Exponential Taylor methods: analysis and implementation

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The problem

We consider the time integration of stiff semilinear initial value problems

\[ u'(t) = Au(t) + g(t, u(t)), \quad u(t_0) = u_0, \]

where \( u(t) \in \mathbb{R}^d, A \in \mathbb{R}^{d \times d} \) (\( d \) large),

\( g \) is a nonlinear function with a moderate Lipschitz constant.

Specifically: problems arising from spatial semidiscretization of partial differential equations.
Exponential integrators are based on the variation-of-constants formula

\[ u(t) = e^{(t-t_0)A}u_0 + \int_{t_0}^{t} e^{(t-\tau)A}g(\tau, u(\tau)) \, d\tau, \]

which gives the exact solution at time \( t \).

Example: exponential Euler method

\[ u_1 = e^{hA}u_0 + h\varphi_1(hA)g(t_0, u_0) \]

where \( h \) denotes the step size and \( \varphi_1 \) is the entire function

\[ \varphi_1(z) = \frac{e^z - 1}{z}. \]
Higher order exponential integrators

For the construction of high order exponential Runge–Kutta methods, and higher order exponential multistep methods, see:


These methods contain the entire functions

$$\varphi_k(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} \, d\theta, \quad k \geq 1.$$ 

For a matrix $A \in \mathbb{R}^{d \times d}$ and a vector $b \in \mathbb{R}^d$, the evaluation of $\varphi_k(A)b$ is often costly.
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Example of state-independent inhomogeneity
Here, we consider multiderivative exponential integrators. We replace the nonlinearity by its Taylor polynomial of degree $p - 1$:

$$g(\tau, u(\tau)) \approx \sum_{k=0}^{p-1} \frac{(\tau - t_0)^k}{k!} \left. \frac{d^k}{dt^k} g(t, u(t)) \right|_{t=t_0}.$$  

Using the chain rule, we see that for $p = 4$ (when $g(t, u) = g(u)$)

$$\frac{d}{dt} g(u) = g'(u)u'$$

$$\frac{d^2}{dt^2} g(u) = g''(u)(u', u') + g'(u)u''$$

$$\frac{d^3}{dt^3} g(u) = g'''(u)(u', u', u') + 3g''(u)(u'', u') + g'(u)u'''$$
By using the known quantity $u_0$, we approximate

$$\left. \frac{d^{k-1}}{dt^{k-1}} g(u(t)) \right|_{t=t_0} \approx w_k,$$

where $w_k$ is defined recursively by

$$u^{(k)}_0 = A u^{(k-1)}_0 + w_k, \quad k \geq 1$$

and

$$
\begin{align*}
    w_1 &= g(u_0) \\
    w_2 &= g'(u_0) u'_0 \\
    w_3 &= g''(u_0)(u'_0, u'_0) + g'(u_0) u''_0 \\
    w_4 &= g'''(u_0)(u'_0, u'_0, u'_0) + 3g''(u_0)(u''_0, u'_0) + g'(u_0) u'''_0
\end{align*}
$$
Exponential Taylor method

We insert the polynomial

\[ g(\tau, u(\tau)) \approx \sum_{k=0}^{p-1} \frac{(\tau - t_0)^k}{k!} w_k \]

to the variation-of-constants formula

\[ u(t) = e^{(t-t_0)A} u_0 + \int_{t_0}^{t} e^{(t-\tau)A} g(\tau, u(\tau)) d\tau \]

to get the exponential Taylor method

\[ u_1 = e^{hA} u_0 + \sum_{k=1}^{p} h^k \varphi_k(hA) w_k. \]
Here the functions $\varphi_k$ are as above:

$$
\varphi_k(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} \, d\theta, \quad k \geq 1.
$$

They satisfy $\varphi_k(0) = 1/k!$ and the recurrence relation

$$
\varphi_{k+1}(z) = \frac{\varphi_k(z) - \varphi_k(0)}{z}, \quad \varphi_0(z) = e^z.
$$
Linearized exponential Taylor method

For an autonomous problem

\[ u'(t) = Au(t) + g(u(t)) = f(u(t)), \quad u(t_0) = u_0, \]

we linearize the differential equation at the numerical approximation \( u_n \) at time \( t_n \):

\[ v'(t) = J_n v(t) + g_n(v(t)), \quad v(t_n) = u_n, \quad (*) \]

where \( J_n \) denotes the Fréchet derivative of \( f \), and \( g_n \) the remainder:

\[
J_n = f'(u_n) = A + g'(u_n), \\
g_n(u) = f(u) - J_n u = g(u) - g'(u_n)u.
\]

Applying an exponential Taylor method to (*) yields a so-called linearized exponential Taylor method.
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Computational advantage

Computation of one time step done as follows:
(Al-Mohy and Higham 2010)

Lemma

Let $A \in \mathbb{R}^{d \times d}$, $W = [w_p, w_{p-1}, \ldots, w_1] \in \mathbb{R}^{d \times p}$, $h \in \mathbb{R}$ and

$$\tilde{A} = \begin{bmatrix} A & W \\ 0 & J \end{bmatrix} \in \mathbb{R}^{(d+p) \times (d+p)}, \quad J = \begin{bmatrix} 0 & I_{p-1} \\ 0 & 0 \end{bmatrix}, \quad v_0 = \begin{bmatrix} u_0 \\ e_p \end{bmatrix} \in \mathbb{R}^{d+p}$$

with $e_p = [0, \ldots, 0, 1]^T$. Then it holds

$$e^{hA}u_0 + \sum_{k=1}^{p} h^k \varphi_k(hA)w_k = \begin{bmatrix} I_d \\ 0 \end{bmatrix} e^{h\tilde{A}}v_0.$$
To compute the appearing matrix exponential times vector product \([I_d \ 0] \ e^{h\tilde{A}} \begin{bmatrix} u_0 \\ e_p \end{bmatrix}\), Krylov methods are used.

The Arnoldi iteration produces an orthogonal basis \(V_k \in \mathbb{R}^{d \times k}\) for the Krylov subspace

\[\mathcal{K}_k(A, b) = \text{span}\{b, Ab, A^2b, \ldots, A^{k-1}b\}\]

and the Hessenberg matrix \(H_k = V_k^T A V_k \in \mathbb{R}^{k \times k}\).

Then the approximation

\[e^{hA} b \approx V_k e^{H_k} V_k^T b = V_k e^{H_k} e_1 \|b\|_2\]

is used.
Krylov approximation

Numerically the convergence is found satisfying for $e^{h\tilde{A}} \begin{bmatrix} u_n \\ e_p \end{bmatrix}$.

Example: here $A \in \mathbb{R}^{500 \times 500}$ is symmetric, $\|hA\|_2 = 80$ and for $W \in \mathbb{R}^{500 \times 5}$, $\|hW\|_2 \approx 2 \cdot 10^5$.

Figure: The errors of the Krylov approximations vs. the dimension of the Krylov subspace.
Adaptive step sizes

An error control for the exponential Taylor integrator

\[ u_1^{[p]} = e^{hA}u_0 + \sum_{k=1}^{p} h^k \varphi_k (hA) w_k \]

can be obtained from the last term of the sum, since for small \( h \) we may approximate

\[ \| u(t_1) - u_1^{[p-1]} \|_2 \approx \| u_1^{[p]} - u_1^{[p-1]} \|_2 = \| h^p \varphi_p (hA) w_p \|_2. \]

\( h^p \varphi_p (hA) w_p \) can be computed also using a single exponential of an augmented matrix.
Computation of the derivatives

For autonomous nonlinearities $g(u)$, the vectors $w_i$ of the exponential Taylor method can be obtained by

\[
\begin{align*}
    w_1 &= g(u_0) \\
    w_2 &= J^{(0)} f^{(0)} \\
    i \geq 2 \quad &\left\{ \begin{array}{l}
        f^{(i-1)} = Af^{(i-2)} + w_i \\
        w_{i+1} = \sum_{k=0}^{i-1} \binom{i-1}{k} J^{(i-1-k)} f^{(k)},
    \end{array} \right.
\end{align*}
\]

where

\[
    f^{(k)} = \frac{d^k}{dt^k} f(u(t))\big|_{u=u_n} \quad \text{and} \quad J^{(k)} = \frac{d^k}{dt^k} g'(u(t))\big|_{u=u_n}.
\]
References for the use of Automatic Differentiation:


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Assumptions

We assume that the involved matrix exponential satisfies the bound

$$\|e^{tA}\| \leq C_0 e^{\omega t}, \quad t \geq 0$$

From this it also follows that

$$\|\varphi_k(tA)\| \leq \frac{C_0 e^{\omega t}}{k!}, \quad t \geq 0.$$

Using these, the convergence bounds depend only on the constants $C_0$ and $\omega$.

We also assume that the nonlinear term $g(t, u(t))$ sufficiently smooth.
For the linear problem

\[ u'(t) = Au(t) + g(t), \quad u(t_0) = u_0, \quad t_0 \leq t \leq T \]

we have the following results

**Theorem**

Let the inhomogeneity \( g \) be \( p \) times differentiable with \( g^{(p)} \in L^1(0, T) \). Then, the exponential Taylor method is convergent of order \( p \).

**Proof:** The exponential Taylor method gives:

\[
    u_{n+1} = e^{hA}u_n + \sum_{k=1}^{p} h^k \varphi_k(hA)g^{(k-1)}(t_n), \quad n \geq 0, 
\]
and we see that the error $e_{n+1} = u_{n+1} - u(t_{n+1})$ satisfies

$$e_{n+1} = e^{hA}e_n - \delta_{n+1},$$

where

$$\delta_{n+1} = \int_0^h e^{(h-\tau)A} \int_0^\tau \frac{(\tau - \xi)^{p-1}}{(p-1)!} g^{(p)}(t_n + \xi) \, d\xi \, d\tau.$$

which can be bounded using bound for $\|\varphi_k(tA)\|$. Solving recursion for $e_n$ and bounding $\|e^{tA}\|$ gives the result.
Convergence for semilinear equation

For the semilinear equation

\[ u'(t) = Au(t) + g(t, u(t)), \quad u(t_0) = u_0. \]

we have:

**Theorem**

*Let the inhomogeneity \( \psi(t) = g(t, u(t)) \) be twice differentiable and \( \psi'' \in L^1(0, T) \). Then, the exponential Taylor method is second order convergent.*

**Proof.** The Taylor scheme with \( p = 2 \) has the form

\[
\begin{align*}
    u_{n+1} &= e^{hA}u_n + h\varphi_1(hA)g(t_n, u_n) \\
    &\quad + h^2\varphi_2(hA)(g_t(t_n, u_n) + g_u(t_n, u_n)(Au_n + g(t_n, u_n))).
\end{align*}
\]
Convergence for semilinear equation

Expressing the exact solution with the second order Taylor polynomial, we get for the global error $e_n = u_n - u(t_n)$ the recursion

$$e_{n+1} = e^{hA}e_n + h\varphi_1(hA)(g(t_n, u_n) - g(t_n, \tilde{u}_n))$$
$$+ h^2\varphi_2(hA)(g_t(t_n, u_n) - g_t(t_n, \tilde{u}_n))$$
$$+ h^2\varphi_2(hA)g_u(t_n, u_n)(Ae_n + g(t_n, u_n) - g(t_n, \tilde{u}_n))$$
$$+ h^2\varphi_2(hA)(g_u(t_n, u_n) - g_u(t_n, \tilde{u}_n))u'(t_n) - \delta_{n+1},$$

where

$$\delta_{n+1} = \int_0^h e^{(h-\tau)A} \int_0^\tau (\tau - \xi) \frac{d^2g}{dt^2}(t, u(t)) \bigg|_{t=t_n+\xi} d\xi d\tau.$$
Convergence for semilinear equation

Multiplying $e_{n+1}$ with $A$ and using $z\varphi_2(z) = \varphi_1(z) - 1$ we get respectively a recursion for $Ae_n$.

Combining these 2 recursions, and using standard Gronwall lemma, we obtain the estimate

$$\|e_n\| + h\|Ae_n\| \leq C \sum_{j=1}^{n} \left( \|e^{(n-j)hA}\delta_j\| + h\|Ae^{(n-j)hA}\delta_j\| \right)$$

where $C$ is independent of $\|A\|$.

Bounding $\delta_j$ gives the result.
Convergence for linearized scheme

When we apply the exponential Taylor method to the linearized equation

\[ v'(t) = J_n v(t) + g_n(v(t)), \quad v(t_n) = u_n, \]

where

\[ J_n = f'(u_n) = A + g'(u_n), \]
\[ g_n(u) = f(u) - J_n u = g(u) - g'(u_n)u, \]

order three is possible. By construction,

\[ g'(u_n) = 0. \]

and therefore the linearized exponential Taylor scheme for \( p = 3 \) has the form

\[ u_{n+1} = e^{hJ_n}u_n + h\varphi_1(hJ_n)g_n(u_n) \]
\[ + h^3\varphi_3(hJ_n)g''(u_n)(J_n u_n + g_n(u_n), J_n u_n + g_n(u_n)) \]
\[ = u_n + h\varphi_1(hJ_n)f(u_n) + h^3\varphi_3(hJ_n)f''(u_n)(f(u_n), f(u_n)). \]
Theorem

Let the inhomogeneity \( \psi(t) = g(u(t)) \) be three times differentiable with \( \psi''' \in L^1(0, T) \). Then, the linearized exponential Taylor method is convergent of order three, i.e.

\[
\| u_n - u(t_n) \| \leq C h^3
\]

with a constant \( C \) that is uniform on compact intervals \( 0 \leq nh \leq T \).
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Example of state-independent inhomogeneity
Consider a simple one-dimensional partial differential equation

$$\partial_t u = u_{xx} + \gamma u(1 - u), \quad x \in \left[-\frac{5}{2}, \frac{5}{2}\right]$$

with periodic boundary conditions and the initial value

$$u(x, 0) = \exp(-10x^2), \quad x \in \left[-\frac{5}{2}, \frac{5}{2}\right].$$

We set $\gamma = 10$. 
Performing spatial semidiscretization with finite differences gives for the linear part:

\[
A := \frac{1}{(\Delta x)^2} \begin{bmatrix}
-2 & 1 & & 1 \\
1 & -2 & 1 & & \\
& \ddots & \ddots & \ddots & \\
& & 1 & -2 & 1 \\
1 & & & 1 & -2
\end{bmatrix},
\]

where \( \Delta x = L/n \).

Eigenvalues of \( A \) are on the negative real axis, the smallest being: \( \lambda_{\text{min}} = -4/(\Delta x)^2 \).
Accumulation of local errors

The term $w_p$ contains the highest powers of $A$, namely 

$$g'(u_n)A^{p-1}u_n.$$ 

Using the inequality 

$$|g'(u)| = \gamma |1 - 2u| \leq \gamma$$ 

the stability of the exponential Taylor scheme is governed by the factor 

$$|\gamma h^p \varphi_p(h\lambda_{\min})\lambda_{\min}^{p-1}|$$ 

which has to be power-bounded, i.e. 

$$\gamma h^p \varphi_p(h\lambda_{\min})|\lambda_{\min}|^{p-1} \leq 1.$$ 

Similarly for $p$th order linearized scheme: 

$$2(p - 1)\gamma h^p \varphi(h\lambda_{\min})|\lambda_{\min}|^{p-2} \leq 1.$$
Accumulation of local errors

<table>
<thead>
<tr>
<th></th>
<th>$p$</th>
<th>$d = 500$</th>
<th>$d = 1000$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>2.3E-3 / 2.4E-3</td>
<td>1.1E-3 / 1.2E-3</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>7.3E-4 / 7.8E-4</td>
<td>2.9E-4 / 3.0E-4</td>
<td></td>
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<tr>
<td>5</td>
<td>4.5E-4 / 4.8E-4</td>
<td>1.5E-4 / 1.6E-4</td>
<td></td>
</tr>
</tbody>
</table>

**Table:** Step sizes determined by the stability condition vs. experimentally observed largest admissible step sizes.
Accumulation of local errors

The spatial discretization $d = 1000$:

Figure: 2-norms of the highest $h^k \varphi_k(hA)w_k$-terms for $p = 3$ and $p = 5$, when the step size larger than the admissible step size.
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Example of state-independent inhomogeneity
A linear example with inhomogeneity

If the nonlinearity is state-independent, no numerical instabilities are expected.

We consider a finite difference spatial discretization (with 500 points) of the equation

$$\partial_t u = \partial_{xx} u + 10 e^{-10t} x (1 - x), \quad x \in [0, 1], \quad t \in [0, 0.1]$$

$$u(x, 0) = 16x^2 (1 - x)^2,$$

$$u(0, t) = u(1, t) = 0.$$
A linear example with inhomogeneity

Figure: Step sizes taken by the exponential Taylor method with $p = 5$, ode15s and ode23s. Number of steps taken 11, 148 and 868, respectively.
Conclusions

- Presented the Exponential Taylor Methods

- Second order convergence for the semilinear equations

- Third order convergence for the linearized semilinear equations

- Methods of arbitrary order for the linear problems