Filtering Spectral Methods with Chebyshev-Padé Approximants

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Abstract: We use Chebyshev-Padé approximants to filtering and estimate singularities of spectral solutions of differential equations.

Key–Words: Spectral methods, Chebyshev-Padé approximants, Filtering spectral solutions.

1 Introduction

It is known that Spectral methods are very efficient to solve differential equations with smooth solutions, they usually exhibit exponential rate of convergence. However, since they usually loose the exponential rate of convergence when the differential equation has a nonsmooth solution, there are several methods to improve the approximation given by the spectral solution, see e.g. general extrapolation methods in [4, 12]. These postprocessings are known by *filtering of spectral solution*.

For certain classes of functions, Chebyshev-Padé approximants present some advantages: they enlarge the domain of convergence [13, 9], and it is possible to localize singularities of the solutions, with the information given by the poles of a sequence of Chebyshev-Padé approximants, [5, 6]. Note, that these "good" properties refer only to Chebyshev-Padé approximants calculated with the coefficients of the orthogonal expansion. In a spectral solution, we only have access to a finite number of coefficientes that do not coincide with the first coefficients of the orthogonal expansion. So, it is not guaranteed that sequences of Chebyshev-Padé approximants calculated with the coefficients obtained by spectral methods has the same properties than the sequences of Chebyshev-Padé approximants computed with the exact coefficients of the orthogonal expansions.

In this paper, we present two numerical examples to show, in a heuristic way, that filtering spectral methods with Chebyshev-Padé approximants allows: to improve the accuracy given by a spectral solution, expand the domain of validity of spectral approximations and localize singularities of solutions of differential equations. In section 2 and 3 we summarize some definitions and notations related with the spectral methods and with the Chebyshev-Padé approximation, respectively. In Section 4 we present the numerical examples and in section 5 we make some observations and conclusions.

2 Spectral Methods

We start with some definitions and notations related with general formulation of spectral methods. Let $L_w(a,b)$ denote the Hilbert space whose elements are mensurable real funtions, u, such that $\int_a^b u^2(x)w(x)dx < \infty$, where w is a given weight function. As usually, we define in $L_w(a,b)$: the inner product by, $(u,v)_w = \int_a^b u(x)v(x)(x)w(x)dx$, for all functions u and v in $L_w(a,b)$ and the associated w-norm

$$\|u\|_w = (u,u)_w^{1/2}. \tag{1}$$

Let $\{\phi_k\}_{k=0}^{\infty}$, be a system of orthogonal polynomials in $L_w(a,b)$. In spectral methods such orthogonal polynomials are called *trial* or *basis functions*. Consider the expansion of a given function u in $L_w(a,b)$ in truncated series

$$u_N(x) = \sum_{k=0}^{N} \hat{u}_k \phi_k(x), \quad x \in [a,b] \tag{2}$$

and the functional equation

$$\mathcal{L}u - f = 0, \tag{3}$$

where, $\mathcal{L}$ denote a functional operator (usually a differential, integral, or integral-differential operator). If u_N is a approximation solution of (3), then the residual R_N is defined by

$$R_N(x) = \mathcal{L}u_N - f.$$

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In spectral methods we determine u_N by setting

$$(R_N, \psi_k)_{\tilde{w}} = 0, \quad k \in I_N, \tag{4}$$

where, $\psi_k(x)$ are *test* functions, $\tilde{w}$ is a weight function related with test functions and I_N is a discrete set that depends on some aditional conditions imposed on the equation (3).

There are three most common spectral methods, namely, the collocation, Galerkin and tau methods. The choice of the test functions, ψ_k and of the weight, $\tilde{w}$ defines the method. In *Galerkin* method we have $\psi_k = \phi_k$, $\tilde{w} = w$ and the basis (and the test) functions satisfy the aditional conditions. In the *tau* method we also have $\psi_k = \phi_k$ and $\tilde{w} = w$ but, we allow that the basis (and the test) functions do not satisfies the aditional conditions. In *collocation* method we have $\psi_k(x) = \delta(x - x_k)$ and $\tilde{w}(x) = 1$. So, in collocation method, we can write equation (4) on the form

$$R_N(x_k) = 0, \quad k \in I_N. \tag{5}$$

In the examples presented in section 4, we will use the Chebyshev-collocation method, i.e., we choose the system of Chebyshev polynomials, $\{T_k\}_{k=0}^{\infty}$ (orthogonal on interval $[-1, 1]$, with weight function $w(x) = (1 - x^2)^{-1/2}$) as the basis functions, and, the collocation points are the Chebyshev-Gauss-Lobatto interior nodes, see e.g. [3].

3 Padé aproximation from orthogonal expansions

Consider a system of orthogonal polynomials $\{\phi_k\}_{k=0}^{\infty}$ under the same conditions of section 2 and let $S(x)$ a formal orthogonal series.

$$S(x) := \sum_{k=0}^{\infty} f_k \phi_k(x) \tag{6}$$

If the formal expansion S represents asimptotically (see e.g. [12]) a function f we have

$$f_k = \frac{1}{\|\phi_k\|_w^2} \int_a^b f(x)\phi_k(x)w(x)dx.$$

We will refer two aproaches to the Padé Aproximation: the linear and the nonlinear Padé Aproximants. Denoting the class of all polynomials of degree up to k, where k is a non negative integer, by $\mathcal{P}_k$ and the class of all rational functions $R = N/D$, where $N \in \mathcal{P}_k$, $D \in \mathcal{P}_\ell$ and $D \not\equiv 0$ by $\mathcal{R}(k, \ell)$.

Definition 1 (Linear Padé Approximant) *Let p and q be two nonnegative integers numbers. A function $\Phi_{p,q} = N_{p,q}/D_{p,q} \in \mathcal{R}(p, q)$ is a linear Padé aproximant of type (p, q) from orhogonal series (6) if it satisfies the condition*

$$\int_a^b \left(D_{p,q}(x)S(x) - N_{p,q}(x)\right) \phi_k(x)w(x)dx = 0, \tag{7}$$

for $k = 0, 1, \ldots, p + q$.

The conditions (7) form a homogeneous system with $p+q+1$ linear equations and $p+q+2$ unknows. Thus linear aproximants always exists. However, generally they are not unique, but if $D_{p,q}$ has degree q and do not vanish in $[a, b]$ the $\Phi_{p,q}$ is unique, [9]. For more details, about the construction of linear Padé aproximantes we refer [10, 11].

Definition 2 (Nonlinear Padé Approximant) *Let p and q be two nonnegative integers numbers. A function $R_{p,q} = N_{p,q}/D_{p,q} \in \mathcal{R}(p, q)$ is a linear Padé aproximant of type (p, q) from orthogonal series (6) if it satisfies the condition*

$$\int_a^b \left(S(x) - R_{p,q}(x)\right) \phi_k(x)w(x)dx = 0, \tag{8}$$

for $k = 0, 1, \ldots, p + q$.

The conditions (8) form a homogeneous system with $p + q + 1$ nonlinear equations and $p + q + 2$ unknows. The existence of the nonlinear Padé aproximants is not garantee, however, if a nonlinear Padé aproximant exist it will be unique, [9].

In next section we will use Chebyshev-Padé approximants (CPA), i.e., we will consider the family of Chebyshev polynomials (the same orthogonal system used as basis functions in the collocation method). To determine a nonlinear CPA, we do not need to solve a system of nonlinear equations. The Clenshaw-Lord alghorithm [7] allows to determine nonlinear CPA solving a linear system, thus avoiding the resolution of a nonlinear system. We remark the following, while to determinate linear CPA we must have the first $p+2q+1$ coefficients of expansion (6) to determinate the nonlinear we only need the first ones $p + q + 1$ coefficients.

4 Numerical examples

We begin with some remarks and notations. Given a differential problem we will represent his solution by $y(x)$, with Chebyshev expansion $S(x)$ =

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$\sum_{k=0}^{\infty} c_k T_k(x)$, where c_k are the Chebyshev coefficients and $S_N(x)$ represents the truncated Chebyshev expansion of $y(x)$, i.e., $S_N(x) = \sum_{k=0}^{N} c_k T_k(x)$. $y_N(x) = \sum_{k=0}^{N} \hat{c}_k T_k(x)$ denotes the spectral solution (or spectral approximation) and the coefficients $\hat{c}_k$ are the spectral coefficients. $\Phi_{p,q}$ ($R_{p,q}$) denotes the linear CPA (nonlinear CPA) of type (p,q) computed with the Chebyshev coefficients c_k and $\hat{\Phi}_{p,q}$ ($\hat{R}_{p,q}$) denotes the linear CPA (nonlinear CPA) of type (p,q) computed with the spectral coefficients $\hat{c}_k$. We will use e_N to denote the spectral error in w-norm (1) defined by

$$\|y - y_N\|_w ,$$

where w is the Chebyshev weight $w(x) = (1 - x^2)^{-1/2}$. To compute the w-norm we use the Chebyshev-Gauss quadrature formula.

Given a spectral solution y_N it is only possible to construct the functions $\hat{\Phi}_{p,q}$, $\hat{R}_{k,\ell}$ such that $p + 2q + 1 \leq N$ and $k + \ell + 1 \leq N$. If we want to compare $\hat{\Phi}_{p,q}$ and $\hat{R}_{k,\ell}$ contructed with the same coeficientes we need to choose (if possible) nonnegative numbers p, q, k and ℓ such that $p + 2q = k + \ell$.

The numerical examples were chosen so that the spectral methods have slow rate of convergence, i.e., the solutions of the differential equations have singularities: near of he orthogonality interval $[-1, 1]$. In the example A, we present a linear differential equation which solution has a brunch cut, and, in example B the solution, of a nonlinear differential equation, is meromorphic with a infinity number of poles..

4.1 Example A

We consider the linear differential equation

$$\left(x - \frac{\alpha^2+1}{2\alpha}\right)\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + \frac{\mathrm{d}y}{\mathrm{d}x} = 0, \quad \alpha \in \mathbb{R}\setminus\{0\}, \quad (9)$$

with Dirichlet boundary conditions

$$y(-1) = 1 - \frac{1}{2}\ln\left(1 + 2\alpha + \alpha^2\right)$$
$$y(1) = 1 - \frac{1}{2}\ln\left(1 - 2\alpha + \alpha^2\right).$$

The solution is

$$y(x) = 1 - \frac{1}{2}\ln\left(1 + \alpha^2 - 2\alpha x\right),$$

where $x_s = \frac{\alpha^2+1}{2\alpha}$ is the nearest branch point from the interval $[-1, 1]$. We know the Chebyshev expansion $y(x) = \sum_{k=0}^{\infty} c_k T_k(x)$, where $c_0 = 1$ and $c_k = \alpha^k/k$, $k \geq 1$ [1].

Setting $\alpha = 9/10$ we have the singularity $x_s = 181/180 \approx 1.00556$ (near from the interval $[-1, 1]$). Using collocation method, we obtained the collocation errors in the w-norm indicated in table (1). These results shows that collocation method exhibit slow rate of convergence.

N	10	20	30	40
e_N	$1.2e-1$	$3.2e-2$	$7.9e-3$	$2.9e-3$
N	50	60	...	100
e_N	$5.3e-4$	$1.5e-4$	...	$1.2e-6$

Table 1: Example A: Errors of the colocation method in w-norm.

Now, if we postprocess the spectral solution with diagonal CPA, i.e., if we compute CPA of type (p,p) we conclude that this process improved, but not significantly, the aproximation given by the collocation method. Settinq $N = 19$, and computing: S_{19}, $\Phi_{6,6}$, $R_{9,9}$, y_{19}, $\hat{\Phi}_{6,6}$ and $\hat{R}_{9,9}$ we obtain the errors indicated in table (2). In the results obtained with the exact coefficients, we can observe that the nonlinear and linear ACP improves significantly the approximation given the collocation solution. However, the non linear CPA has mores accuracy than the linear CPA. In the results obtained with the spectral coefficients both CPA have the same accuracy.

If we compute the coefficients relative errors

$$Er_k = \left|\frac{c_k - \hat{c}_k}{c_k}\right|, \quad k = 0, \ldots, 19$$

we can see that these errors are "almost" crescent, i.e. for small values of k we have $Er_k \approx 7e-3$ then they increase till reach the maximum at $Er_{18} \approx 7.5e-1$. So, in practice it is advisable not to use the last spectral coefficients in this filtering method. We will use this "practical" rule to compute $\hat{\Phi}_{p,q}$ and $\hat{R}_{p,q}$.

In order to estimate x_s, we begin with an observation about the solution of equation (9). All numeric results suggest that the function $y(x)$ has similar properties to the so called Markov type functions. Here, we only will refer two properties. The first propertie is that nonlinear or linear, Padé aproximantes of type $(p+\ell, p)$, $\ell \geq -1$, from Markov type functions always exist, are unique and have exactly p real (simple) poles and all poles lie on the branch cut of the Markov type function, the second one is that the Padé aproximantes from orthogonal series of type $(p+\ell, p)$, $\ell \geq -1$ of Markov type functions accelerate the rate of convergence of truncated orthogonal series on orthogonal

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interval and for fixed $\ell \geq -1$ any paradiagonal sequence of orthogonal Padé approximants, converges uniformly in any compact that does not contains the branch cut of the Markov type function. However we must consider the condition $\ell \geq 0$ for the function y. To more details related with the above results we refer to [9]. In fact, we observed the above properties in all numerical tests, (with $\ell \geq 0$) for the linear aproximations $\Phi_{p+\ell,p}$ and $\hat{\Phi}_{p+\ell,p}$ and for nonlinear approximants $R_{p+\ell,p}$. In Table (3) we present the smallest pole ζ_p, i.e., the nearest pole of the interval $[-1,1]$ (and from x_s) of some diagonal linar ACP $\hat{\Phi}_{p,p}$ computed from y_{31}. Note that, if we increase the value of p the pole ζ_p are close to x_s.

$\|\|y-S_{19}\|\|_w$	$\|\|y-\Phi_{6,6}\|\|_w$	$\|\|y-R_{9,9}\|\|_w$
$1.0e-2$	$8.1e-4$	$1.2e-6$
$\|\|y-y_{19}\|\|_w$	$\|\|y-\hat{\Phi}_{6,6}\|\|_w$	$\|\|y-\hat{R}_{9,9}\|\|_w$
$3.4e-2$	$2.0e-2$	$2.3e-2$

Table 2: Example A: Errors of computed approximations in w-norm.

p	2	3	4
ζ_p	1.0805	1.0347	1.0207
p	5	...	8
ζ_p	1.0147	...	1.0073

Table 3: Example A: Nearest pole of $\hat{\Phi}_{p,p}$ from singularity $x_s = 1.00556\ldots$.

On figure (1), we show the advantages to filter the collocation solution to extend the validity of the approximation interval. While spectral approximation does not make sense outside from orthogonality interval, the CPA is lower than 10^{-2} on interval $[-5,1]$.

4.2 Example B

We consider the Burguers equation

$$\epsilon \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - \frac{\mathrm{d}y}{\mathrm{d}x} y = 0, \quad \epsilon > 0, \tag{10}$$

with Dirichlet boundary conditions

$$y(-1) = -\sqrt{2\epsilon}\tan(\alpha)$$
$$y(1) = \sqrt{2\epsilon}\tan(\alpha),$$

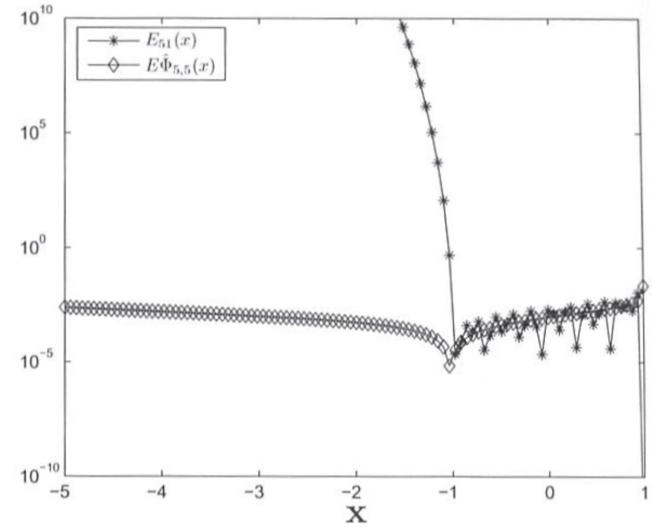

Figure 1: Example A; Error $E_{51}(x) = |y(x) - y_{51}(x)|$ *versus* Error $E\Phi\hat{R}_{5,5}(x) = |y(x) - \hat{\Phi}_{7,6}(x)|$ on expanded interval $[-5,1]$.

with $\alpha = (2\epsilon)^{-1/2}$. The solution is the meromorphic (odd) function $y(x) = \sqrt{2\epsilon}\tan(\alpha x)$,
with an infinite number of (single) poles at points

$$x_k = \sqrt{2\epsilon}\left(k + \frac{1}{2}\pi\right), \tag{11}$$

for all integer k. Thus we have two symetric syngularities, $x_s^+ = \alpha$ and $x_s^- = -\alpha$, nearest from interval $[-1,1]$. For values of $\epsilon > \frac{2}{\pi^2}$, we have $x_s^+ > 1$ (and $x_s^- = -x_s^- < -1$). Considering, in (11), $k=-2$ and $k=1$ we get the singularities represented by y_s^- and y_s^+. Setting, $\epsilon = \frac{2}{\pi^2} + t$ we have that $x_s^+ \to 1$ (and $x_s^- \to -1$) as $t \to 0^+$.

Fixing $t = 1/200$, we computed the collocation approximations y_N, for some values of N, and for each value of N, we computed $\hat{\Phi}_{5,4}$ and $\hat{R}_{7,6}$. Note that we only use the first 14 spectral coefficients from each CPA. We will denote the w-norms of: spectral approximation error, linear CPA error and nonlinear CPA error by e_N, $e\hat{\Phi}_{5,4}$ and $e\hat{R}_{7,6}$, respectively. Observing the data presented in table (4), we can conclude that this filtering technique accelerated the covergence given by collocation method. The CPA errors are similars, thus it is better using the linear approximation to avoid to solve a nonlinear system. In figure (2), we compare the absolute error functions $E_{71}(x) = |y(x) - y_{71}(x)|$ and $E\hat{R}_{7,6} = \left|y(x) - \hat{R}_{7,6}(x)\right|$ on $[-1,1]$. In figure (2) we just extend to the range $[-2,2]$ and we see that outside the orthogonality interval the error of the nonlinear CPA, although worse, remains below 10^{-2}.

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N	31	41	51	61
e_N	$9.6e-1$	$1.6e-1$	$3.0e-2$	$5.9e-3$
$e\hat{\Phi}_{5,4}$	$2.9e-1$	$1.0e-2$	$8.4e-4$	$1.1e-4$
$e\hat{R}_{7,6}$	$3.0e-1$	$1.0e-2$	$8.0e-4$	$1.1e-4$

Table 4: Example B: Errors of computed approximations in w-norm.

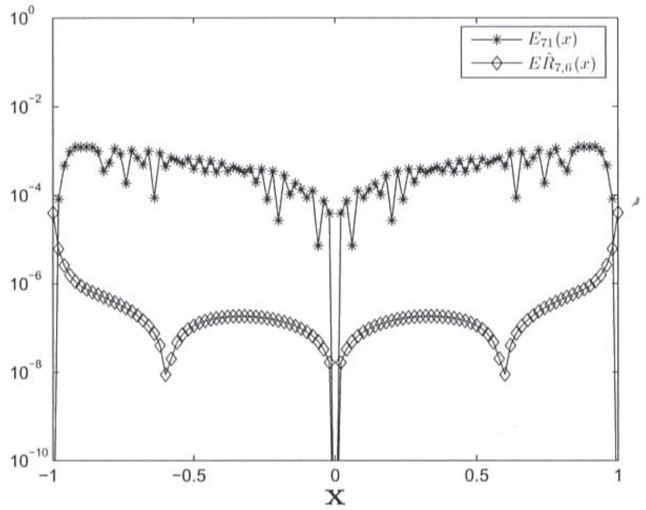

Figure 2: Example B; Error $E_{71}(x) = |y(x) - y_{71}(x)|$ *versus* Error $E\hat{R}_{7,6}(x) = |y(x) - \hat{R}_{7,6}(x)|$. The filtering method improves the spectral solution on interval of orthogonality.

For the estimation of the singularities, we begin to note that usually the matrices, that represents the linear systems that compute the linear and nonlinear CPA, have a bad condition number. Thus we are limited to compute CPA of type (p,q) when the value of $p+q$ is "small" (in ours examples when $p+q<20$). One way to overcome this limitation is to compute the poles of line sequences of CPA $\{\Phi_{p,1}\}_{p\geq 0}$, $\{\Phi_{p,2}\}_{p\geq 0}$. It is easy to see that

$$r_{p,1} = \frac{c_p + c_{p+2}}{2c_{p+1}}, \quad c_{p+1} \neq 0, \tag{12}$$

are the poles of $\Phi_{p,1}$, $p = 0, 1, \ldots$. And if the matrix

$$\begin{bmatrix} c_{p+1} & c_p + c_{p+2} \\ c_p & c_{p+1} + c_{p+3} \end{bmatrix}$$

is regular, then we have

$$r_{p,2}^{(i)} = \frac{-b_1 \pm \sqrt{b_1^2 - 8(b_0 - 1)}}{4}, \quad i \in \{-1, 1\}, \quad p \geq 1, \tag{13}$$

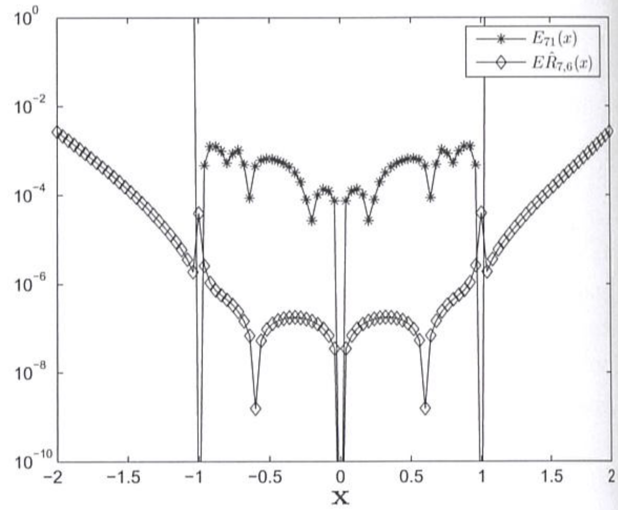

Figure 3: Example BError $E_{71}(x) = |y(x) - y_{71}(x)|$ *versus* Error $E\hat{R}_{7,6}(x) = |y(x) - \hat{R}_{7,6}(x)|$. The filtering method improves the spectral solution on interval of orthogonality. Same plot as figure (2) on the extended range, $[-2, 2]$, that contains the singularities x_s^- and x_s^+. While the error of spectral approximation $E_{71}(x)$ tends rapidly to infinity, the error of nonlinear CPA $E\hat{R}_{7,6}(x)$ (computed only with the first fourteen coefficients of $y_{71}(x)$) remains below 10^{-2}, except in a neighborhood of the singularities.

where: setting $i = -1$ means that we choose the signal minus, setting $i = 1$ means that we choose the signal plus, $b_0 = N_0/D_0$ with,

$$\begin{aligned} N_0 =& (c_{p+1} + c_p)c_{p+4} - c_{p+3}^2 - (c_{p+1} + c_{p-1})c_{p+3} + \\ & + (c_p - c_{p-1})c_{p+1} + c_p^2, \\ D_0 =& 2\left[c_{p+1}c_{p+3} - (c_{p+1} + c_p)c_{p+2} + c_{p+1}^2\right], \end{aligned}$$

and $b_1 = N_1/D_1$ with,

$$\begin{aligned} N_1 =& c_{p+2}c_{p+3} + c_{p-1}c_{p+2} - c_p c_{p+1} - c_{p+1}c_{p+4} \\ D_1 =& c_{p+1}c_{p+3} - (c_{p+1} + c_p)c_{p+2} + c_{p+1}^2. \end{aligned}$$

Observing that the even spectral coefficients $\hat{c}_{2k}$, are, numerically, zero (remember that $y(x)$ is an odd function) it is advisible use the relation (13) instead the relation (12). We remark that for odd and even functions (series) the relation (13) could be simplified. Thus using the spectral coefficients in relation (13), and taking into account the "practical rule" (see example A) we present the results, only the poles $\hat{r}_{p,2}^{(1)}$ for p odd (the poles $\hat{r}_{p,2}^{(-1)}$ are symmetric) on table (5), where we only show the correct digits, note that we have $x_s^+ = 1.0122618$. More, computing $\hat{\Phi}_{p,q}$, with

$q \geq 4$, it is possible to estimate the sigularities: $y_s^+ = 3.0367854$ and $y_s^- = -y_s^+$, although, we lose accuracy. For example, Computing $\hat{\Phi}_{7,4}$ we get the poles: -3.0940919, -1.0122618, 1.0122618 and 3.0940919.

p	5	15	25
$\hat{r}^{(1)}_{p,2}$	1.01226	1.012261	1.0122618

Table 5: Example B: Positive pole of $\hat{\Phi}_{p,2}$ (only exact digits).

5 Conclusions

In both examples, this filtering method improves the accuracy of the collocation aproximation. We note, as was said before, that we did not use all available data to determinate CPA coefficients. This filtering method allows to estimate singularities, being more efficient to meromorphic functions (example B) than to functions with branch cuts (example A). Finally, in both examples the filtering methods expand the range of validity of the collocation solution.

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