

Singularity-based Approach in a Padé-Chebyshev Resolution of the Gibbs Phenomenon

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Abstract— We present a singularity-based approach to resolve the Gibbs phenomenon that appears in Padé-Chebyshev approximation of functions with jump discontinuities. In this paper, we consider the more difficult case where the locations of the jump discontinuities are not known. The identification of unknown singularities is carried out using a Padé-Chebyshev approximation. We provide numerical examples to illustrate the method, including an application on postprocessing computational data corrupted by the Gibbs phenomenon.

Keywords: Gibbs phenomenon, function reconstruction, Padé-Chebyshev approximation

1 Introduction

Approximation of smooth functions by Fourier series or by truncated orthogonal polynomial expansions in general is known to be exponentially convergent and highly accurate [2,4]. For functions with singularities, however, convergence of a partial sum of orthogonal series is adversely affected in the area over which the singularities occur, a problem which has come to be known as the Gibbs phenomenon. This phenomenon manifests in an oscillatory behavior at the vicinity of the jumps.

A class of techniques aimed at resolving Gibbs phenomenon comprises Padé-type approximations. An approximant of this type enjoys the advantage of utilizing a rational function as this kind of function is broader and richer in form than a polynomial and is considered the simplest function that can have singularities, and hence the likelihood of the poles of a rational approximant being close enough to the singularities of the function being approximated [2,5].

Some Padé-based methods work without requiring information about the jump locations. However, locating jump discontinuities can become a relevant issue when the actual function is not explicitly known. In many

cases, for instance, involving spectral approximations of nonsmooth solutions to some partial differential equations, the solution comes in the form of computational data that are contaminated by Gibbs phenomenon. As these data are noisy, the standard procedure is to post-process them to correct the phenomenon. One way this can be done, as demonstrated in [1,5], is to use Padé-type approximation. This Padé postprocessing approach, however, may turn out to be less successful unless fed with some information about the possible jump positions which, as noted in [5], can be advantageous for its effective implementation. As computational data may not show explicitly the existence and whereabouts of possible jumps, to somehow locate them can become imperative.

A study by Driscoll and Fornberg [2] reveals just how significant the knowledge of the jump locations can be in correcting the Gibbs phenomenon. Realizing that the poles available in a rational approximant do not intrinsically and adequately reproduce the jump behaviors of a discontinuous function f , they devised an approach that incorporates the jump locations into the approximation process. A similar approach that imbibes this concept in the context of Padé-Chebyshev approximation is discussed in [9].

This paper is anchored on the Singular Padé - Chebyshev approximation discussed in [9], a brief review of which is presented in the next section. Section 3 discusses a Padé-based approach in identifying singularities of the function. Section 4 focuses on the numerical results of the SPC implementation in reconstructing a test function and postprocessing computational data.

2 A Singularity-based Padé-Chebyshev Resolution

The Chebyshev expansion of a function f can be written as

$$f(x) = \frac{c_0}{2} + \sum_{n=1}^{\infty} c_n T_n(x), \quad (1)$$

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where $T_n(x)$ are the Chebyshev polynomials defined as $T_n(x) = \cos(n\theta)$, $\theta = \cos^{-1}(x)$, and $x \in [-1, 1]$. The coefficients c_n are given by

$$c_n = \frac{2}{\pi} \int_{-1}^1 \frac{f(x)T_n(x)}{\sqrt{1-x^2}} dx$$

and may be approximated using the following Gauss-Chebyshev quadrature rule

$$\int_{-1}^1 h(x)\omega(x)dx \cong \sum_{k=1}^m A_k h(x_k), \quad (2)$$

where $\{x_k\}$ are the zeros of the Chebyshev polynomials $T_m(x) = \cos(m\theta)$, $h(x) = f(x)T_n(x)$, $\omega(x) = \frac{1}{\sqrt{1-x^2}}$, and $A_k = \frac{\pi}{m}$ for all k .

By the substitution $z = e^{i\theta}$, expansion (1) is transformed into

$$f(z) = \frac{1}{2} \left(\sum'_{n=0}^{\infty} c_n z^n + \sum'_{n=0}^{\infty} c_n z^{-n} \right),$$

where the primed sum indicates that the first term is halved. Let

$$g(z) = \sum'_{k=0}^{\infty} c_n z^n. \quad (3)$$

We refer to $g(z)$ as the *transformed Chebyshev series associated with $f(z)$* , and consequently with $f(x)$.

Let $f(x)$ be a piecewise analytic function defined on $[-1, 1]$ with s jump locations at $x = \xi_k \in [-1, 1]$, $k = 1, \dots, s$, and consider its associated transformed Chebyshev series (3). The *Singular Padé-Chebyshev (SPC) approximant* to $f(x)$ of order (N, M, V_1, \dots, V_s) is defined by the rational function

$$\mathcal{R}(z) = \frac{P_N(z) + \sum_{k=1}^s R_{V_k}(z) \log \left(1 - \frac{z}{e^{i\theta_k}} \right)}{Q_M(z)}, \quad (4)$$

where $z = e^{i \cos^{-1}(x)}$ and

$$P_N(z) = \sum_{j=0}^N p_j z^j, \quad Q_M(z) = \sum_{j=0}^M q_j z^j \neq 0,$$

$$R_{V_k}(z) = \sum_{j=0}^{V_k} r_j^{(k)} z^j, \quad k = 1, \dots, s,$$

such that

$$Q_M(z)g(z) - [P_N(z) + U(z)] = \mathcal{O}(z^{\eta+1}),$$

with

$$U(z) = \sum_{k=1}^s R_{V_k}(z) \log \left(1 - \frac{z}{e^{i\theta_k}} \right)$$

and

$$\eta = N + M + s + \sum_{k=1}^s V_k.$$

The unknown coefficients of polynomials P_N , Q_M , and R_{V_k} are then computed through the following linear system of $\eta + 1$ equations in $\eta + 2$ variables:

$$\sum_{j=0}^M c_{N-j+t} q_j - \sum_{j=0}^{V_1} a_{N-j+t}^{(1)} r_j^{(1)} - \dots - \sum_{j=0}^{V_s} a_{N-j+t}^{(s)} r_j^{(s)} = 0,$$

$$\sum_{j=0}^M c_{l-j} q_j - \sum_{j=0}^{V_1} a_{l-j}^{(1)} r_j^{(1)} - \dots - \sum_{j=0}^{V_s} a_{l-j}^{(s)} r_j^{(s)} = p_l,$$

where $t = 1, \dots, \eta - N$, $l = 0, \dots, N$, and the asterisk-marked summation indicates that the term with c_0 is halved. We note that in this system, $c_n = 0$, for $n < 0$. It should be noted too that the $a_n^{(k)}$ are the coefficients in the Taylor expansion of $\log \left(1 - \frac{z}{e^{i\theta_k}} \right)$ and $a_n^{(k)} = 0$, for $n \leq 0$. Accordingly, $\mathcal{R}_{(N,M)}(z)$ approximates $g(z)$ which implies that the real part of \mathcal{R} approximates $f(x)$.

3 Approximate Jump Locations of a Discontinuous Function

There have been studies on locating jump discontinuities of a function [3,7] and some of these explore the connection between jump locations and the differentiated series expansion of the function. Estimating jump locations using Padé approximation is introduced in [2] and its applicability is based on the idea that a Padé approximation of the differentiated series expansion of a discontinuous function f likely leads to an ordinary pole at a jump location. As our approach is founded on Padé-Chebyshev approximation, we further pursue this idea to generate information about the jump locations of discontinuous functions.

For the derivative of f , a Padé-Chebyshev approximant of order (N, M) may be defined as

$$\mathcal{R}_{f'}(z) = \frac{(P_{f'})_N(z)}{(Q_{f'})_M(z)}, \quad (5)$$

where $z = e^{i \cos^{-1}(x)}$ and

$$(P_{f'})_N(z) = \sum_{j=0}^N (p_{f'})_j z^j,$$

$$(Q_{f'})_M(z) = \sum_{j=0}^M (q_{f'})_j z^j \neq 0,$$

such that

$$(Q_{f'})_M(z)g'(z) - (P_{f'})_N(z) = \mathcal{O}(z^{N+M+1}).$$

Finding the unknown coefficients of polynomials $(P_{f'})_N$ and $(Q_{f'})_M$ is tantamount to solving the following linear

system:

$$\begin{cases} \sum_{j=0}^M i(N + \lambda - j + 1)c_{N+\lambda-j+1} (q_{f'})_j = 0, \\ \lambda = 0, 1, 2, \dots, M - 1, \\ \sum_{j=0}^M i(\lambda - j)c_{\lambda-j} (q_{f'})_j = (p_{f'})_\lambda, \\ \lambda = 1, 2 \dots, N, \end{cases}$$

where $i = \sqrt{-1}$ and the expansion coefficients $c_t = 0$ for each $t < 0$. We remark that $\mathcal{R}_{f'}$ approximates $g'(z)$ which is the derivative of the transformed Chebyshev series associated with $f(x)$ which implies the real part of $\mathcal{R}_{f'}$ approximates $f'(x)$.

Recalling the definition of the Chebyshev polynomial, we know that $\theta = \cos^{-1}(x)$ with $x \in [-1, 1]$ and $\theta \in [0, \pi]$. This defines a mapping from $[-1, 1]$ onto $[0, \pi]$. The transformation $z = e^{i\theta}$ consequently maps $[-1, 1]$ to the upper half of the unit circle in the complex plane at which $|e^{i\theta}| = 1$. Now consider the Padé-Chebyshev approximant $R_{f'}$ to g' . Let z_0 be a zero of $(Q_{f'})_M$ or a pole of $R_{f'}$. We have $z_0 = e^{i\theta_0}$ for some $\theta_0 \in [0, \pi]$. By the inverse mapping, $|z_0| = 1$ implies that z_0 corresponds to a point x_0 in $[-1, 1]$. As z_0 is a singularity, x_0 must be a jump of $f(x)$ in $[-1, 1]$. Furthermore, since $z_0 = \cos \theta_0 + i \sin \theta_0$, the jump is located at $x_0 = \cos \theta_0 = \Re(z_0)$.

The immediately preceding discussion may be summarized by stating that a pole z_0 of $R_{f'}$ for which $|z_0| = 1$ corresponds to a jump discontinuity of $f(x)$ in $[-1, 1]$ which occurs at $x = \Re(z_0)$. This provides a simple criterion by which we may be able to locate a jump discontinuity of a piecewise continuous function using the Padé-Chebyshev approximant of its differentiated series expansion. As stated, we only need to consider those zeros of $(Q_{f'})_M$ for which the modulus is equal to (or approximately) 1 in order to identify the zeroth-order jumps of the function.

4 Numerical Results

We first implement the SPC method to reconstruct the following test function

$$f(x) = \begin{cases} \sqrt{1-x^2}, & 0 \leq x \leq 1 \\ 0, & -1/2 \leq x < 0 \\ -x-1, & -1 \leq x < -1/2. \end{cases} \quad (6)$$

As a second example, we show how the method recovers a function from a computational data set that is contaminated by the Gibbs phenomenon. For this case, we consider a function given in terms of computational data from the numerical solution to the following viscous Burgers' equation:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \epsilon \frac{\partial^2 u}{\partial x^2}, \quad x \in [-1, 1], \quad \epsilon = 0.001 \quad (7)$$

with boundary conditions

$$u(-1, t) = u(1, t) = 0 \quad (8)$$

and initial condition

$$u(x, 0) = -\tanh\left(\frac{x+0.5}{2\epsilon}\right) + 1. \quad (9)$$

4.1 Reconstructing f

The exact Chebyshev coefficients of the function f defined by (6) are given by

$$c_n = \begin{cases} -\frac{2}{3} + \frac{2+\sqrt{3}}{\pi}, & n = 0 \\ \frac{1+\sqrt{3}}{\pi} - \frac{\sqrt{3}}{4\pi} - \frac{1}{3}, & n = 1 \\ k, & n \geq 2, \end{cases}$$

where

$$k = \frac{2n \sin \frac{n\pi}{2} - n \sin \frac{2n\pi}{3} - \sqrt{3} \cos \frac{2n\pi}{3} - 2}{(n^2 - 1)\pi} + \frac{2}{n\pi} \sin \frac{2n\pi}{3}.$$

Since f has known discontinuity at $x = 0$ and $x = -\frac{1}{2}$, its SPC approximant is determined by

$$\frac{P(z) + R_1(z)L_1(z) + R_2(z)L_2(z)}{Q(z)},$$

where

$$L_1(z) = \log\left(1 - \frac{z}{i}\right)$$

and

$$L_2(z) = \log\left[1 - \frac{z}{\exp\left(\frac{2\pi i}{3}\right)}\right].$$

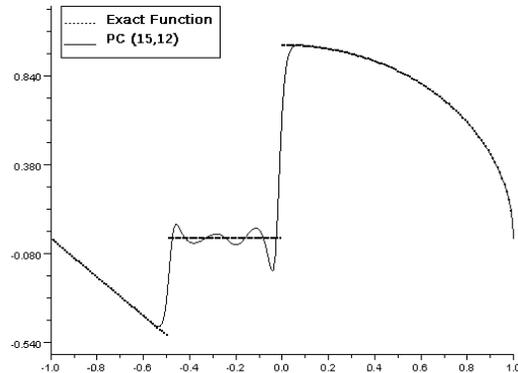


Figure 1: Contrast between the exact f and its PC(15, 12) approximant

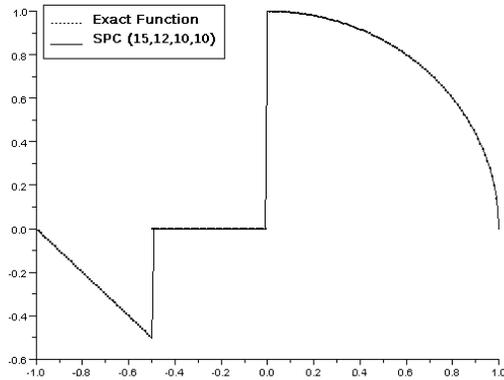


Figure 2: Contrast between the exact f and its SPC (15,12,10,10) approximant

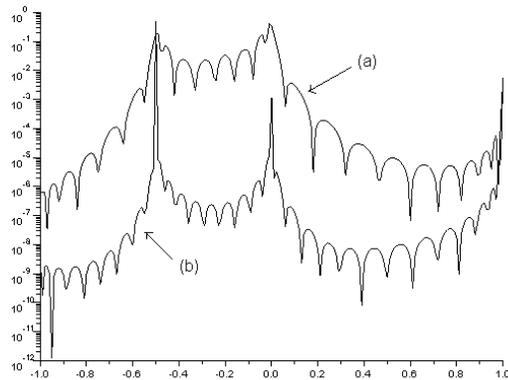


Figure 3: Comparison of the pointwise error convergence of the (a) PC(15,12) and (b) SPC (15,12,10,10) approximants to f

In the following discussion, we denote by SPC (N, M, V_1, \dots, V_s) an SPC approximant of order (N, M, V_1, \dots, V_s) while its corresponding Padé-Chebyshev (PC) approximant of order (N, M) is denoted by PC (N, M) .

Figure 1 shows the Gibbs phenomenon in a PC approximation of f . The oscillation caused by the phenomenon is practically eliminated upon the inclusion of the function's singularities into the approximation process as shown in Figure 2. An SPC approximant of f is shown in Figure 2 against the graph of the exact function. The reconstruction is remarkably good that the graph of the exact function is hardly noticeable. As shown in Figure 3, this impressive result by the SPC approximation is clearly marked by an improved convergence of the pointwise error drawn in logarithmic scale.

4.2 Recovering Solution to Burger's Equation

Numerical solution to the Burgers' equation by spectral method generates a set of computational data that is corrupted by the Gibbs phenomenon in the sense that solutions to such equation are known to develop sharp gradient in time [1]. Here we present some results on the use of the SPC approximation to postprocess or "clean up" the data in order to recover the solution to the viscous Burger's equation defined in (7)-(9). This equation is a suitable model for testing computational algorithms for flows where steep gradients or shocks are anticipated because it allows exact solutions for many combinations of initial and boundary conditions [1]. It should be noted that the postprocessing needs only to be applied at time levels at which a "clean" solution is desired, and not at every time step [8].

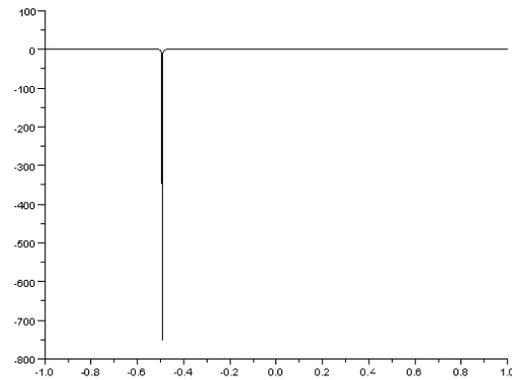


Figure 4: Approximate shock location of u at $x = -0.4932143$ when $t = 0$, using PC-IC (3,3) with $m = 100$

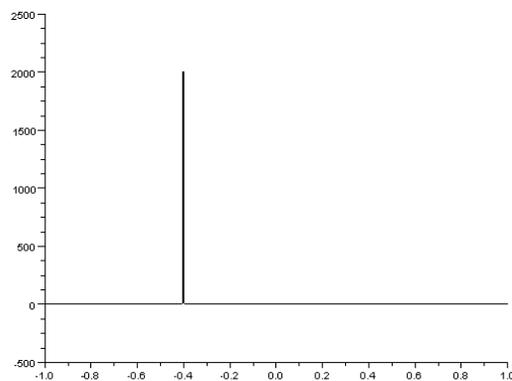


Figure 5: Approximate shock location of u at $x = -0.4066582$ when $t = 0.1$, using PC (3,3) with $m = 100$

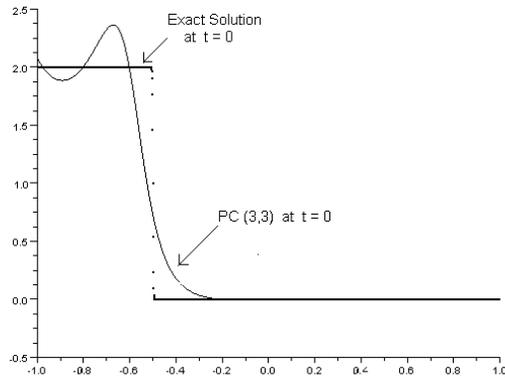


Figure 6: Contrast between the exact solution and its PC(3,3) approximant at $t = 0$

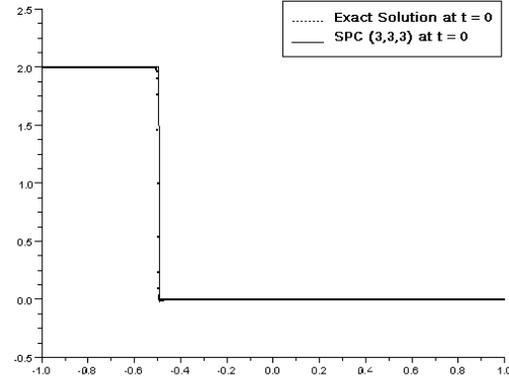


Figure 8: Contrast between exact solution and its SPC(3,3,3) approximant at $t = 0$

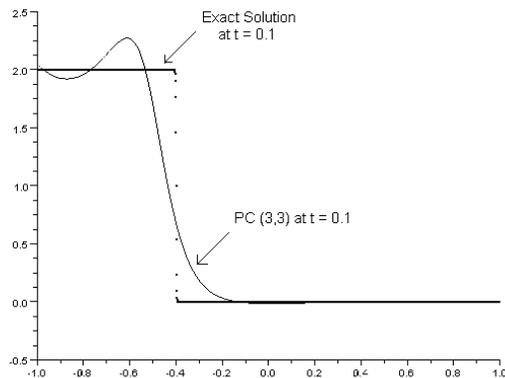


Figure 7: Contrast between the exact solution and its PC(3,3) approximant at $t = 0.1$

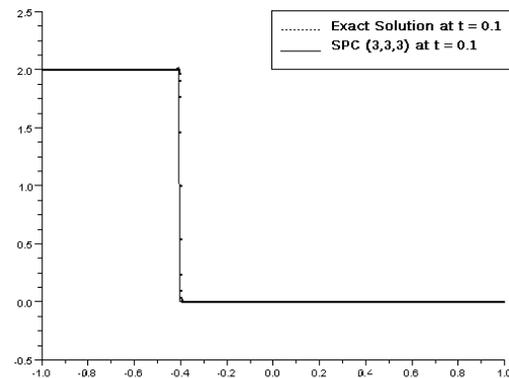


Figure 9: Contrast between exact solution and its SPC(3,3,3) approximant at $t = 0.1$

In this case, the transformed Chebyshev series for the solution assumes expansion coefficients that are approximated using (2). The input data are given at the m Gauss-Chebyshev quadrature points. Working on the assumption that there may be some inherent jump discontinuities or sharp gradient not known or readily observable from the data, we first seek the locations of these possible jumps or shocks in the data by way of the Padé approximation applied to the differentiated expansion that represents the solution u . Incorporating the resulting shock information into the SPC approximation generates a reconstructed u . For illustration, let us consider the case when time $t = 0$ and $t = 0.1$. Under each case, we take as inputs some computed data that serve as values of u at the given m Gauss-Chebyshev points.

Figure 4 produced by the PC(3,3) approximant to the differentiated transformed Chebyshev expansion associated with u shows that at $t = 0$ a possible jump or

shock occurs somewhere very close to $x = -0.5$. The zeros of the denominator of the PC(3,3) approximant are -0.0076362 and $-0.4932143 \pm 0.8696562i$. The complex zero gives a modulus of 0.9997811 which strongly indicates that a shock occurs at $x = -0.4932143$. This confirms what the plot shows. For the case when $t = 0.1$, the PC(3,3) approximation shown in Figure 5 indicates that there is a shock very near $x = -0.4$. The zeros of the denominator of the PC(3,3) approximant in this case are $-0.4066582 \pm 0.9140550i$ and -1.6168483 . The complex zero gives a modulus of 1.0004337 implying that a shock location is at $x = -0.4066582$, which is what the plot seems to suggest. In consideration of the two different shock positions at two different points in time, we note that the Burgers' solution involves time evolution of a shock or a sharp gradient.

We present the PC(3,3) and SPC(3,3,3) reconstructions of u in Figures 6 and 8 for the case $t = 0$ and in

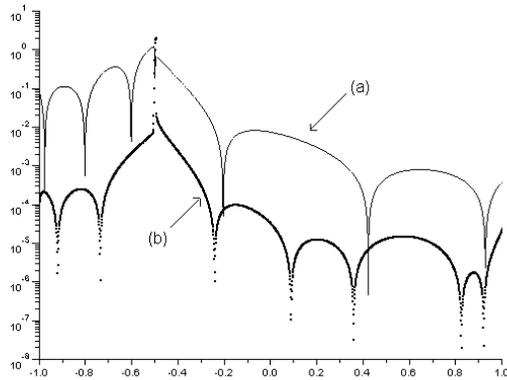


Figure 10: Comparison of pointwise error convergence of the (a) PC(3,3) and (b) SPC (3,3,3) approximants at $t = 0$

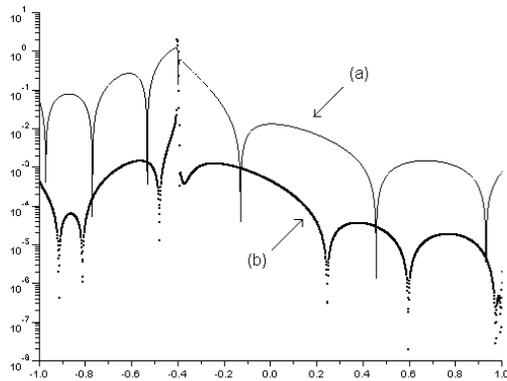


Figure 11: Comparison of pointwise error convergence of the (a) PC(3,3) and (b) SPC (3,3,3) approximants at $t = 0.1$

Figures 7 and 9 for $t = 0.1$. They are plotted against the exact solution. Both approximants in the two cases take the PC approximated jump locations, that is, the jump at $x = -0.4932143$ for $t = 0$ and the jump at $x = -0.4066582$ for $t = 0.1$. The SPC results are quite impressive notwithstanding the fact the we only use low order approximants to generate them. Comparisons of their respective pointwise error convergence are shown in Figures 10 and 11.

5 Conclusion

The Singular Padé-Chebyshev (SPC) approximation demonstrates how a Padé-Chebyshev (PC) reconstruction of a function with singularities is greatly enhanced by utilizing its singularities in the approximation pro-

cess. If the singularities are known, the Singular Padé-Chebyshev (SPC) approximation remarkably reconstructs such function. Under restrictive conditions where only approximated expansion coefficients for the transformed Chebyshev series of the function and approximated jump locations are used, as in the case of postprocessing computational data, numerical results still reveal that the SPC approximant successfully resolves the Gibbs phenomenon that occurs in the process of recovering the function.

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