

P-stable Exponentially fitted Obrechhoff methods

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Outline

- Introduction on exponentially fitted (EF) methods
- 2-step Obrechhoff methods for $y'' = f(x, y)$
- P-stable Obrechhoff methods for $y'' = f(x, y)$
- P-stable EF Obrechhoff methods for $y'' = f(x, y)$
- Conclusions

Exponentially fitted methods

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 or 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)

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

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

$$\begin{aligned} \mathcal{L}[z(x); h] := & z(x+h) + \alpha_0 z(x) + \alpha_{-1} z(x-h) \\ & - h^2 (\beta_1 z''(x+h) + \beta_0 z''(x) + \beta_{-1} z''(x-h)) \end{aligned}$$

Exponential fitting

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

$$y(x) \approx \alpha \cos(\omega x + \phi)$$

To mimic this oscillatory behaviour, one could replace polynomials by trigonometric (in the complex case : exponential) functions.

EF Numerov method

Construction : impose $\mathcal{L}[z(x); h] = 0$ for

$$z(x) = 1, x, x^2, \sin(\omega x), \cos(\omega x)$$

$$\begin{aligned} \mathcal{L}[z(x); h] := & z(x+h) + \alpha_0 z(x) + \alpha_{-1} z(x-h) \\ & - h^2 (\beta_1 z''(x+h) + \beta_0 z''(x) + \beta_{-1} z''(x-h)) \end{aligned}$$

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

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

EF methods

Generalisation : to determine the coefficients of a method, we impose conditions on a linear functional. These conditions are related to

- polynomials :

$$\{x^q | q = 0, \dots, K\}$$

- exponential or trigonometric functions, multiplied with powers of x :

$$\{x^q \exp(\pm \mu x) | q = 0, \dots, P\}$$

or, with $\omega = i \mu$,

$$\{x^q \cos(\omega x), x^q \sin(\omega x) | q = 0, \dots, P\}$$

Classical method : $P = -1$

Choice of ω

- local optimization
based on local truncation error (lte)
 ω is step-dependent
- global optimization
Preservation of geometric properties (periodicity, energy, ...)
 ω is constant over the interval of integration

Obrechhoff methods



Nikola Obrechhoff (1896-1963)

Obrechhoff methods (OM) : °1940 for quadrature

Milne : OM for solving diff. eq. : 1949

Obrechhoff methods for $y'' = f(x, y)$

Two-step methods

$$y_{n+1} - 2y_n + y_{n-1} = \sum_{i=1}^m h^{2i} \left(\beta_{i0} y_{n+1}^{(2i)} + 2\beta_{i1} y_n^{(2i)} + \beta_{i0} y_{n-1}^{(2i)} \right)$$

$$\mathcal{L}[z(x); h] := z(x+h) - 2z(x) + z(x-h)$$

$$- \sum_{i=1}^m h^{2i} \left(\beta_{i0} z^{(2i)}(x+h) + 2\beta_{i1} z^{(2i)}(x) + \beta_{i0} z^{(2i)}(x-h) \right)$$

symmetric method : $\mathcal{L}[z(x); h] \equiv 0$ if $z(x)$ is odd

$$\mathcal{L}[1; h] \equiv 0$$

order $p \iff \mathcal{L}[x^q; h] = 0, q = 0, 1, \dots, p+1$

$$\text{lte} = C_{p+2} h^{p+2} y^{(p+2)}(x_n) + \mathcal{O}(h^{p+3}) \quad C_{p+2} = \frac{\mathcal{L}[x^{p+2}; h]}{(p+2)! h^{p+2}}$$

Two-step OM

- $m = 1 : p = 4, C_6 = -\frac{1}{240}$ (Numerov method)

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

- $m = 2 : p = 8, C_{10} = \frac{59}{76204800}$

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{252} \left(11y_{n+1}^{(2)} + 230y_n^{(2)} + 11y_{n-1}^{(2)} \right) - \frac{h^4}{15120} \left(13y_{n+1}^{(4)} - 626y_n^{(4)} + 13y_{n-1}^{(4)} \right)$$

Two-step OM

- $m = 3 : p = 12, C_{14} = -\frac{45469}{1697361329664000}$

$$y_{n+1} - 2y_n + y_{n-1} =$$

$$\frac{h^2}{7788} \left(229 y_{n+1}^{(2)} + 7330 y_n^{(2)} + 229 y_{n-1}^{(2)} \right)$$

$$- \frac{h^4}{25960} \left(11 y_{n+1}^{(4)} - 1422 y_n^{(4)} + 11 y_{n-1}^{(4)} \right)$$

$$+ \frac{h^6}{39251520} \left(127 y_{n+1}^{(6)} + 4846 y_n^{(6)} + 127 y_{n-1}^{(6)} \right)$$

- ...

method of order $p = 4m$

Stability of two-step OM

$$y_{n+1} - 2y_n + y_{n-1} = \sum_{i=1}^m h^{2i} \left(\beta_{i0} y_{n+1}^{(2i)} + 2\beta_{i1} y_n^{(2i)} + \beta_{i0} y_{n-1}^{(2i)} \right)$$

applied to $y'' = -\lambda^2 y$ gives

$$y_{n+1} - 2R_{mm}(\nu^2) y_n + y_{n-1} = 0 \quad \nu := \lambda h$$

$$R_{mm}(\nu^2) = \frac{1 + \sum_{i=1}^m (-1)^i \beta_{i1} \nu^{2i}}{1 + \sum_{i=1}^m (-1)^{i+1} \beta_{i0} \nu^{2i}}$$

The stability function R_{mm} uniquely determines the method.

A method has the interval of periodicity $(0, \nu_0^2)$ if

$$|R_{mm}(\nu^2)| < 1 \text{ for } 0 < \nu^2 < \nu_0^2.$$

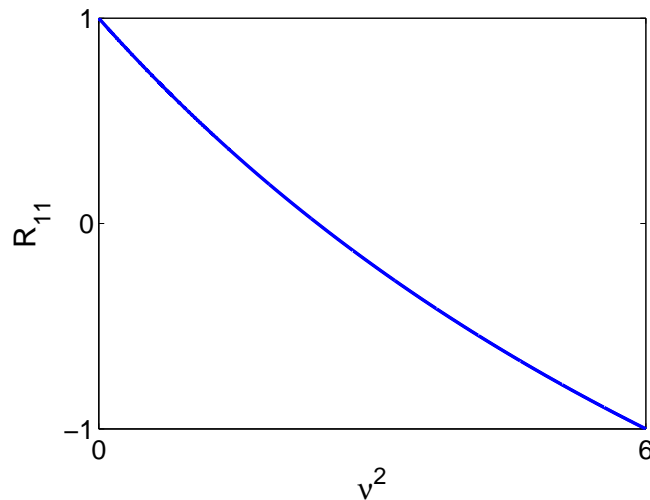
The method is *P-stable* if $|R_{mm}(\nu^2)| \leq 1$ for all real $\nu \neq 0$.

Stability of two-step OM

• $m = 1 : p = 4, C_6 = -\frac{1}{240}$ (Numerov)

$$\nu_0^2 = 6$$

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



Stability of two-step OM

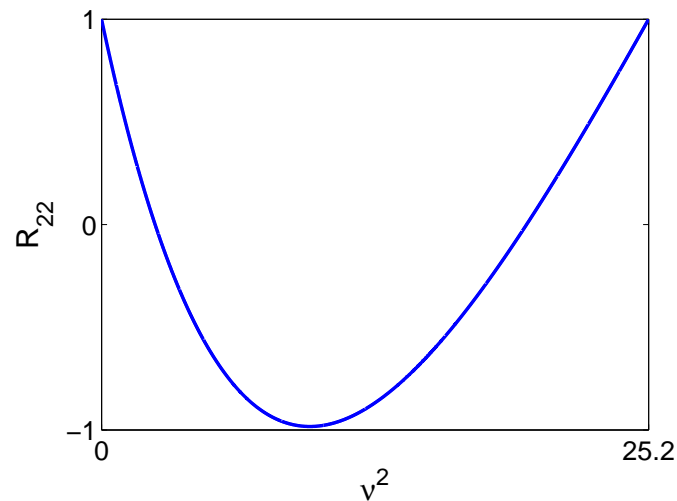
• $m = 2 : p = 8, C_{10} = \frac{59}{76204800}$

$$\nu_0^2 = 25.2$$

$$y_{n+1} - 2y_n + y_{n-1} =$$

$$\frac{h^2}{252} \left(11 y_{n+1}^{(2)} + 115 y_n^{(2)} + 11 y_{n-1}^{(2)} \right)$$

$$- \frac{h^4}{15120} \left(13 y_{n+1}^{(4)} - 626 y_n^{(4)} + 13 y_{n-1}^{(4)} \right)$$

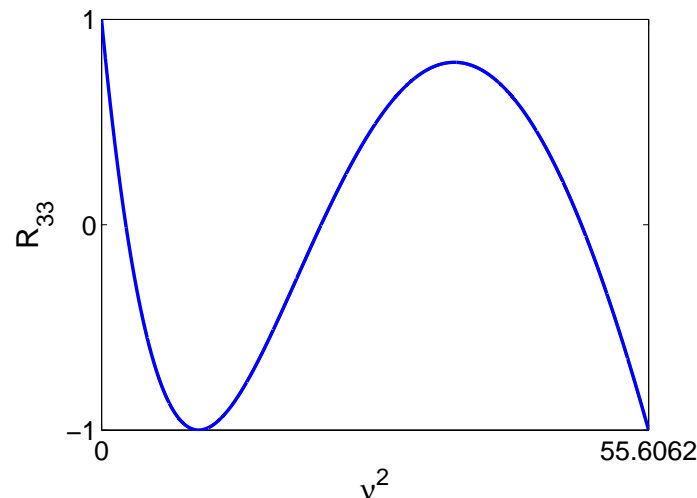


Stability of two-step OM

• $m = 3 : p = 12, C_{14} = -\frac{45469}{1697361329664000} \quad \nu_0^2 = 55.60 \dots$

$$y_{n+1} - 2y_n + y_{n-1} =$$

$$\begin{aligned} & \frac{h^2}{7788} \left(229 y_{n+1}^{(2)} + 7330 y_n^{(2)} + 229 y_{n-1}^{(2)} \right) \\ & + \frac{h^4}{25960} \left(-11 y_{n+1}^{(4)} + 1422 y_n^{(4)} - 11 y_{n-1}^{(4)} \right) \\ & + \frac{h^6}{39251520} \left(127 y_{n+1}^{(6)} + 4846 y_n^{(6)} + 127 y_{n-1}^{(6)} \right) \end{aligned}$$



P-stable 2-step OM

Ananthakrishnaiah (1987)

idea : use some parameters to obtain P-stability.

$$m = 3 \text{ and } m = 4$$

$$\text{e.g. } m = 3$$

$$y_{n+1} - 2y_n + y_{n-1} =$$

$$h^2 \left(\beta_{10} y_{n+1}^{(2)} + 2 \beta_{11} y_n^{(2)} + \beta_{10} y_{n-1}^{(2)} \right)$$

$$+ h^4 \left(\beta_{20} y_{n+1}^{(4)} + 2 \beta_{21} y_n^{(4)} + \beta_{20} y_{n-1}^{(4)} \right)$$

$$+ h^6 \left(\beta_{30} y_{n+1}^{(6)} + 2 \beta_{31} y_n^{(6)} + \beta_{30} y_{n-1}^{(6)} \right)$$

impose $p = 6 : \{x^2, x^4, x^6\}$,

then 3 parameters (β_{20} , β_{30} and β_{31}) remain

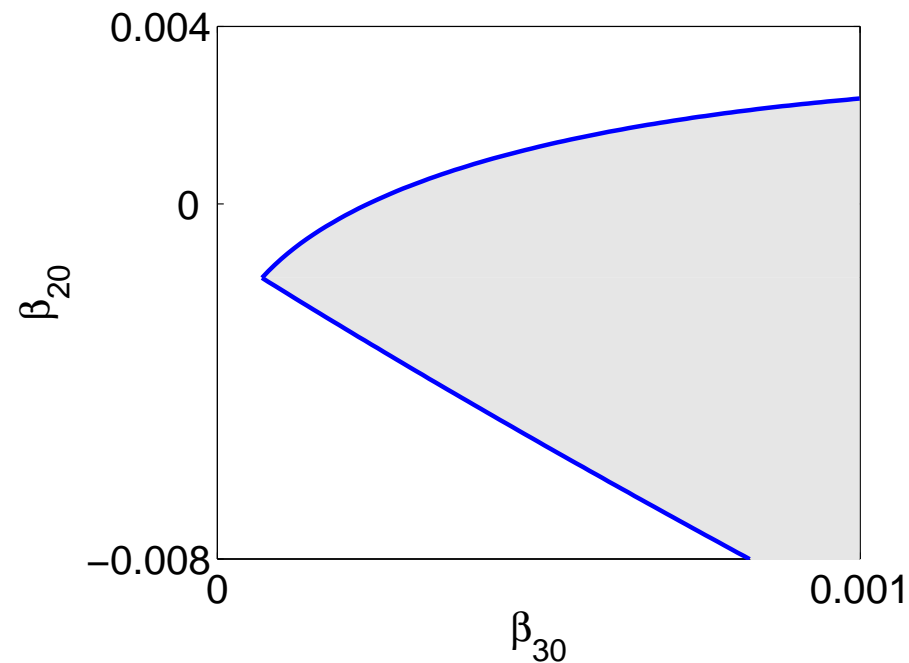
$$R_{33} = \frac{1 - \beta_{11} \nu^2 + \beta_{21} \nu^4 - \beta_{31} \nu^6}{1 + \beta_{10} \nu^2 - \beta_{20} \nu^4 + \beta_{30} \nu^6}$$

$$\text{let } \beta_{31} = \beta_{30}$$

Ananthakrishnaiah's idea

Choose these 2 remaining parameters β_{20} , β_{30} such that the method becomes P-stable

$$|R_{33}| = \left| \frac{N_3}{D_3} \right| < 1 \iff (D_3 - N_3)(D_3 + N_3) > 0$$

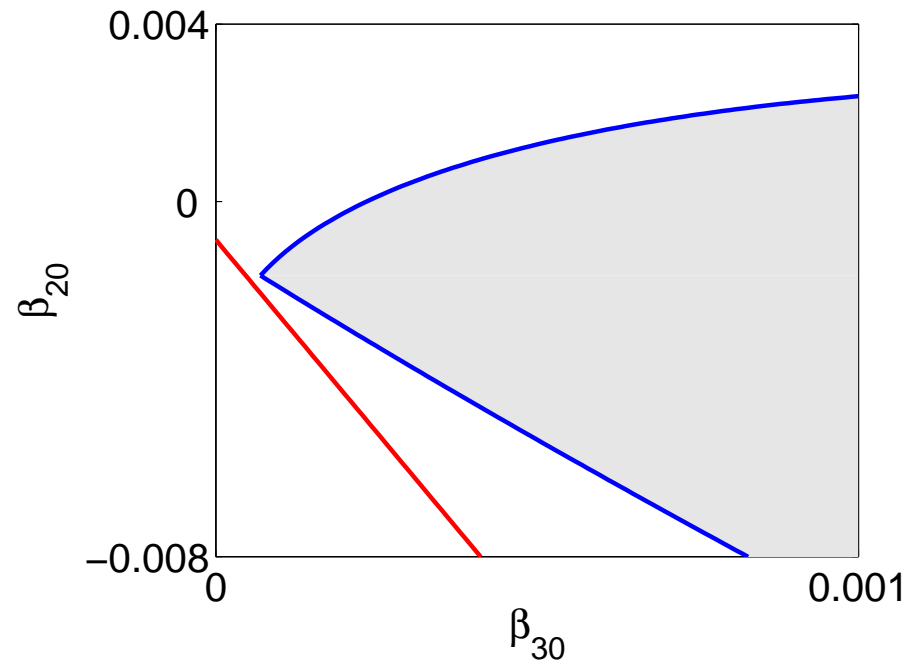


Ananthakrishnaiah's idea

Find the solution for which the phase-lag,

$$\nu - \arccos R_{33} = \left(\frac{13}{604800} + \frac{13}{30} \beta_{30} + \frac{1}{40} \beta_{20} \right) \nu^7 + \mathcal{O}(\nu^9)$$

becomes minimal.

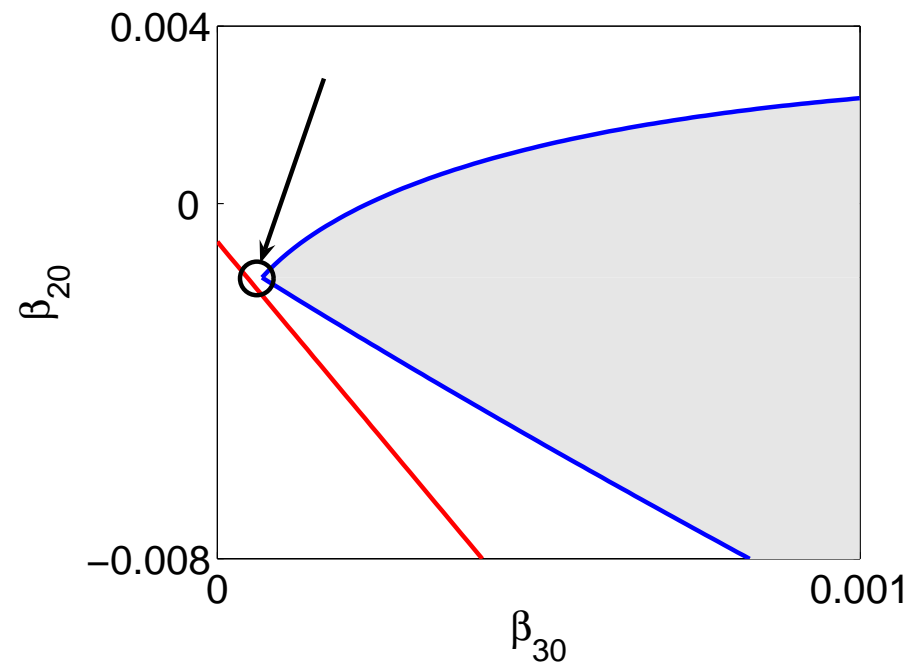


Ananthakrishnaiah's idea

Find the solution for which the phase-lag,

$$\nu - \arccos R_{33} = \left(\frac{13}{604800} + \frac{13}{30} \beta_{30} + \frac{1}{40} \beta_{20} \right) \nu^7 + \mathcal{O}(\nu^9)$$

becomes minimal.



$$\text{This gives } (\beta_{30}, \beta_{20}) = \left(\frac{1}{14400}, -\frac{1}{600} \right).$$

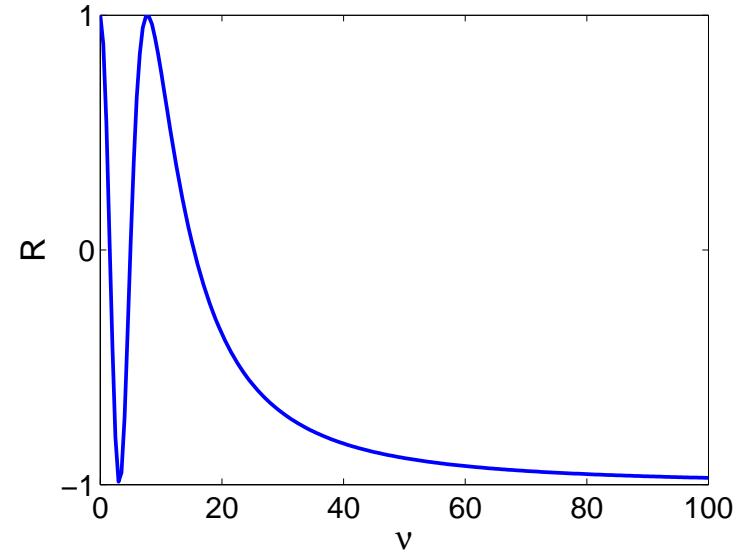
Ananthakrishnaiah's idea

Ananthakrishnaiah $m = 3 : p = 6$, P-stable, $C_8 = -\frac{1}{50400}$

$$\begin{aligned} y_{n+1} - 2y_n + y_{n-1} = & \\ & \frac{h^2}{20} \left(y_{n+1}^{(2)} + 18 y_n^{(2)} + y_{n-1}^{(2)} \right) \\ & - \frac{h^4}{600} \left(y_{n+1}^{(4)} - 22 y_n^{(4)} + y_{n-1}^{(4)} \right) \\ & + \frac{h^6}{14400} \left(y_{n+1}^{(6)} + 2 y_n^{(6)} + y_{n-1}^{(6)} \right) \end{aligned}$$

Ananthakrishnaiah's idea

$$R_{33} = \frac{1 - \frac{9}{20} \nu^2 + \frac{11}{600} \nu^4 - \frac{1}{14400} \nu^6}{1 + \frac{1}{20} \nu^2 + \frac{1}{600} \nu^4 + \frac{1}{14400} \nu^6}$$



$$|R_{33}| = \left| \frac{N_3}{D_3} \right| < 1 \text{ since}$$

$$(D_3 - N_3)(D_3 + N_3) = \frac{\nu^2 (\nu^2 - 10)^2 (\nu^2 - 60)^2}{360000}$$

P-stable 2-step OM

We were able to generalise Ananthakrishnaiah's idea in

M. Van Daele and G. Vanden Berghe, P-stable Obrechhoff methods of arbitrary order for second-order differential equations, Numerical Algorithms **44**, 2007, 115-131

Algorithm to construct a P-stable OM for a given m :

- impose order $2m$
- $D_m - N_m$ and $D_m + N_m$ should both be halves of perfect squares

This leads to a system of **non-linear** equations.

Theorem : the approximant $R_{mm}(\nu^2)$, obtained by generalising Ananthakrishnaiah's approach, is given by the real part of the (m, m) -Padé approximant of $\exp(i\nu)$.

This leads to a system of **linear** equations.

Example

$$\begin{aligned} R_{33}(\nu^2) &= \frac{1 - \frac{9}{20} \nu^2 + \frac{11}{600} \nu^4 - \frac{1}{14400} \nu^6}{1 + \frac{1}{20} \nu^2 + \frac{1}{600} \nu^4 + \frac{1}{14400} \nu^6} \\ &= \Re \left(\frac{1 + \frac{1}{2} i \nu - \frac{1}{10} \nu^2 - \frac{1}{120} i \nu^3}{1 - \frac{1}{2} i \nu - \frac{1}{10} \nu^2 + \frac{1}{120} i \nu^3} \right) \\ &= \frac{\left(1 - \frac{1}{10} \nu^2\right)^2 - \left(\frac{1}{2} \nu - \frac{1}{120} \nu^3\right)^2}{\left(1 - \frac{1}{10} \nu^2\right)^2 + \left(\frac{1}{2} \nu - \frac{1}{120} \nu^3\right)^2} \end{aligned}$$

$$\text{where } \frac{1 + \frac{1}{2} \nu + \frac{1}{10} \nu^2 + \frac{1}{120} \nu^3}{1 - \frac{1}{2} \nu + \frac{1}{10} \nu^2 - \frac{1}{120} \nu^3} = \exp(\nu) + \mathcal{O}(\nu^7)$$

$$|R_{33}(\nu^2)| = \left| \frac{\left(1 - \frac{1}{10} \nu^2\right)^2 - \left(\frac{1}{2} \nu - \frac{1}{120} \nu^3\right)^2}{\left(1 - \frac{1}{10} \nu^2\right)^2 + \left(\frac{1}{2} \nu - \frac{1}{120} \nu^3\right)^2} \right| \leq 1$$

Conclusion

How does the P-stable Obrechhoff method

$$y_{n+1} - 2y_n + y_{n-1} = \sum_{i=1}^m h^{2i} \left(\beta_{i0} y_{n+1}^{(2i)} + 2\beta_{i1} y_n^{(2i)} + \beta_{i0} y_{n-1}^{(2i)} \right)$$

of order $2m$ look like ?

$$\left\{ \begin{array}{l} \beta_{i0} = (-1)^{i+1} a_i^2 + 2 \sum_{j=0}^{i-1} (-1)^{j+1} a_j a_{2i-j} \\ \beta_{i1} = a_i^2 + 2 \sum_{j=0}^{i-1} a_j a_{2i-j} \end{array} \right. \quad i = 1 \dots, m$$

$$\text{where } a_j = \begin{cases} \frac{\binom{m}{j}}{\binom{2m}{j}} & \text{for } 0 \leq j \leq m \\ 0 & \text{for } j > m \end{cases}$$

P-stable Expon. fitted OM

How to obtain P-stable exponentially-fitted Obrechhoff methods ?

$$y_{n+1} - 2y_n + y_{n-1} = \sum_{i=1}^m h^{2i} \left(\beta_{i0} y_{n+1}^{(2i)} + 2\beta_{i1} y_n^{(2i)} + \beta_{i0} y_{n-1}^{(2i)} \right)$$

applied to $y'' = -\lambda^2 y$ gives

$$y_{n+1} - 2R_{mm}(\theta, \nu^2) y_n + y_{n-1} = 0$$

with $\theta := \omega h$ and $\nu := \lambda h$

Padé-approximants \implies exponentially-fitted Padé approximants

Construction of Polynomially-fitted (m, m) Padé approximants :

$$\frac{P_m(x)}{P_m(-x)} = \exp(x) + \mathcal{O}(x^{2m+1})$$

$$\iff \exp(x) P_m(-x) - P_m(x) = \mathcal{O}(x^{2m+1})$$

$$\iff \frac{d^{2q}}{dx^{2q}} (\exp(x) P_m(-x) - P_m(x)) \Big|_{x=0} = 0 \quad q = 1, \dots, m$$

EF Padé approximants

$$\mathcal{F}(x, t) = \exp(tx) V_m(-tx) - V_m(tx) \qquad V_m(x) = 1 + \sum_{j=1}^m a_j x^j$$

$$\begin{cases} \frac{\partial^{2q}}{\partial x^{2q}} \mathcal{F}(x, t) \Big|_{(x,t)=(0,\theta)} = 0 & q = 1, \dots, K \\ \Re \left(\frac{\partial^q}{\partial t^q} \mathcal{F}(x, t) \Big|_{(x,t)=(i,\theta)} \right) = 0 & q = 0, \dots, P \end{cases}$$

where $0 \leq K \leq m$ and $P + K + 1 = m$.

This leads to a system of m linear equations in the unknowns a_i ,

$$i = 1, \dots, m.$$

The EF (K, P) Padé approximant to $\exp(\nu)$ is then given by

$${}^{(K,P)}\hat{P}_m^m(\nu) = V_m(\nu)/V_m(-\nu).$$

EF Padé approximants : $m = 1$

$$\mathcal{F}(x, t) = \exp(tx) V_1(-tx) - V_1(tx) \qquad V_m(x) = 1 + a_1 x$$

- $(K = 1, P = -1)$

$$\frac{\partial^2}{\partial x^2} \mathcal{F}(x, t) \Big|_{(x,t)=(0,\theta)} = 0 \iff \theta^2 (1 - 2a_1) = 0 \iff a_1 = \frac{1}{2}$$

- $(K = 0, P = 0)$ ${}^{(1,-1)}\hat{P}_1^1(\nu) = \frac{1 + \frac{1}{2}x}{1 - \frac{1}{2}x}$

$$\Re(\mathcal{F}(i, \theta)) = 0 \iff \Re\left(e^{i\theta} (1 - i a_1 \theta) - (1 + i a_1 \theta)\right) = 0$$

$$\iff a_1 = \frac{\sin \theta}{\theta (\cos \theta + 1)} = \frac{1}{2} \frac{\tan(\theta/2)}{\theta/2}$$

$${}^{(0,0)}\hat{P}_1^1(\nu) = \frac{1 + \frac{1}{2} \frac{\tan(\theta/2)}{\theta/2} x}{1 - \frac{1}{2} \frac{\tan(\theta/2)}{\theta/2} x}$$

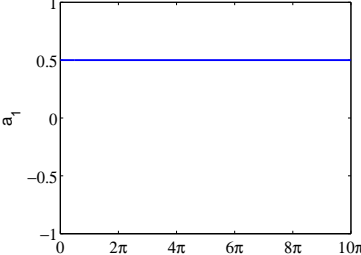
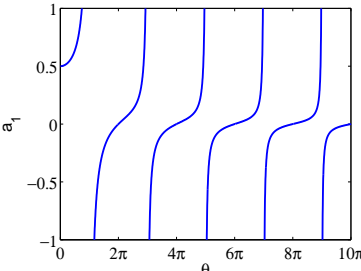
EF Padé approximants : $m = 1$

$m = 1$	
(K, P)	a_1
$(1, -1)$	$\frac{1}{2}$
$(0, 0)$	$\frac{\tan \frac{\theta}{2}}{\theta}$

EF Padé approximants : $m = 1$

$m = 1$	
(K, P)	a_1
$(1, -1)$	$\frac{1}{2}$
$(0, 0)$	$\frac{1}{2} + \frac{\theta^2}{24} + \mathcal{O}(\theta^4)$

EF Padé approximants : $m = 1$

$m = 1$	
(K, P)	a_1
$(1, -1)$	 <p>A plot showing the function a_1 versus θ for the Padé approximant $(1, -1)$. The x-axis (θ) ranges from 0 to 10π with major ticks at $0, 2\pi, 4\pi, 6\pi, 8\pi, 10\pi$. The y-axis ($a_1$) ranges from -1 to 1 with major ticks at -1, -0.5, 0, 0.5, 1. The plot shows a single horizontal blue line at $a_1 = 0.5$.</p>
$(0, 0)$	 <p>A plot showing the function a_1 versus θ for the Padé approximant $(0, 0)$. The x-axis (θ) ranges from 0 to 10π with major ticks at $0, 2\pi, 4\pi, 6\pi, 8\pi, 10\pi$. The y-axis ($a_1$) ranges from -1 to 1 with major ticks at -1, -0.5, 0, 0.5, 1. The plot shows a periodic function with vertical asymptotes at $\theta = 2\pi, 4\pi, 6\pi, 8\pi, 10\pi$. The function passes through $a_1 = 0$ at $\theta = 0, 2\pi, 4\pi, 6\pi, 8\pi, 10\pi$ and has a local maximum of $a_1 = 1$ at $\theta = \pi$ and a local minimum of $a_1 = -1$ at $\theta = 3\pi, 5\pi, 7\pi, 9\pi$.</p>

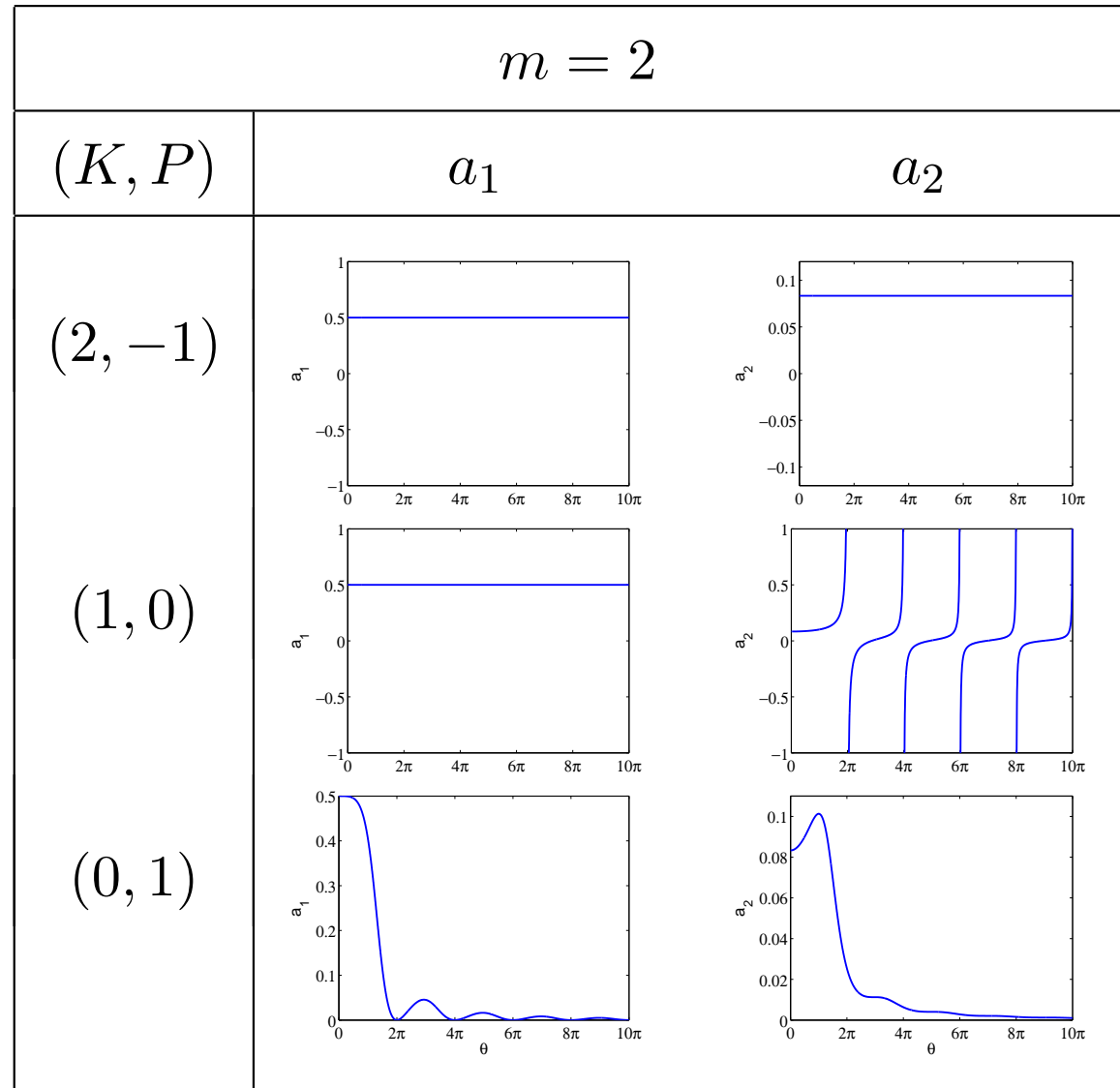
EF Padé approximants : $m = 2$

$m = 2$		
(K, P)	a_1	a_2
$(2, -1)$	$\frac{1}{2}$	$\frac{1}{12}$
$(1, 0)$	$\frac{1}{2}$	$\frac{2 \tan \frac{\theta}{2} - \theta}{2 \theta^2 \tan \frac{\theta}{2}}$
$(0, 1)$	$\frac{2 (1 - \cos \theta)}{(\theta + \sin \theta) \theta}$	$\frac{\theta - \sin \theta}{(\theta + \sin \theta) \theta^2}$

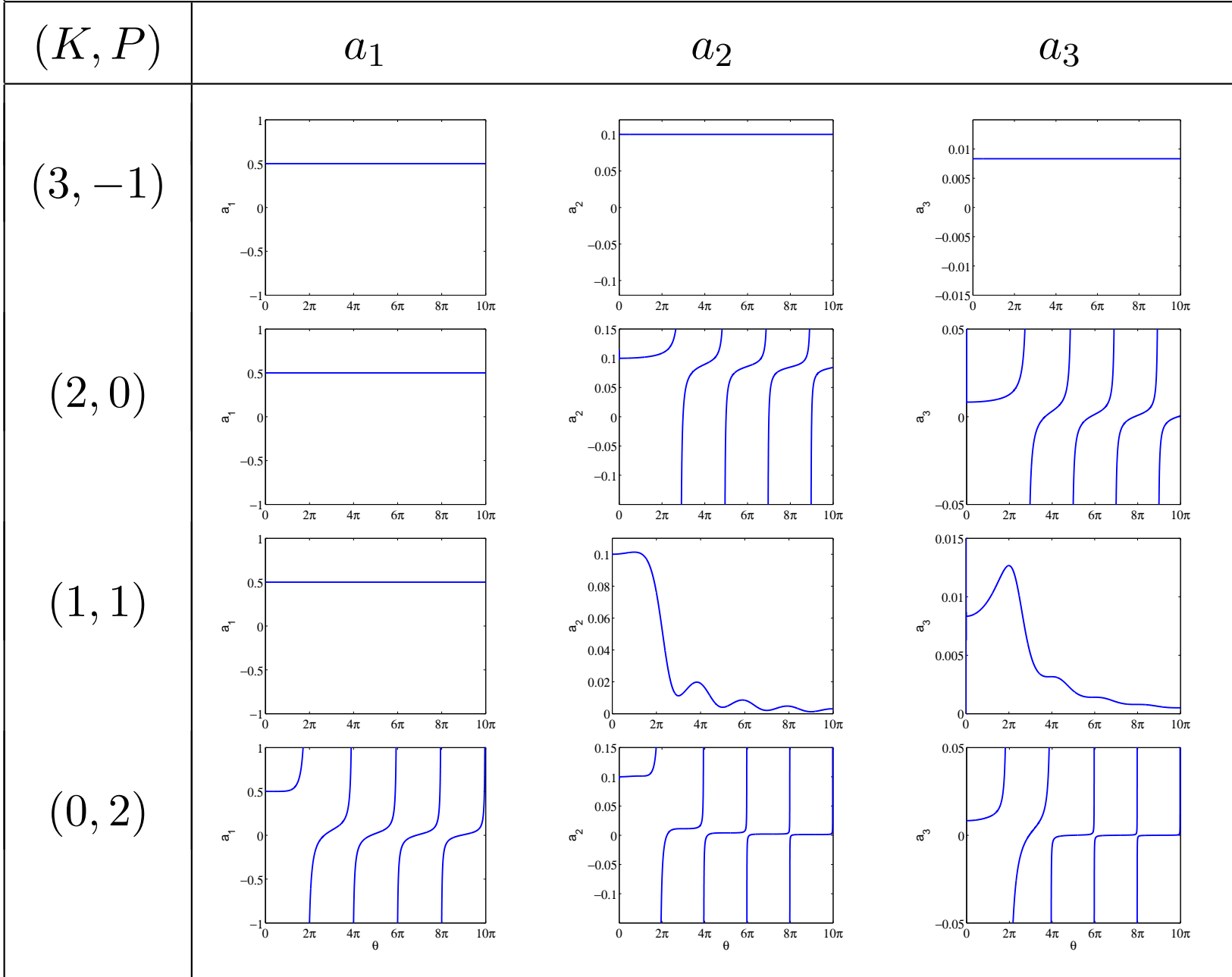
EF Padé approximants : $m = 2$

$m = 2$		
(K, P)	a_1	a_2
$(2, -1)$	$\frac{1}{2}$	$\frac{1}{12}$
$(1, 0)$	$\frac{1}{2}$	$\frac{1}{12} + \frac{\theta^2}{720} + \mathcal{O}(\theta^4)$
$(0, 1)$	$\frac{1}{2} + \mathcal{O}(\theta^4)$	$\frac{1}{12} + \frac{\theta^2}{360} + \mathcal{O}(\theta^4)$

EF Padé approximants : $m = 2$



$$m = 3$$



The Stiefel-Bettis problem

$$z'' + z = 0.001 \exp(ix) \quad z(0) = 1 \quad z'(0) = 0.995i \quad 0 \leq x \leq 40\pi$$

equivalent real form

$$\begin{cases} u'' + u = 0.001 \cos(x), & u(0) = 1, & u'(0) = 0, \\ v'' + v = 0.001 \sin(x), & v(0) = 0, & v'(0) = 0.9995. \end{cases}$$

$$z(x) = u(x) + i v(x)$$

$$u(x) = \cos(x) + 0.0005x \sin(x)$$

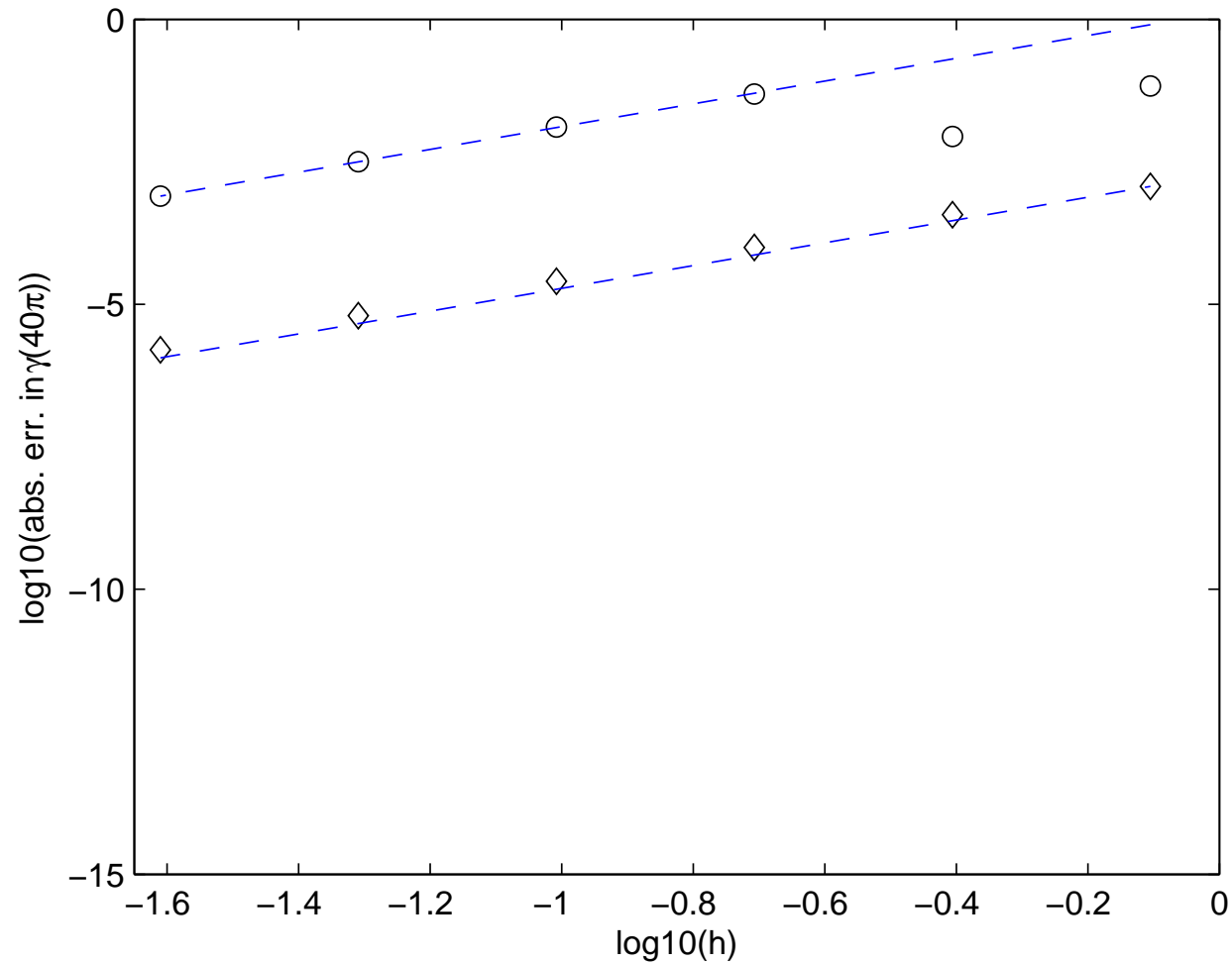
$$v(x) = \sin(x) - 0.0005x \cos(x)$$

$$\gamma(x) = \sqrt{u^2(x) + v^2(x)} = \sqrt{1 + (0.0005x)^2}$$

$$\gamma(40\pi) \quad h = 2^{-i} \pi \quad \omega = 1$$

The Stiefel-Bettis problem

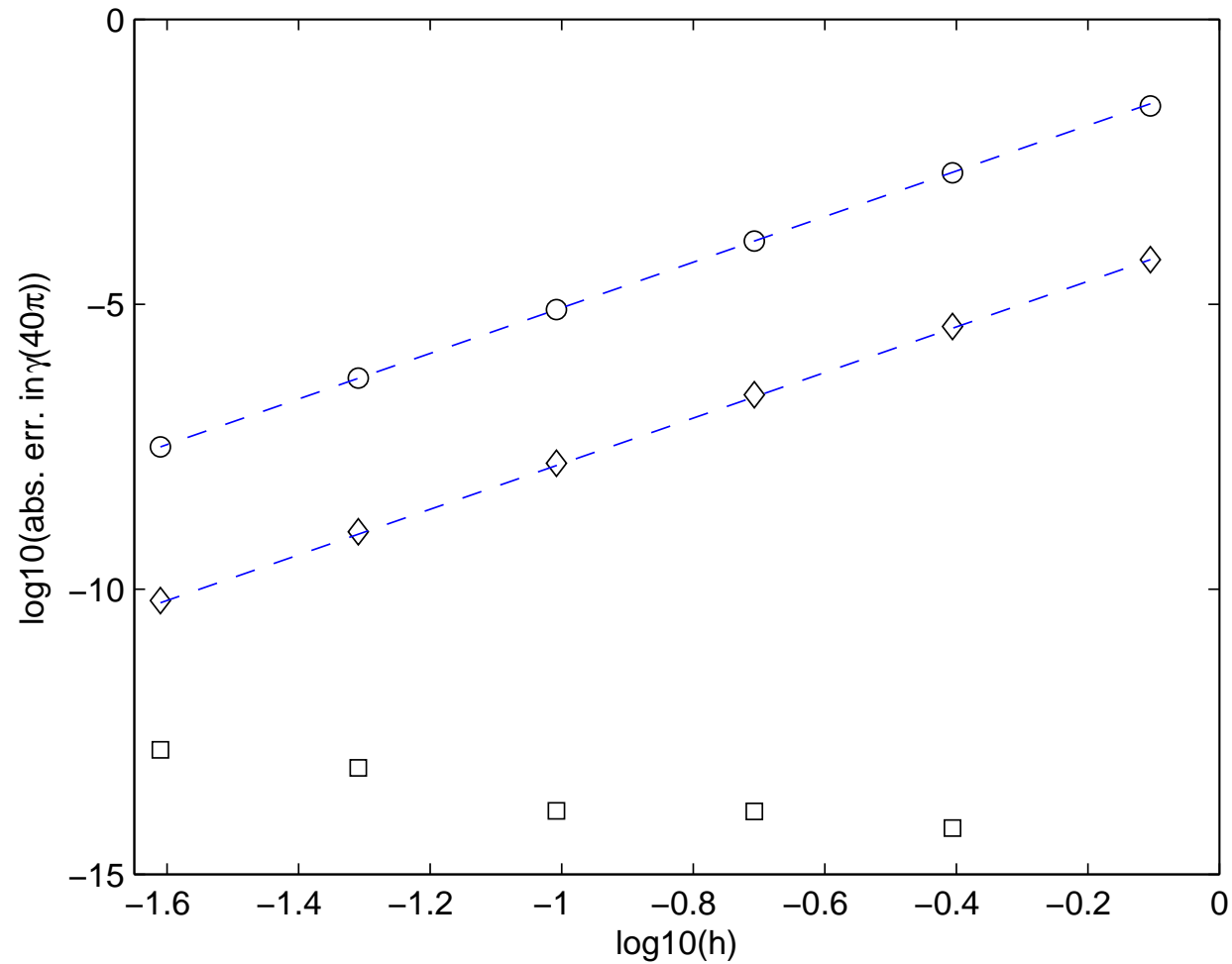
$$m = 1$$



$\circ : P = -1$ $\diamond : P = 0$

The Stiefel-Bettis problem

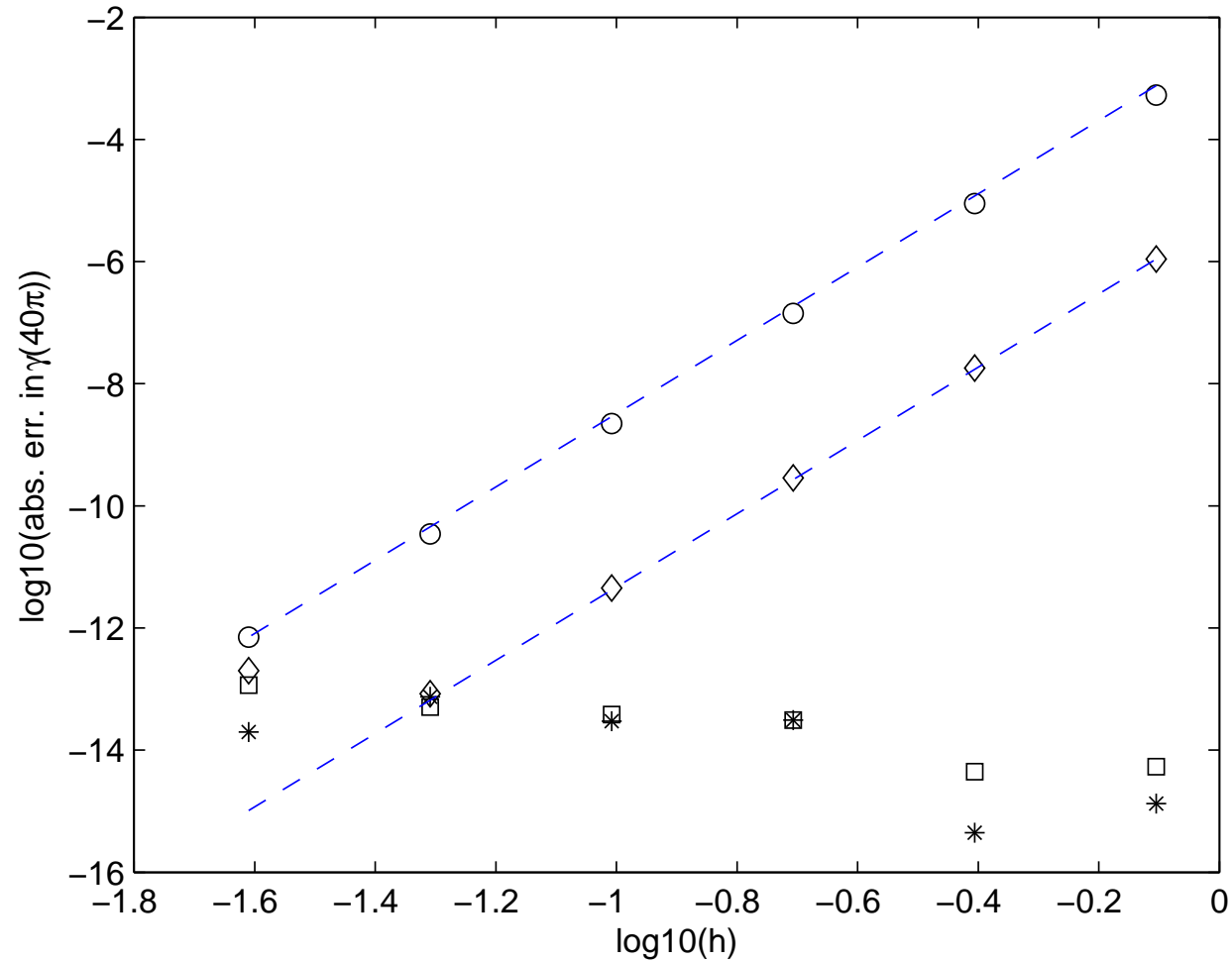
$$m = 2$$



$\circ : P = -1$ $\diamond : P = 0$ $\square : P = 1$

The Stiefel-Bettis problem

$$m = 3$$



$\circ : P = -1$ $\diamond : P = 0$ $\square : P = 1$ $\star : P = 2$

Conclusion

two-step P-stable exponentially fitted Obrechhoff methods :

- for any given m , P-stable EF (K, P) -methods of order $2m$ exist
- the construction is based on EF Padé approximants to the exponential function
- the coefficients depend on a parameter θ
- the coefficients are continuous functions of θ iff P is odd
- numerical example was given to illustrate the theory