODEs)

This method will be accurate if $B(u)$ varies slowly over the time step.

Note that if $u^{n+1} = u^{n}$ (fixed point) then $f^{n} = 0$. This means that this method can be used to quickly find stable fixed points of ODEs/PDEs.

This is not true for another class of "Integrating Factor" Exponential Integrators which are used in some fields

We can improve the order of accuracy with the same ideas we used for RK methods;

$$u^{n+1} = \left(e^{A^n \Delta t}\right) u^n + \int_{t^n}^{t^{n+1}} e^{A^n (t_{n+1} - \tau)} B^n(u(\tau))\, d\tau$$

$$B^n(u(\tau)) \simeq B^n + \frac{\tau - t^n}{\Delta t}\left(B^n - B^{n-1}\right)$$

Now do the integral (assume A is normal & diagonalize it)

Exponential Time Differencing ETD2:

$$u^{n+1} = e^{A^n \Delta t} u^n + A_n^{-1}\left(e^{A_n \Delta t} - I\right) B^n + \underbrace{\frac{A_n^{-2}}{\Delta t}\left(e^{A_n \Delta t} - I - A_n \Delta t\right)\left(B^n - B^{n-1}\right)}_{O(\Delta t^2)\ 2^{nd}\text{ order correction}}$$

This is an exponential multistep scheme (two step like AB2)

If we want an RK2 scheme instead, say explicit midpoint:

① Midpoint ETDRK1 (exponential Euler) <u>predictor</u> step:

$$u^{n+1/2,*} = \left(e^{A_n \Delta t/2}\right) u^n + A_n^{-1}\left(e^{A_n \Delta t/2} - I\right) B^n$$

② ETDRK2 corrector:

$$u^{n+1} = \left(e^{A_n \Delta t}\right) u_n + A_n^{-1}\left(e^{A_n \Delta t} - I\right) B^n$$

$$+ 2 A_n^{-2} \underbrace{\left(\frac{e^{A_n \Delta t} - I - A_n \Delta t}{\Delta t}\right)\left(B^{n+1/2,*} - B^n\right)}_{\text{ETD2}}$$

Cox and Matthews also derive a set of ETD methods based on Runge–Kutta time-stepping, which they call ETDRK schemes. In this report we consider only the fourth-order scheme of this type, known as ETDRK4. According to Cox and Matthews, the derivation of this scheme is not at all obvious and requires a symbolic manipulation system. The Cox and Matthews ETDRK4 formulae are: 13

$$\boxed{\begin{aligned}
a_n &= e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})\mathbf{N}(u_n, t_n),\\
b_n &= e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})\mathbf{N}(a_n, t_n + h/2),\\
c_n &= e^{\mathbf{L}h/2}a_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})(2\mathbf{N}(b_n, t_n + h/2) - \mathbf{N}(u_n, t_n)),\\
u_{n+1} &= e^{\mathbf{L}h}u_n + h^{-2}\mathbf{L}^{-3}\{[-4 - \mathbf{L}h + e^{\mathbf{L}h}(4 - 3\mathbf{L}h + (\mathbf{L}h)^2)]\mathbf{N}(u_n, t_n)\\
&\quad + 2[2 + \mathbf{L}h + e^{\mathbf{L}h}(-2 + \mathbf{L}h)](\mathbf{N}(a_n, t_n + h/2) + \mathbf{N}(b_n, t_n + h/2))\\
&\quad + [-4 - 3\mathbf{L}h - (\mathbf{L}h)^2 + e^{\mathbf{L}h}(4 - \mathbf{L}h)]\mathbf{N}(c_n, t_n + h)\}.
\end{aligned}}$$

FROM PAPER BY KASSAM & TREFETHEN (linked on course webpage)

PROBLEM: Roundoff in $|z| \ll 1$ $\dfrac{e^z - 1}{z}$ (use complex contour integration)