Multiparameter exponentially-fitted methods applied to second-order boundary value problems

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

Department of Applied Mathematics and Computer Science
Ghent University

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Outline

Introduction

In the past 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 second-order BVP

$$y'' = f(y) \qquad y(a) = y_a \qquad y(b) = y_b$$

Numerov method :

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

$$n = 1, 2, \ldots, N \qquad h = \frac{b-a}{N+1}$$

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

$$\begin{aligned}\mathcal{L}[z(t);h] := {} & z(t+h) + a_0\,z(t) + a_{-1}\,z(t-h) \\ & -h^2\left(b_1\,z''(t+h) + b_0\,z''(t) + b_{-1}\,z''(t-h)\right)\end{aligned}$$

$$\mathcal{L}[z(t);h] = -\frac{1}{240}h^6\,z^{(6)}(t) + \mathcal{O}(h^8) \qquad \Longrightarrow \text{order } 4$$

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A model problem

Consider

$$y'' + \omega^2 y = g(y) \qquad y(a) = y_a \qquad y(b) = y_b\,.$$

If $|g(y)| \ll |\omega^2 y|$ (and if unique solution exists) 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.

This leads to exponentially-fitted (EF) methods

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$$\lambda \;=\; \frac{1}{4\sin^2\frac{\theta}{2}} - \frac{1}{\theta^2} = \frac{1}{12} + \frac{1}{240}\theta^2 + \frac{1}{6048}\theta^4 + \dots \qquad \theta := \omega\, h$$

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L. Ixaru and G. Vanden Berghe
Exponential fitting
Kluwer Academic Publishers, Dordrecht, 2004

$$\xi(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z < 0 \\ \cosh(Z^{1/2}) & \text{if } Z \geq 0 \end{cases}$$

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

Extension to $Z \in \mathbb{C}$:

$$\xi(Z) = \cos(\mathrm{i}\sqrt{Z}) \quad \text{and} \quad \eta(Z) = \begin{cases} \dfrac{\sin(\mathrm{i}\sqrt{Z})}{\mathrm{i}\sqrt{Z}} & \text{if } Z \neq 0 \\ 1 & \text{if } Z = 0 \end{cases}$$

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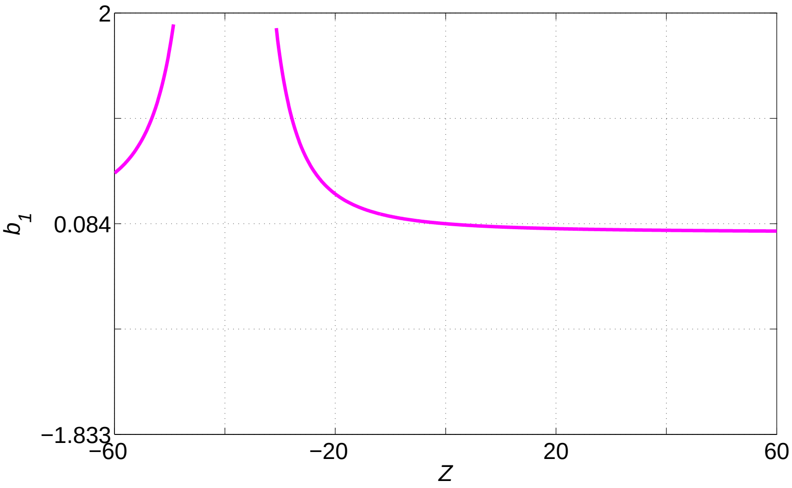
λ as a function of Z



Parameter selection

- local optimization
  based on local truncation error (lte)
  Z is step-dependent

- global optimization
  Preservation of geometric properties (periodicity, energy, ...)
  Z is constant over the interval of integration

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Generalisations

To determine the coefficients of a method, we impose conditions on a linear functional. These conditions are related to the fitting space $\mathcal{S}$ which contains $\{1, t, t^2, \ldots, t^K\}$ and

- possibility 1 (Calvo et al.) : trigonometric polynomials $\{\exp(\pm\mu t), \exp(\pm 2\mu t), \ldots, \exp(\pm(P+1)\mu t)\}$
- possibility 2 (Ixaru, Vanden Berghe, V.D., ...) : exponential-fitting $\{\exp(\pm\mu t), t\,\exp(\pm\mu t), \ldots, t^P\exp(\pm\mu t)\}$

A method can be characterized by the couple (K, P)
Classical method : $P = -1$
number of basis functions : $M = 2P + K + 3$
Numerov $M = 6$: $(K, P) = (5, -1), (3, 0), (1, 1)$ or $(-1, 2)$
Here, we consider a generalisation of both classes :

- possibility 3 : $\{\exp(\pm\mu_0 t), \exp(\pm\mu_1 t), \ldots, \exp(\pm\mu_P t)\}$

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Numerov $M = 6$: $(K, P) = (5, -1), (3, 0), (1, 1)$ or $(-1, 2)$
Here, we consider a generalisation of both classes :

- possibility 3 : $\{\exp(\pm\mu_0 t), \exp(\pm\mu_1 t), \ldots, \exp(\pm\mu_P t)\}$

Generalisations

To determine the coefficients of a method, we impose conditions on a linear functional. These conditions are related to the fitting space $\mathcal{S}$ which contains $\{1, t, t^2, \ldots, t^K\}$ and

- possibility 1 (Calvo et al.) : trigonometric polynomials $\{\exp(\pm\mu t), \exp(\pm 2\mu t), \ldots, \exp(\pm(P+1)\mu t)\}$
- possibility 2 (Ixaru, Vanden Berghe, V.D., . . .) : exponential-fitting $\{\exp(\pm\mu t), t\ \exp(\pm\mu t), \ldots, t^P \exp(\pm\mu t)\}$

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

Classical method : $P = -1$

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Motivation

recent work by Hollevoet, V.D. and Vanden Berghe

- "On the leading error term of exponentially fitted Numerov methods", ICNAAM 2008
- "The optimal exponentially-fitted Numerov method for solving two-point boundary value methods", J. CAM 2009

EF-approach of Ixaru and Vanden Berghe :

$$\begin{aligned}\mathcal{L}[z(t);h] := {} & z(t+h) + a_0\, z(t) + a_{-1}\, z(t-h) \\ & -h^2 \left(b_1\, z''(t+h) + b_0\, z''(t) + b_{-1}\, z''(t-h)\right)\end{aligned}$$

$$\begin{aligned} z(t) \in {} & \mathcal{S}_{K,P}(\mu) = \\ & \{1, t, t^2, \ldots, t^K\} \cup \{\exp(\pm\mu\, t),\ t\ \exp(\pm\mu\, t),\ \ldots,\ t^P \exp(\pm\mu\, t)\}\end{aligned}$$

Motivation

μ is determined from the lte :

$$h^6\,\phi_P(Z)\,D^{K+1}\,(D^2-\mu^2)^{P+1}\,y(t_j)+\mathcal{O}(h^8) \qquad \phi_P(Z)=-\frac{1}{240}+\mathcal{O}(Z)$$

At $t=t_j$, $\mu^2 := \mu_j^2$ such that

$$E_{P,j} := D^{K+1}\,(D^2-\mu_j^2)^{P+1}\,y(t_j)=0$$

- $P=0 : y^{(6)}(t_j)-\mu_j^2\,y^{(4)}(t_j)=0 \Longrightarrow \mu_j^2\in\mathbb{R}$
- $P=1 : y^{(6)}(t_j)-2\,\mu^2\,y^{(4)}(t_j)+\mu^4\,y^{(2)}(t_j)=0$ may only have complex roots μ_j^2, such that $y_j\in\mathbb{C}$.

To solve this problem, we propose a new type of EF methods.

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  To solve this problem, we propose a new type of EF methods.

Multiparameter exponentially-fitted methods

Replace

$$\mathcal{S}_{K,P}(\mu) = \{1, t, t^2, \ldots, t^K\} \cup \{\exp(\pm\mu\, t), t\ \exp(\pm\mu\, t), \ldots, t^P \exp(\pm\mu\, t)\}$$

by

$$\widehat{\mathcal{S}}_{K,P}(\mu_0, \mu_1, \ldots, \mu_P) = \{1, t, t^2, \ldots, t^K\} \cup \{\exp(\pm\mu_0\, t), \exp(\pm\mu_1\, t), \ldots, \exp(\pm\mu_P\, t)\}$$

The parameters μ_q, $q = 0, \ldots, P$ are either real or appear as complex conjugate pairs

Coefficients

(i) $P = -1$: Classical Numerov method

$$a_0 = -2 \qquad b_0 = \frac{5}{6} \qquad b_1 = \frac{1}{12}$$

(ii) $P = 0$: already known EF Numerov method

$$a_0 = -2 \quad b_0 = \frac{2 - 2\,\xi_0 + \xi_0 Z_0}{Z_0\,(\xi_0 - 1)} \quad b_1 = \frac{2\,\xi_0 - Z_0 - 2}{2\,Z_0\,(\xi_0 - 1)} = 1 - 2\,b_0$$

$Z_0 := (\mu_0\,h)^2$, $\xi_0 := \xi(Z_0)$ and $\eta_0 := \eta(Z_0)$

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Coefficients

(iii) $P = 1$: a new 2-parameter method

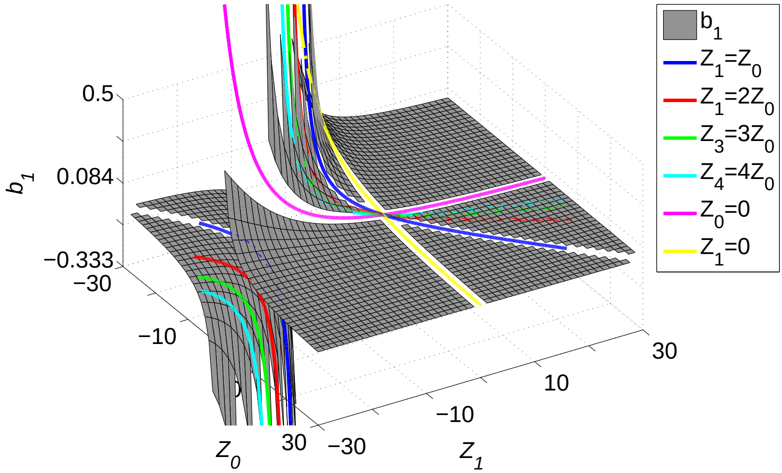
$$a_0 = -2 \qquad b_0 = -2\frac{\xi_0\,(\xi_1 - 1)\,Z_0 + \xi_1\,(1-\xi_0)\,Z_1}{Z_1 Z_0\,(\xi_1 - \xi_0)}$$

$$b_1 = \frac{(\xi_1 - 1)\,Z_0 + (1-\xi_0)\,Z_1}{Z_1 Z_0\,(\xi_1 - \xi_0)} = 1 - 2\,b_0$$

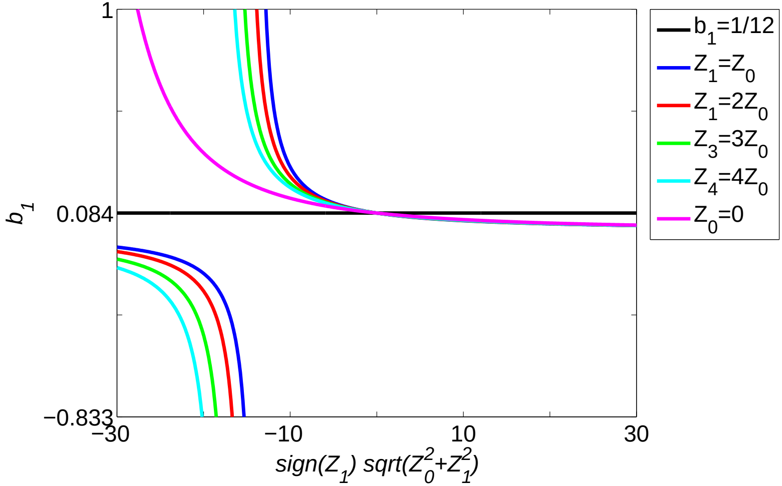
$Z_q := (\mu_q\, h)^2$, $\xi_q := \xi(Z_q)$ and $\eta_q := \eta(Z_q)$

assuming $Z_0 \cdot Z_1 \neq 0$ and $Z_0 - Z_1 \neq 0$

b_1 as a function of Z_0 and Z_1



b_1 as a function of $\mathrm{sign}(Z_1)\sqrt{Z_0^2+Z_1^2}$



Coefficients

(iv) $P = 2$: a new 3-parameter method

$$a_0 = 2\,\frac{\xi_0\,(\xi_1-\xi_2)\,Z_1Z_2+\xi_1\,(\xi_2-\xi_0)\,Z_0Z_2+\xi_2\,(\xi_0-\xi_1)\,Z_0Z_1}{(\xi_2-\xi_1)\,Z_1\,Z_2+(\xi_1-\xi_0)\,Z_0\,Z_1+(\xi_0-\xi_2)\,Z_0Z_2}$$

$$b_0 = 2\,\frac{\xi_1\,(\xi_0-\xi_2)\,Z_1+\xi_2\,(-\xi_0+\xi_1)\,Z_2+\xi_0\,(\xi_2-\xi_1)\,Z_0}{(\xi_2-\xi_1)\,Z_1\,Z_2+(\xi_1-\xi_0)\,Z_0\,Z_1+(\xi_0-\xi_2)\,Z_0Z_2}$$

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assuming $Z_0 \cdot Z_1 \cdot Z_2 \neq 0$ and
$(Z_0 - Z_1)(Z_1 - Z_2)(Z_2 - Z_0) \neq 0$

Special cases

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$$a_0 = -2 \qquad b_0 = -2\frac{\xi_0\,(\xi_1 - 1)\,Z_0 + \xi_1\,(1-\xi_0)\,Z_1}{Z_1 Z_0\,(\xi_1 - \xi_0)}$$

$$b_1 = \frac{(\xi_1 - 1)\,Z_0 + (1-\xi_0)\,Z_1}{Z_1 Z_0\,(\xi_1 - \xi_0)} = 1 - 2\,b_0$$

$$\lim_{Z_1\to Z_0} b_0 = \frac{4\,{\xi_0}^2 - 4\,\xi_0 - 2\,\eta_0 Z_0}{{Z_0}^2 \eta_0} \qquad \lim_{Z_1\to Z_0} b_1 = \frac{\eta_0 Z_0 + 2 - 2\,\xi_0}{{Z_0}^2\eta_0}$$

same expressions as in the case

$\mathcal{S}_{1,1}(\mu_0) = \{1,\, t,\, \exp(\pm\mu_0\, t),\, t\ \exp(\pm\mu_0\, t)\}$

$$\lim_{\mu_1\to\mu_0} \widehat{\mathcal{S}}_{K,1}(\mu_0,\mu_1) = \mathcal{S}_{K,1}(\mu_0)$$

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$$a_0 = 2\,\frac{\xi_0\,(\xi_1-\xi_2)\,Z_1Z_2+\xi_1\,(\xi_2-\xi_0)\,Z_0Z_2+\xi_2\,(\xi_0-\xi_1)\,Z_0Z_1}{(\xi_2-\xi_1)\,Z_1\,Z_2+(\xi_1-\xi_0)\,Z_0\,Z_1+(\xi_0-\xi_2)\,Z_0Z_2}$$

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$$\lim_{\substack{Z_1\to Z_0\\ Z_2\to Z_0}} b_0 = 2\,\frac{\eta_0\xi_0+{\xi_0}^2-2}{Z_0\,(\xi_0+3\,\eta_0)}$$

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same coefficients as in the case $\mathcal{S}_{-1,2}(\mu_0) = \{\exp(\pm\mu_0\,t),\ t\,\exp(\pm\mu_0\,t),\ t^2\,\exp(\pm\mu_0\,t)\}$

$$\lim_{\substack{\mu_1\to\mu_0\\ \mu_2\to\mu_0}} \widehat{\mathcal{S}}_{K,2}(\mu_0,\mu_1,\mu_2) = \mathcal{S}_{K,2}(\mu_0)$$

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Selecting values for parameters

$$\widehat{lte} = h^6\, \widehat{\phi}_P(Z_0, \ldots, Z_P)\widehat{E}_{P,j} + \mathcal{O}(h^8)$$

$$\widehat{E}_{P,j} := D^{K+1}(D^2 - \mu_0^2)(D^2 - \mu_1^2)\cdots(D^2 - \mu_P^2)y(t_j)$$

$$\widehat{\phi}_P(Z_0, \ldots, Z_P) = -\frac{1}{240} + \mathcal{O}(Z_0, Z_1, \ldots, Z_P)$$

(i) $P = 0 : \widehat{E}_{0,j} := y^{(6)}(t_j) - \mu_0^2 y^{(4)}(t_j)$

(ii) $P = 1 : \widehat{E}_{1,j} := y^{(6)}(t_j) - (\mu_0^2 + \mu_1^2)y^{(4)}(t_j) + \mu_0^2\mu_1^2 y^{(2)}(t_j)$

(iii) $P = 2 :$

$$\begin{aligned}\widehat{E}_{2,j} \;:=\; & y^{(6)}(t_j) - (\mu_0^2 + \mu_1^2 + \mu_2^2)y^{(4)}(t_j) \\ & + (\mu_0^2\mu_1^2 + \mu_0^2\mu_2^2 + \mu_1^2\mu_2^2)y^{(2)}(t_j) - \mu_0^2\mu_1^2\mu_2^2 y(t_j)\end{aligned}$$

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$$\begin{aligned}\widehat{E}_{2,j} \;:=\; & y^{(6)}(t_j) - (\mu_0^2+\mu_1^2+\mu_2^2)\,y^{(4)}(t_j)\\ & +(\mu_0^2\,\mu_1^2+\mu_0^2\,\mu_2^2+\mu_1^2\,\mu_2^2)\,y^{(2)}(t_j) - \mu_0^2\,\mu_1^2\,\mu_2^2\,y(t_j)\end{aligned}$$

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$$\widehat{E}_{1,j} = y^{(6)}(t_j) - (\mu_0^2 + \mu_1^2)\, y^{(4)}(t_j) + \mu_0^2\, \mu_1^2\, y^{(2)}(t_j)$$

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$\widehat{E}_{P,j}$ contains $y^{(6)}(t_j)$, $y^{(4)}(t_j)$, ...

- these can be expressed in terms of y and y' by means of the differential equation
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Example

$$y'' = \frac{3}{4}y - e^t \sin(t/2) \qquad y(0) = 1 \qquad y(\pi) = 0$$

$$y(t) = e^t \cos(t/2)$$

$$y(t) \in \text{Span}\, \widehat{\mathcal{S}}_{1,1}(1 + i/2, 1 - i/2)$$

but there exists no $\mu \in \mathbb{C}$ such that

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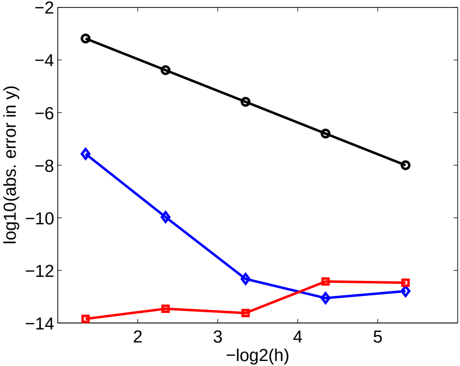

$\max_{j\in\{1,\ldots,N\}} \|y(t_j) - y_j\|$ for the classical method (black), the 2-parameter method with exact values for μ_i^2 (red) and the 2-parameter method with numerically computed values for μ_i^2 (blue).

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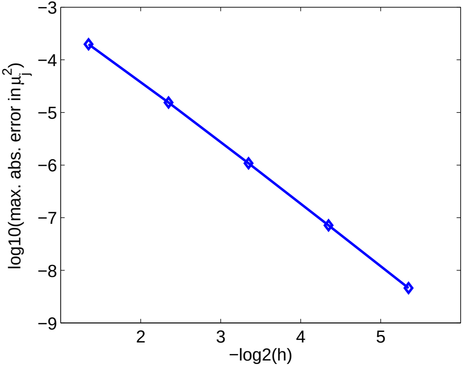

max-norm of the error in μ_i^2

Conclusions

- we constructed a new family of exponentially-fitted variants of the well-known Numerov method
- these methods contain $P + 1$ parameters $\mu_0, \mu_1, \ldots, \mu_P$ that can be determined either by local arguments of by global arguments and this resp. leads to variable or constant parameter values
- special case $\mu_0 = \mu_1 = \ldots = \mu_P = \mu$ gives a known family of EF methods
- methods can be constructed that give much more accurate results than those obtained by the classical Numerov method