Exponentially fitted methods applied to fourth-order boundary value problems

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SCICADE, Beijing, 2009
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Introduction

In the past 15 years, our research group has constructed modified versions of well-known

- linear multistep methods
- Runge-Kutta methods

Aim: build methods which perform very good when the solution has a known exponential of trigonometric behaviour.
A model problem

Consider the initial value problem

\[ y'' + \omega^2 y = g(y) \quad y(a) = y_a \quad y'(a) = y'_a. \]

If \(|g(y)| \ll |\omega^2 y|\) then

\[ y(t) \approx \alpha \cos(\omega t + \phi) \]

To mimic this oscillatory behaviour, we construct methods which yield exact results when the solution is of trigonometric (in the complex case: exponential) type. These methods are called Exponentially-fitted methods.
EF methods

To determine the coefficients of a method, we impose conditions on a linear functional. These conditions are related to the fitting space $S$ which contains

- polynomials:
  \[ \{ t^q | q = 0, \ldots, K \} \]

- exponential or trigonometric functions, multiplied with powers of $t$:
  \[ \{ t^q \exp(\pm \mu t) | q = 0, \ldots, P \} \]
  or, with $\omega = i \mu$,
  \[ \{ t^q \cos(\omega t), t^q \sin(\omega t) | q = 0, \ldots, P \} \]

EF method can be characterized by the couple $(K, P)$

Classical method : $P = -1$

number of basis functions : $M = 2P + K + 3$
\[ M = 2P + K + 3 \]

<table>
<thead>
<tr>
<th>((K, P))</th>
<th>(M = 2)</th>
<th>(M = 4)</th>
<th>(M = 6)</th>
<th>(M = 8)</th>
<th>(M = 10)</th>
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<tbody>
<tr>
<td>((1, -1))</td>
<td>((3, -1))</td>
<td>((5, -1))</td>
<td>((7, -1))</td>
<td>((9, -1))</td>
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<tr>
<td>((-1, 1))</td>
<td>((1, 0))</td>
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\((1, 2) \implies S = \left\{ 1, t, e^{\pm \mu t}, t e^{\pm \mu t}, t^2 e^{\pm \mu t} \right\} \)
Exponential Fitting

L. Ixaru and G. Vanden Berghe

*Exponential fitting*


\[ \eta_{-1}(Z) = \begin{cases} 
\cos(|Z|^{1/2}) & \text{if } Z < 0 \\
\cosh(Z^{1/2}) & \text{if } Z \geq 0 
\end{cases} \]

\[ \eta_0(Z) = \begin{cases} 
\sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0 \\
1 & \text{if } Z = 0 \\
\sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0 
\end{cases} \]

\[ \eta_n(Z) := \frac{1}{Z} [\eta_{n-2}(Z) - (2n - 1)\eta_{n-1}(Z)], \quad n = 1, 2, 3, \ldots \]

\[ \eta'_n(Z) = \frac{1}{2} \eta_{n+1}(Z), \quad n = 1, 2, 3, \ldots \]

\[ Z := (\mu h)^2 = -(\omega h)^2 \]
Choice of $\omega$

- local optimization
  based on local truncation error (lte)
  $\omega$ is step-dependent

- global optimization
  Preservation of geometric properties (periodicity, energy, . . .)
  $\omega$ is constant over the interval of integration
Fourth-order boundary value problem

\[ y^{(4)} = F(t, y) \quad a \leq t \leq b \]
\[ y(a) = A_1 \quad y''(a) = A_2 \]
\[ y(b) = B_1 \quad y''(b) = B_2 \]

- special case: \( y^{(4)} + f(t) y = g(t) \)
- mathematical modeling of viscoelastic and inelastic flows, deformation of beams, plate deflection theory, . . .
- work by Doedel, Usmani, Agarwal, Cherruault et al., Van Daele et al., . . .
- finite differences, B-splines, . . .
The formulae

t_j = a + j h, j = 0, 1, \ldots, N + 1 \quad N \geq 5 \quad h := \frac{b - a}{N + 1}

- **central formula** for $j = 2, \ldots, N - 1$

  \[ y_{j-2} + a_1 y_{j-1} + a_0 y_j + a_1 y_{j+1} + y_{j+2} = \]
  \[ h^4 \left( b_2 F_{j-2} + b_1 F_{j-1} + b_0 F_j + b_1 F_{j+1} + b_2 F_{j+2} \right) \]

  whereby $y_j$ is approximate value of $y(t_j)$ and $F_j := F(t_j, y_j)$.

- **begin formula**

  \[ c_1 y_0 + c_2 y_1 + c_3 y_2 + y_3 = \]
  \[ d_1 h^2 y_0'' + h^4 \left( d_2 F_0 + d_3 F_1 + d_4 F_2 + d_5 F_3 + d_6 F_4 + d_7 F_5 \right) \]

- **end formula**
Central formula

\[ \mathcal{L}[y] := y(t - 2h) + a_1 y(t - h) + a_0 y(t) + a_1 y(t + h) + y(t + 2h) \]
\[ - h^4 \left( b_2 y^{(4)}(t - 2h) + b_1 y^{(4)}(t - h) + b_0 y^{(4)}(t) + b_1 y^{(4)}(t + h) + b_2 y^{(4)}(t + 2h) \right) \]

\[ P = -1 : \quad S = \left\{ 1, t, t^2, \ldots, t^{M-1} \right\} \]

case \( M = 10 \) : order 6

\[ y_{p-2} - 4y_{p-1} + 6y_p - 4y_{p+1} + y_{p+2} = \]
\[ \frac{h^4}{720} \left( -y^{(4)}_{p-2} + 124y^{(4)}_{p-1} + 474y^{(4)}_p + 124y^{(4)}_{p+1} - y^{(4)}_{p+2} \right) \]

\[ \mathcal{L}[y](t) = \frac{1}{3024} h^{10} y^{(10)}(t) + O(h^{12}) \]

case \( M = 8 \) and \( b_2 = 0 \) : order 4
EF Central formula

\[ \mathcal{L}[y] := y(t - 2h) + a_1 y(t - h) + a_0 y(t) + a_1 y(t + h) + y(t + 2h) \]
\[ - h^4 \left( b_2 y^{(4)}(t - 2h) + b_1 y^{(4)}(t - h) + b_0 y^{(4)}(t) + b_1 y^{(4)}(t + h) + b_2 y^{(4)}(t + 2h) \right) \]

\[ P = 0 : \quad S = \{ \cos(\omega t), \sin(\omega t), 1, t, t^2, \ldots, t^{M-3} \} \]

case \( M = 10 \) :

\[ y_{p-2} - 4 y_{p-1} + 6 y_p - 4 y_{p+1} + y_{p+2} = \]
\[ h^4 \left( b_2 y_{p-2}^{(4)} + b_1 y_{p-1}^{(4)} + b_0 y_p^{(4)} + b_1 y_{p+1}^{(4)} + b_2 y_{p+2}^{(4)} \right) \]

\[ b_0 = \frac{4 \cos^2 \theta - 2 - 11 \cos \theta}{6 (\cos \theta - 1)^2} + \frac{6}{\theta^4}, \quad b_1 = \frac{\cos^2 \theta + 5}{6 (\cos \theta - 1)^2} - \frac{4}{\theta^4}, \quad b_2 = -\frac{\cos \theta + 2}{12 (\cos \theta - 1)^2} + \frac{1}{\theta^4} \]

\[ \mathcal{L}[y](t) = \frac{1}{3024} h^{10} \left( y^{(10)}(t) + \omega^2 y^{(8)}(t) \right) + \mathcal{O}(h^{12}) \]
EF Central formula

\[ L[y] := y(t - 2h) + a_1 y(t - h) + a_0 y(t) + a_1 y(t + h) + y(t + 2h) - h^4 \left( b_2 y^{(4)}(t - 2h) + b_1 y^{(4)}(t - h) + b_0 y^{(4)}(t) + b_1 y^{(4)}(t + h) + b_2 y^{(4)}(t + 2h) \right) \]

\[ P = 1 : \quad S = \{ \cos(\omega t), \sin(\omega t), t \cos(\omega t), t \sin(\omega t), 1, t, t^2, \ldots, t^{M-5} \} \]

case \( M = 6 \) and \( b_1 = b_2 = 0 \):

\[ y_{p-2} + a_1 y_{p-1} + a_0 y_p + a_1 y_{p+1} + y_{p+2} = b_0 h^4 y_p^{(4)} \]

\[ a_0 = 2 \frac{-8 \sin^2 \theta + \theta (4 \cos \theta - 1) \sin \theta - 4 \cos \theta + 4}{\theta \sin \theta + 4 \cos \theta - 4} \]

\[ a_1 = -4 \frac{\sin \theta (\theta \cos \theta - 2 \sin \theta)}{\theta \sin \theta + 4 \cos \theta - 4} \]

\[ b_0 = 4 \frac{\sin \theta \left( \sin^2 \theta - 2 + 2 \cos \theta \right)}{\theta^3 (\theta \sin \theta + 4 \cos \theta - 4)} \]
Coefficients of central formula

e.g. case $M = 6$:

$$y_{p-2} + a_1 y_{p-1} + a_0 y_p + a_1 y_{p+1} + y_{p+2} = b_0 h^4 y_p^{(4)}$$

$$Z = (\mu h)^2 = - (\omega h)^2$$
Coefficients of central formula

e.g. case $M = 6$

- $P = -1$ :
  \[ b_0 = 1 \]

- $P = 0$ :
  \[ b_0 = 4 \frac{(\cos \theta - 1)^2}{\theta^4} \]

- $P = 1$ :
  \[ b_0 = -4 \frac{\sin \theta (\cos \theta - 1)^2}{\theta^3 (4 \cos \theta - 4 + \theta \sin \theta)} \]

- $P = 2$ :
  \[ b_0 = -2 \frac{\sin^3 \theta}{\theta^2 (\theta \cos \theta - 3 \sin \theta)} \]
Central formula: coefficients

e.g. case $M = 6$

- $P = -1$:
  \[ b_0 = 1 \]

- $P = 0$:
  \[ b_0 = 1 - \frac{1}{6} \theta^2 + \frac{1}{80} \theta^4 + O(\theta^6) \]

- $P = 1$:
  \[ b_0 = 1 - \frac{1}{3} \theta^2 + \frac{37}{720} \theta^4 + O(\theta^6) \]

- $P = 2$:
  \[ b_0 = 1 - \frac{1}{2} \theta^2 + \frac{7}{60} \theta^4 + O(\theta^6) \]
Central formula: local truncation error

\[ \text{Lte} = \mathcal{L}[y](t) \]

As an infinite series:

\[ \text{Lte} = h^M C_M D^{K+1} (D^2 + \omega^2)^{P+1} y(t) + \mathcal{O}(h^{M+2}) \]

In closed form: (Coleman and Ixaru)

\[ \text{Lte} = h^M \Phi_{K,P}(Z) D^{K+1} (D^2 + \omega^2)^{P+1} y(\xi) \]

\(Z \in \text{some interval} \quad \Phi_{K,P}(0) \neq 0 \quad \xi \in (t - 2h, t + 2h)\)
Local truncation error

\[ \text{lte} = h^M C_M D^{K+1} (D^2 + \omega^2)^{P+1} y(t) + \mathcal{O}(h^{M+2}) , \]

At \( t_j : D^{(K+1)} (D^2 + \omega_j^2)^{(P+1)} y(t) \bigg|_{t=t_j} = 0 \quad j = 2, \ldots, N - 1 \)

- \( P = 0 : \)
  \[ y^{(K+3)}(t_j) + y^{(K+1)}(t_j) \omega_j^2 = 0 \]

- \( P = 1 : \)
  \[ y^{(K+5)}(t_j) + 2 y^{(K+3)}(t_j) \omega_j^2 + y^{(K+1)}(t_j) \omega_j^4 = 0 \]

- \( P = 2 : \)
  \[ y^{(K+7)}(t_j) + 3 y^{(K+5)}(t_j) \omega_j^4 + 3 y^{(K+3)}(t_j) \omega_j^4 + y^{(K+1)}(t_j) \omega_j^6 = 0 \]
Local truncation error

$$lte = h^M C_M D^{K+1} (D^2 + \omega^2)^{P+1} y(t) + O(h^{M+2}) ,$$

At \( t_j \): 
$$D^{(K+1)} (D^2 + \omega_j^2)^{(P+1)} y(t) \bigg|_{t=t_j} = 0 \quad j = 2, \ldots, N - 1$$

\( \omega_j^2 \) is solution of equation of degree \( P + 1 \).

- Which value of \( P \) should be chosen?
- Which root \( \omega_j \) should be chosen?
Parameter selection

\[ \text{lt}e = h^M C_M D^{K+1} (D^2 - \mu^2)^{P+1} y(t) + \mathcal{O}(h^{M+2}) \]

Suppose \( y(t) \) takes the form \( t^{P_0} e^{\mu_0 t} \)

Then \( \text{lt}e = 0 \) for any EF rule with \( P \geq P_0 \) and \( \mu_j = \mu_0 \)

**Theorem**

If \( y(t) = t^{P_0} e^{\mu_0 t} \) then \( \nu = \mu_0^2 \) is a root of multiplicity \( P - P_0 + 1 \) of \( D^{K+1} (D^2 - \nu)^{P+1} y(t) = 0. \)

- if \( P = P_0 \), then \( \mu = \mu_0 \) will be a single root
- if \( P = P_0 + 1 \), then \( \mu = \mu_0 \) will be a double root
- if \( P = P_0 + 2 \), then \( \mu = \mu_0 \) will be a triple root
- \ldots
Parameter selection

\[ \text{Iter} = h^M C_M D^{K+1} (D^2 - \mu^2)^{P+1} y(t) + O(h^{M+2}) \]

Suppose \( y(t) \) does not take the form \( t^{P_0} e^{\mu_0 t} \).

Then \( y(t) \not\in S \) for any \( P \).

For a given value of \( P \):

\[ D^{(K+1)} (D^2 - \mu_j^2)^{(P+1)} y(t) \bigg|_{t=t_j} = 0 \]

At each point \( t_j \), this gives \( P + 1 \) values for \( \mu_j^2 \).

Idea: keep \( |\mu_j h| \) as small as possible.

If possible, choose \( P \geq 1 \) to avoid too large values for \( |\mu_j| \).
Numerical Illustrations
Problem 1

\[ y^{(4)} - \frac{384 t^4}{(2 + t^2)^4} y = 24 \frac{2 - 11 t^2}{(2 + t^2)^4} \]

\[
\begin{align*}
    y(-1) &= \frac{1}{3} & y(1) &= \frac{1}{3} \\
    y''(-1) &= \frac{2}{27} & y''(1) &= \frac{2}{27}
\end{align*}
\]

Solution : \[ y(t) = \frac{1}{2 + t^2} \]

Since \( y(t) \) does not belong to the fitting space of a EF-rule, the parameter \( \mu \) will not be constant over the interval of integration.
Solution obtained by a fourth-order EF method

Computation of $\mu_j$ with $M = 8$:

$$P = 0 : y^{(8)}(t_j) - y^{(6)}(t_j) \mu_j^2 = 0$$

- re-express higher order derivatives in terms of $y$, $y'$, $y''$ and $y'''$
- approximate $y'$, $y''$ and $y'''$ in terms of $y$
- an initial approximation for $y$ can be computed with the classical, polynomial rule
Solution obtained by a fourth-order EF method

Computation of $\mu_j$ with $M = 8$ :

$$P = 1 : y^{(8)}(t_j) - 2 y^{(6)}(t_j) \mu_j^2 + y^{(4)}(t_j) \mu_j^4 = 0$$

Real and imaginary part of $\mu_j$ with smallest norm

Real and imag. part of $\mu_{1,j}$ and $\mu_{2,j}$
Solution obtained by a fourth-order EF method

Computation of $\mu_j$ with $M = 8$:

$$P = 1 : y^{(8)}(t_j) - 2 y^{(6)}(t_j) \mu_j^2 + y^{(4)}(t_j) \mu_j^4 = 0$$

error obtained with $\mu_{1,j}$, $\mu_{2,j}$ and $\mu$ with smallest norm
Global error

\[ M = 6 : \quad (K, P) = (5, -1) : \text{second-order method} \]
\[ (K, P) = (1, 1) : \text{fourth-order method} \]
Global error

\[ M = 8 : \quad (K, P) = (7, -1) \quad : \text{fourth-order method} \]
\[ (K, P) = (3, 1) \quad : \text{sixth-order method} \]
Global error

\[ M = 10 : \]

\[ (K, P) = (9, -1) \quad : \text{sixth-order method} \]

\[ (K, P) = (5, 1) \quad : \text{eighth-order method} \]
Condition number of the coefficient matrix

![Graph showing the condition number of the coefficient matrix as a function of h.]
Condition number of the coefficient matrix

The (classical) discretisation of $y_p^{(4)}$ gives rise to the coefficient matrix

$$
\begin{pmatrix}
5 & -4 & 1 \\
-4 & 6 & -4 & 1 \\
1 & -4 & 6 & -4 & 1 \\
& & & & \\
& & & & \\
1 & -4 & 6 & -4 & 1 \\
1 & -4 & 5 \\
\end{pmatrix}
$$

$$
\begin{pmatrix}
-2 & 1 \\
1 & -2 & 1 \\
& & & & \\
& & & & \\
1 & -2 & 1 \\
\end{pmatrix}
$$

$$
\text{cond}(A) \\
\text{cond}(B)
$$
Factorisation of the coefficient matrix

\[
\begin{pmatrix}
  c_2 & c_3 & 1 \\
  a_1 & a_2 & a_1 & 1 \\
  1 & a_1 & a_2 & a_1 & 1 \\
  & \vdots & \vdots & \vdots & \vdots \\
  1 & a_1 & a_2 & a_1 & 1 \\
  1 & a_1 & a_2 & a_1 \\
  1 & c_3 & c_2 \\
\end{pmatrix}
= 
\begin{pmatrix}
  a_2 - 1 & a_1 & 1 \\
  a_1 & a_2 & a_1 & 1 \\
  1 & a_1 & a_2 & a_1 & 1 \\
  & \vdots & \vdots & \vdots & \vdots \\
  1 & a_1 & a_2 & a_1 \\
  1 & a_1 & a_2 - 1 \\
\end{pmatrix}
\begin{pmatrix}
  \alpha & 1 \\
  1 & \alpha & 1 \\
  & \vdots & \vdots & \vdots \\
  1 & \alpha & 1 \\
  1 & \alpha \\
\end{pmatrix}
= 
\begin{pmatrix}
  \beta & 1 \\
  1 & \beta & 1 \\
  & \vdots & \vdots & \vdots \\
  1 & \beta \\
\end{pmatrix}
\begin{pmatrix}
  P \\
  \alpha \\
  \beta
\end{pmatrix}
\]

\[
M = 6: 
\begin{array}{ccc}
-1 & -2 & -2 \\
0 & -2 & -2 \\
1 & \frac{-2 - 4 \sin \theta (2 \cos \theta - 2 + \theta \sin \theta)}{4 \sin \theta - \theta (1 + \cos \theta)} & -2 \\
\end{array}
\]
Problem 2

\[ y^{(4)} - t = 4 e^t \]

\[ y(-1) = -1/e \quad y(1) = e \]
\[ y''(-1) = 1/e \quad y''(1) = 3e \]

Solution: \[ y(t) = e^t t \]

In theory, this problem is solved up to machine accuracy by any EF-rule with \( P \geq 1 \) and \( \mu_j = 1 \).
\( M = 6 \)

\[ P = 1 : y^{(6)}(t_j) - 2 y^{(4)}(t_j) \mu_j^2 + y^{(2)}(t_j) \mu_j^4 = 0 \]

differentiating the differential equation:

\[ (y^{(2)}(t_j) + 4 e^{t_j}) - 2 (y_j + 4 e^{t_j}) \mu_j^2 + y^{(2)}(t_j) \mu_j^4 = 0 \]

approximating \( y^{(2)}(t_j) \) by \( O(h^2) \) finite difference scheme

two real roots \( \mu^{(1)} \) and \( \mu^{(2)} \)
How to improve the accuracy?

\[ y^{(0)} \xrightarrow{\mu^{(1)}} y^{(1)} \xrightarrow{\mu^{(2)}} y^{(2)} \ldots \]

- \( y^{(0)} \) is obtained from classical, second order method
- compute \( \mu^{(1)} \) from \( y^{(0)} \) with classical second order schemes to approximate the derivatives that appear in the lte
- \( y^{(1)} \) is obtained from EF method with \( P = 1 \) and \( \mu = \mu^{(1)} \)
- compute \( \mu^{(2)} \) from \( y^{(1)} \) with EF schemes \( (P = 1) \) to approximate the derivatives that appear in the lte
- \( y^{(2)} \) is obtained from EF method with \( P = 1 \) and \( \mu = \mu^{(2)} \)
  \ldots
How to improve the accuracy?

**case $M = 6, h = 1/4$**

Abs. error in approx. of $y$, $h=1/4$

Computed values of $\mu$, $h=1/4$
How to improve the accuracy?

case $M = 6, \, h = 1/8$
How to improve the accuracy?

case $M = 6$, $h = 1/16$
How to improve the accuracy?

**case \( M = 6 \)**

Max. abs. error in \( y \) for \( h = 1/4, 1/8, h = 1/16 \)
How to improve the accuracy?

**case \( M = 8 \)**

Max. abs. error in \( y \) for \( h = \frac{1}{4}, \frac{1}{8}, h = \frac{1}{16} \)
Conclusions

- Fourth-order boundary value problems are solved by means of parameterized exponentially-fitted methods.
- A suitable value for the parameter can be found from the roots of the leading term of the local truncation error.
- If a constant value is found, then a very accurate solution can be obtained.
- However, the methods strongly suffer from the fact that the system to be solved is ill-conditioned for small values of the mesh size.