Exponentially-fitted methods applied to fourth-order boundary value problems

M. Van Daele, D. Hollevoet and G. Vanden Berghe

Department of Applied Mathematics and Computer Science

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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.
Linear multistep methods

A well known method to solve

\[ y'' = f(y) \quad y(a) = y_a \quad y'(a) = y'_a \]

is the Numerov method (order 4)

\[
y_{n+1} - 2y_n + y_{n-1} = \frac{1}{12} h^2 \left( f(y_{n-1}) + 10 f(y_n) + f(y_{n+1}) \right)
\]

Construction:

impose \( \mathcal{L}[z(t); h] = 0 \) for \( z(t) \in S = \{1, t, t^2, t^3, t^4\} \) where

\[
\mathcal{L}[z(t); h] := z(t + h) + \alpha_0 z(t) + \alpha_{-1} z(t - h) - h^2 \left( \beta_1 z''(t + h) + \beta_0 z''(t) + \beta_{-1} z''(t - h) \right)
\]
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, one could replace polynomials by trigonometric (in the complex case: exponential) functions.
EF Numerov method

Construction: impose $\mathcal{L}[z(t); h] = 0$ for $z(t) \in S$ with

$$S = \{1, t, t^2, \sin(\omega t), \cos(\omega t)\}$$

$$\mathcal{L}[z(t); h] := z(t + h) + \alpha_0 z(t) + \alpha_{-1} z(t - h)$$
$$- h^2 \left( \beta_1 z''(t + h) + \beta_0 z''(t) + \beta_{-1} z''(t - h) \right)$$

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left( \lambda f(y_{n-1}) + (1 - 2\lambda) f(y_n) + \lambda f(y_{n+1}) \right)$$

$$\lambda = \frac{1}{4 \sin^2 \frac{\theta}{2}} - \frac{1}{\theta^2}$$
$$\theta := \omega h$$

$$= \frac{1}{12} + \frac{1}{240} \theta^2 + \frac{1}{6048} \theta^4 + \ldots$$
EF methods

Generalisation: 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: $M = 2P + K + 3$
Examples

\[ M = 2P + K + 3 \]

\[
\begin{array}{|c|c|c|c|c|}
\hline
(K, P) & (K, P) & (K, P) & (K, P) & (K, P) \\
\hline
M = 2 & M = 4 & M = 6 & M = 8 & M = 10 \\
(1, -1) & (3, -1) & (5, -1) & (7, -1) & (9, -1) \\
(-1, 1) & (1, 0) & (3, 0) & (5, 0) & (7, 0) \\
 & (-1, 1) & (1, 1) & (3, 1) & (5, 1) \\
 & & (-1, 2) & (1, 2) & (3, 2) \\
 & & & (-1, 3) & (1, 3) \\
 & & & & (-1, 4) \\
\hline
\end{array}
\]

\[ (1, 2) \implies S = \left\{ 1, t, \exp(\pm \mu t), t \exp(\pm \mu t), t^2 \exp(\pm \mu t) \right\} \]
Exponential Fitting

L. Ixaru and G. Vanden Berghe

Exponential fitting


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

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

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

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

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

\[ t_j = a + jh, \quad j = 0, 1, \ldots, N + 1 \quad N \geq 3 \quad h := \frac{b-a}{N+1} \]

- **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**

\[
y_0 + \alpha_1 y_1 + \alpha_2 y_2 + a_3 y_3 = \gamma h^2 y''_0 + h^4 \left( \beta_0 F_0 + \beta_1 F_1 + \beta_2 F_2 + \beta_3 F_3 + \beta_4 F_4 + \beta_5 F_5 \right)
\]

- **end formula**
Central formula

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

\[ P = -1 : \quad \mathcal{L}[y] = 0 \quad \text{for} \quad y \in S = \{1, t, t^2, \ldots, t^{M-1}\} \]

\[ M = 10 : \]
\[ y_{p-2} - 4 y_{p-1} + 6 y_p - 4 y_{p+1} + y_{p+2} = \]
\[ h^4 \frac{1}{720} \left( -y_{p-2}^{(4)} + 124 y_{p-1}^{(4)} + 474 y_p^{(4)} + 124 y_{p+1}^{(4)} - y_{p+2}^{(4)} \right) \]
\[ \mathcal{L}[y](t) = \frac{1}{3024} h^{10} y^{(10)}(t) + O(h^{12}) \]

\[ M = 8 \text{ and } b_2 = 0 : \]
\[ h^4 \left( \text{central formula} \right) \]
EF Central formula

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

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

\[ M = 10 : \]
\[ y_{p-2} - 4 y_{p-1} + 6 y_p - 4 y_{p+1} + y_{p+2} = \]
\[ h^4 \left( b_2 y^{(4)}_{p-2} + b_1 y^{(4)}_{p-1} + b_0 y^{(4)}_p + b_1 y^{(4)}_{p+1} + b_2 y^{(4)}_{p+2} \right) \]

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

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

\( \mathcal{L}[y] := y(t - 2h) + a_1 y(t - h) + a_0 y(t) + a_1 y(t + h) + y(t + 2h) \)

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

\( P = 1 : \mathcal{L}[y] = 0 \text{ for } y \in S = \left\{ \cos(\omega t), \sin(\omega t), t \cos(\omega t), t \sin(\omega t), 1, t, t^2, \ldots, t^{M-5} \right\} \)

\( M = 6 \text{ and } b_1 = b_2 = 0 : \)

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

\[ a_0 = 2 \frac{-8 \sin^2 \theta + \theta \left( 4 \cos \theta - 1 \right) \sin \theta - 4 \cos \theta + 4}{\theta \sin \theta + 4 \cos \theta - 4} \quad a_1 = -4 \frac{\sin \theta \left( \theta \cos \theta - 2 \sin \theta \right)}{\theta \sin \theta + 4 \cos \theta - 4} \]

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

\( \mathcal{L}[y](t) = \frac{1}{6} h^6 \left( y^{(6)}(t) + 2 \omega^2 y^{(4)}(t) + \omega^4 y^{(2)}(t) \right) + \mathcal{O}(h^8) \)
Coefficients of Central formula $M = 6$

- $a_0$ and $a_1$ for $P = -1, 0, 1, 2$.
- $b_0$ for $P = -1, 0, 1, 2$.
Coefficients of Central formula $M = 8$
Coefficients of Central formula $M = 10$
Central formula: coefficients

E.g. $b_0$ in case $M = 6$

In closed form . . .

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

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

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

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

E.g. \( b_0 \) in case \( M = 6 \)

As a series . . .

- \( P = -1 : \)
  \[ b_0 = 1 \]

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

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

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

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

As an infinite series:

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

In closed form: (Coleman and Ixaru)

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

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

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

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

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

At \( t_j : \left. D^{(K+1)} (D^2 + \omega_j^2)^{(P+1)} y(t) \right|_{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

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

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

Then \( \ell(t) = 0 \) 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
- ...
Parameter selection

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 $|\mu_j|$. 
First example

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

\[ y(-1) = \frac{1}{3} \quad y(1) = \frac{1}{3} \]

\[ y''(-1) = \frac{2}{27} \quad y''(1) = \frac{2}{27} \]

Solution: \[ y(t) = \frac{1}{2 + t^2} \]
\( \mu_j \) for \( M = 8 \)

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

- 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 a polynomial rule

Real and imaginary part of \( \mu_j \)
\( \mu_j \) for \( M = 8 \)

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

Real and imaginary part of \( \mu_j \) with smallest norm

Real and imag. part of \( \mu_{1,j} \) and \( \mu_{2,j} \)
$\mu_j$ for $M = 8$

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

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

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

\( M = 10 : \)

\((K, P) = (9, -1)\) : sixth-order method  
\((K, P) = (5, 1)\) : eighth-order method
Condition number

\[ \text{cond}(A) \]

\[ 10^{-3} \quad 10^{-2} \quad 10^{-1} \quad 10^{4} \quad 10^{6} \quad 10^{8} \quad 10^{10} \quad 10^{12} \]

\[ h \]
Second example

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

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

Solution: \[ y(t) = e^t t \]
\( \mu_j \) for \( M = 6 \)

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

differentiating the differential equation:

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

\( y^{(2)}(t_j) \) approximated by fourth-order finite difference scheme

two real roots \( \mu^{(1)} \) and \( \mu^{(2)} \)
\( M = 6 \)

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

differentiating the differential equation:

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

\( y^{(2)}(t_j) \) approximated by sixth-order finite difference scheme

two real roots \( \mu^{(1)} \) and \( \mu^{(2)} \)
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.