How well do the Hermite-Padé approximants reduce the Gibbs phenomenon?

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The Gibbs phenomenon
Hermite-Padé approach
Particular sequences of HP approximants
Numerical experiments

OUTLINE OF THE TALK

- the problem: *accelerating partial sums of Fourier series of functions with jumps* (spectral methods in PDE)
- definition of the Gibbs phenomenon and some classical approaches
- new approach: use of Hermite-Padé forms
  - definition of Hermite-Padé approximants and motivation
  - rate of convergence for a model problem
  - comparison with Padé approximants
  - numerical experiments
The Gibbs phenomenon

Definition
Some different approaches

Hermite-Padé approach
Particular sequences of HP approximants
Numerical experiments

The Gibbs phenomenon

Problem

Given a small number of coefficients of a real–valued Fourier series construct point values of \( f(t) = \text{Re}(\sum_{j=0}^{\infty} c_j e^{ijt}) \)

If we consider the partial sums

\[
S_n(f)(t) = \text{Re}\left(\sum_{j=0}^{n} c_j e^{ijt}\right) = \frac{a_0}{2} + \sum_{j=1}^{n} [a_j \cos(jt) + b_j \sin(jt)],
\]

how good is the approximation?
Convergence results

- \( f \) smooth and periodic: exponential accuracy
  \[
  \max_{-\pi \leq x \leq \pi} |f(x) - f_N(x)| \leq e^{-\alpha N}, \quad \alpha > 0
  \]

- \( f \in C^{m-1}([-\pi, \pi]) \) periodic (\( \hat{f}_k = O(|k|^{-(m+1)}), k \to \pm\infty \))
  \[
  \max_{-\pi \leq x \leq \pi} |f(x) - f_N(x)| = O(N^{-m}), \quad N \to \infty
  \]

- \( f \) discontinuous or non periodic: nonuniform convergence of the Fourier series
  \[
  |f(x_0) - f_N(x_0)| \sim O\left(\frac{1}{N}\right) \text{ away from discontinuity}
  \]
  \[
  \max_{[-\pi, \pi]} |f(x) - f_N(x)| \text{ doesn’t tend to } 0
  \]

  \( \Rightarrow \) Gibbs phenomenon: oscillations and bad convergence
Example: the saw-tooth function

How to overcome this phenomenon?
Some different approaches

1. **Linear summation methods**: Cesàro means, De la Vallée-Poussin means;

2. **Gottlieb approach**: to obtain exponential accuracy in the maximum norm in any interval of analyticity of a discontinuous piecewise analytic function - uses Gegenbauer polynomials;

3. **Eckhoff approach**: split a singular function into two parts, one presenting some regularity and the other corresponding to the singularities, modelled by some prototype functions (more details later)

4. **Fourier-Padé approach**
Consider the following procedure (C. Brezinski, P. Wynn):

- construct

\[ S_n(f)(t) + i\tilde{S}_n(f)(t) = G_n(f)(e^{it}), \text{ with} \]

- \( \tilde{S}_n(f)(t) = \sum_{j=1}^{n} [a_j \sin(jt) - b_j \cos(jt)] \),
- \( G_n(f) \) the \( n \)th Taylor sum of the (formal) series

\[ G(f)(z) = \sum_{j=0}^{\infty} c_j(f)z^j, \quad c_0(f) = \frac{a_0}{2}, \quad c_j(f) = a_j - ib_j. \]

- compute Padé approximants of this power series \( [n + k/k]_f(z) \)
Definition of the Fourier-Padé approximants

- use the real part for approaching $f(t) = \text{Re} \left( G(f)(e^{it}) \right)$.

$$\epsilon_{2k}^{(n)}(t) = \frac{p}{q}(t) = \text{Re} \left( [n + k/k]G(f)(e^{it}) \right)$$

where $p$ and $q$ are trigonometric polynomials of degrees $n + k$ and $k$ respectively.

- we showed that for $f \in L_2$ and $Q(z) \neq 0$ (denominator polynomial) for $|z| \leq 1$ then $f - \frac{p}{q}$ is orthogonal to $\sin(jt)$, $\cos(jt)$ for $j = 0, 1, \ldots, m + k$. $\iff$ non linear Fourier-Padé approximants

- numerical examples for functions with jumps show very good acceleration properties and strong reduction of Gibbs oscillations
s(t) = \pi + t \quad \text{for } t \in (-\pi, 0], \quad \text{s(t)} = -\pi + t \quad \text{for } t \in (0, \pi],

the 2\pi periodic saw tooth function, having one jump of absolute value 2\pi at t = 0 in [-\pi, \pi), approximants computed with 18 Fourier coefficients.
Convergence results (B. Beckermann, AM, F. Wielonsky, 2008)

- we consider a class of test functions

\[ G^{(\alpha,\beta)}(z) = 2F_1 \left( \begin{array}{c} \alpha + 1, 1 \\ \alpha + \beta + 2 \end{array} \bigg| z \right), \quad \alpha, \beta > -1 \]

- some examples are

\[
\begin{align*}
  f(t) &= \text{sign}(\cos(t)) \\
  f(t) &= |\sin(t/2)| \in C^0 \setminus C^1 \\
  f(t) &= (1 - \cos(s))s(t)
\end{align*}
\]
Convergence results

- Convergence for **columns**

\[
\max_{t \in I} \left| f(t) - \Re \left( [n|k](e^{it}) \right) \right| = O(n^{-2k})_{n \to \infty} \quad \text{for fixed } k
\]

even after perturbation of \( f \) with \( C^m \) function, \( m \) sufficiently large.

- Convergence of **ray sequences**: for some \( \gamma \geq 1 \)

\[
\lim_{k \to \infty, n = \gamma k} \max_{t \in I} \left| f(t) - \Re \left( [n|k](e^{it}) \right) \right|^{1/k} < 1.
\]
Why does it work so well?

\[ s(t) = -2 \sum_{j=1}^{\infty} \frac{\sin(jt)}{j} = \text{Re}\left( G(s)(e^{it}) \right), \quad \text{with} \]

\[ G(s)(z) = 2i \sum_{j=1}^{\infty} \frac{z^j}{j} = -2i \log(1 - z) = 2iz \int_{0}^{1} \frac{dx}{1 - xz}. \]

\[ s_1(t) = |\sin(t/2)|, \quad G(s_1)(z) = \frac{2}{\pi} - \frac{z}{\pi} \int_{0}^{1} \frac{1 - x}{\sqrt{x}} \frac{dx}{1 - xz}, \]

Stieltjes functions \( g_\sigma(z) = \int_{0}^{1} \frac{d\sigma(x)}{1 - zx} \) are very well approximated by Padé approximants in compact subsets of \( \mathbb{C} \setminus [1, +\infty) \), in particular all poles are on \( (1, +\infty) \).
Hypothesis:

We know location of singularity but not amplitude of jumps!

If \( f \in C^{n_1+1}([-\pi, 0) \cup (0, \pi]) \) periodic has left- and right-hand side derivatives of order \( 0, 1, \ldots, n_1 \) at \( t = 0 \):

\[
\exists d_j \in \mathbb{R} : \quad e(t) = f(t) - \sum_{j=0}^{n_1} d_j \sin^j(t)s(t) \in C^{n_1+1}([-\pi, \pi])
\]

In terms of \( z = e^{it} \):

\[
f(t) = \text{Re} \left( F(z) \right), \quad \sum_{j=0}^{n_1} d_j \sin^j(t) = \text{Re} \left( \frac{i}{2} p_1(z) \right),
\]

\[
s(t) = \text{Re} \left( \frac{2}{i} \log(1 - z) \right)
\]
Why Hermite-Padé forms?

thus reasonable approximation:

\[ f(t) \approx \text{Re} \left( -p_0(z) - p_1(z) \log(1 - z) \right) \]

with

\[ p_0 \in \mathcal{P}_{n_0}, \quad p_1 \in \mathcal{P}_{n_1}, \]

\[ p_0(z) + p_1(z) \log(1 - z) + F(z) = O(z^{n_0+n_1+2})_{z \to 0}. \]

particular case of Hermite-Padé approximants
Hermite–Padé approximant

Find $p_j \in \mathcal{P}_{n_j}$ for $j = 0, 1, 2$ such that

$$p_0(z) + p_1(z)g_1(z) + p_2(z)g_2(z) = \mathcal{O}(z^{n_0+n_1+n_2+2})_{z \to 0},$$

The Hermite–Padé approximant of $g_2(z)$ (or in short HP approximant) of order $\vec{n} = (n_0, n_1, n_2)$ is defined as

$$\Pi_{\vec{n}}(z) = -\frac{p_0(z) + p_1(z)g_1(z)}{p_2(z)}.$$
Hermite-Padé approximation

In our case

\[ g_1(z) = \log(1 - z), \quad g_2(z) = F(z) \]

and approach \( f(t) = \text{Re}(g_2(e^{it})) \) by

\[ f(t) \approx \text{Re} \left( \prod_{n_0, n_1, n_2} (e^{it}) \right) \]

Approximant with built-in singularity
Hermite-Padé approximation

- approach first proposed by Driscoll and Fornberg - singular Fourier-Padé approximant - with very convincing numerical experiments
- we can obtain rates of convergence by studying convergence of HP-approximants
- $n_2 = 0$: the Eckhoff approach: subtracting the singular part
- $n_1 = -1$: Fourier-Padé approximants (find themselves singularities)
Model problems \( (\text{logarithmic singularity at } z = 1) \)

\[
g_1(z) = \log(1 - z) = z \int_0^1 \frac{dx}{1-xz}.
\]
\[
g_2(z) = z \int_0^1 \frac{u(x) \, dx}{1-xz}, \quad u(x) = \int_c^d \frac{d\tau(y)}{x-y}, \quad [c, d] \cap [0, 1] = \emptyset.
\]

Property

\((1, g_1(1/z), g_2(1/z))\) form a **Nikishin system**.

\[
\Rightarrow \text{polynomials and residuals involved in their Hermite–Padé approximants satisfy orthogonality relations with respect to varying weights}
\]

\[
\Rightarrow \text{their } n\text{-th root asymptotics can be given in terms of the solution of a vector equilibrium problem in potential theory.}
\]
some results of potential theory

rate of convergence of Hermite-Padé approximants

error estimates for particular cases
  - diagonal sequences
  - row sequences
  - linear HP-approximants
  - comparison with Padé approximants

numerical experiments
Definitions of potential theory

- $\mathcal{M}_\rho(\Delta) = \{\mu \text{ measure} : \text{supp}(\mu) \subset \Delta, \mu(\mathbb{C}) = \rho\}$
- Logarithmic potential $U^\mu(x) := \int \log\left(\frac{1}{|x-y|}\right) d\mu(y)$.
- Consider $\sigma \in \mathcal{M}_1([\alpha, \beta])$ and $w_n \in \mathcal{C}([\alpha, \beta])$ sequence of weight functions. The corresponding orthonormal polynomials with varying weights $\{p_{k,n}\}, k, n \geq 0$ satisfy

$$j, k = 0, 1, \ldots : \int w_n(x)p_{j,n}(x)p_{k,n}(x) d\sigma(x) = \delta_{j,k},$$

with zero counting measures $\chi_k(p_{k,n}) = \frac{1}{k} \sum_{p_{k,n}(\xi)=0} \delta_\xi$. 
Weak asymptotics for OP with varying weight

Lemma (Stahl & Totik ’92)

If $w_n^{1/n} \to \exp(-2Q)$ uniformly in $[\alpha, \beta]$ and $\sigma \in \text{Reg}$ then we have the weak star convergence

$$\chi_n(p_{n,n}) \to \sigma_\mu$$

where $\sigma_\mu \in \mathcal{M}_1([\alpha, \beta])$ is the unique minimizer in $\mathcal{M}_1([\alpha, \beta])$ of

$$I_Q(\nu) = \int \log\left(\frac{1}{|x - y|}\right) d\nu(x)d\nu(y) + 2 \int Q d\nu$$
The minimizer $\sigma_\mu$ is uniquely characterized by the equilibrium conditions: $\exists W \in \mathbb{R}$

$$U^{\sigma_\mu}(x) + Q(x) \begin{cases} 
\geq W & \text{if } x \in [\alpha, \beta], \\
= W & \text{if } x \in \text{supp} \,(\sigma_\mu).
\end{cases}$$

$Q = 0$, $\text{supp} \,(\sigma) = [\alpha, \beta]$: $\sigma \in \text{Reg}$ iff $\sigma_\mu = \omega_{[\alpha, \beta]}$ equilibrium measure.
we consider sequences of Hermite-Padé approximants satisfying

- the total degree $n = n_0 + n_1 + n_2 \to \infty$;
- $n_0 \geq n_1 \geq n_2$;
- ray sequences $n_0, n_1, n_2$ such that
  
  \[
  \frac{n_0}{n} \to \rho_0, \quad \frac{n_1}{n} \to \rho_1, \quad \frac{n_2}{n} \to \rho_2.
  \]

Then the $n$-th root asymptotic behavior for the error function is given by
Theorem

Assume that \([c, d]\) is a compact interval and that \(\tau \in \text{Reg}\). Then, the error function \((g_2 - \Pi_{\vec{n}})(1/z)\) satisfies, locally uniformly for \(z \in \mathbb{C} \setminus ([0, 1] \cup [c, d])\),

\[
\lim_{n \to \infty} \frac{1}{n} \log |(g_2 - \Pi_{\vec{n}})(1/z)| =
\]

\[
(\rho_1 + \rho_2)U^\mu(z) + \rho_2 U^\nu(z) + (\rho_0 - \rho_2)U^{\delta_0}(z) - W - w,
\]

the probability measures \(\mu\) and \(\nu\), and the constants \(W\) and \(w\), solve the following vector equilibrium problem in potential theory.
Theorem (cont.)

μ, ν are the unique measures in \( \mathcal{M}_1([0, 1]) \), and \( \mathcal{M}_1([c, d]) \), respectively, satisfying the **equilibrium conditions**

\[
2(\rho_1 + \rho_2)U^\mu(x) - \rho_2 U^\nu(x) + (\rho_0 - \rho_1)U^{\delta_0}(x) \geq W \quad x \in [0, 1],
\]

\[
= W \quad x \in \text{supp}(\mu)
\]

\[
-(\rho_1 + \rho_2)U^\mu(x) + 2\rho_2 U^\nu(x) + (\rho_1 - \rho_2)U^{\delta_0}(x) \geq w \quad x \in [c, d],
\]

\[
= w \quad x \in \text{supp}(\nu).
\]

where \( W, w \in \mathbb{R} \).
idea of the proof

- Let \( A_n(z) = z^{n_1} p_1(1/z) \), \( B_n(z) = z^{n_2} p_2(1/z) \) monic,
  \[
  C_n(z) = A_n(z) + z^{n_1-n_2} B_n(z) u(z)
  \]

- Orthogonality relations for \( C_n(x) \):
  \[
  \int_0^1 x^{n_0-n_1} C_n(x) x^k dx = 0, \quad k = 0, \ldots, n_1 + n_2
  \]

- Denote \( H_n \in \mathcal{P}_{n_1+n_2+1} \) monic with roots the simple zeros of \( C_n \); orthogonality of \( H_n \) with respect to the varying weights \( n^{n_0-n_1} C_n(x)/H_n(x) \);

- Orthogonality relations for \( B_n(x) \):
  \[
  k = 0, 1, \ldots, n_2 - 1 : \quad \int_c^d y^{n_1-n_2} y^k \frac{B_n(y)}{H_n(y)} d\tau(y) = 0.
  \]
• applying the lemma we obtain existence and uniqueness of two measures \( \mu_1 \) and \( \mu_2 \)

\[
\chi_n(H_n) \to \mu, \quad \chi_n(B_n) \to \nu.
\]

satisfying the previous system of equilibrium conditions

• integral representation of the error:

\[
B_n(z)z^{n_0-n_2}(g_2(1/z) - \Pi_n(1/z)) = \frac{1}{H_n(z)} \int_0^1 x^{n_0-n_1} H_n(x) \frac{C_n(x)}{z-x} \, dx.
\]
Aim:
compare the rate achieved by HP-approximants of type \((n_0, n_1, n_2)\) as \((n \to \infty), \ n = n_0 + n_1 + n_2, \ n_0 \geq n_1 \geq n_2\) with that of Padé approximants of type \((m_0, -1, m_2)\) as \(m \to \infty, \ m = m_0 + m_2, \ m_0 \geq m_2\)

- constructed from the same number of Taylor coefficients of \(g_2\)
  \[ \Rightarrow \quad m = n + 1 \]

- based on the solution of linear systems of equal dimensions
  \[ \Rightarrow \quad m_0 = n_0, \quad m_2 = n_1 + n_2 + 1 \]
Let $\Theta_{\vec{m}} = -\tilde{P}_0/\tilde{P}_2$ is the Padé approximant of type $(m_0, -1, m_2)$ of the function $g_2$ at the origin. We consider a ray sequence
\[
\frac{m_0}{m} \to \sigma_0 > 0, \quad \frac{m_2}{m} \to \sigma_2 > 0,
\]

**Theorem**

*for* $z \in \mathbb{C} \setminus [0, 1]$,

\[
\lim_{m \to \infty} \frac{1}{m} \log |(g_2 - \Theta_{\vec{m}})(1/z)| = 2\sigma_2 U_{\tilde{\mu}}(z) + (\sigma_0 - \sigma_2) U_{\delta_0}(z) - \tilde{W}.
\]

*where* $\tilde{\mu}$ *measure, supported on* $[0, 1]$, *solution of an equilibrium problem in potential theory*

\[
2\sigma_2 U_{\tilde{\mu}}(x) + (\sigma_0 - \sigma_2) U_{\delta_0}(x) \begin{cases} 
\geq \tilde{W}, & x \in [0, 1], \\
= \tilde{W}, & x \in \text{supp} (\tilde{\mu}).
\end{cases}
\]
Diagonal HP-approximants \((n_1 = n_2)\)

- Ray sequences

  - for \(\Pi_{\vec{n}}\) (HP): \(\vec{n} = (n_0, n_1, n_1)\) as \((n \to \infty)\), \(\rho_0 \geq \rho_1 = \rho_2\)
  - for \(\Theta_{\vec{m}}\) (Padé): \(\vec{m} = (n_0, -1, 2n_1 + 1)\), \(\rho_0 \geq 2\rho_1\)

\[
\lim_{z \to 1} \lim_{n \to \infty} |(g_2 - \Pi_{\vec{n}})(z)|^{1/n} < 1,
\]

\[
\lim_{z \to 1} \lim_{m \to \infty} |(g_2 - \Theta_{\vec{m}})(z)|^{1/m} = 1.
\]

\(\Rightarrow\) there exists a neighborhood of 1 in \(\mathbb{C} \setminus (0, 1)\) in which the Hermite–Padé approximants achieve a rate of convergence which is better than the rate of the Padé approximants.
Linear HP-approximants ($n_2 = 0$)

- for $\Pi_{\vec{n}}$ (HP): $\vec{n} = (n_0, n_1, 0)$ as ($n \to \infty$), $\rho_0 \geq \rho_1 > 0$
  - HP approximants without denominator (Eckhoff approximants)
- for $\Theta_{\vec{m}}$ (Padé): $\vec{m} = (n_0, -1, n_1 + 1)$

\[
\lim_{z \to 1} \lim_{n \to \infty} \left| \frac{g_2 - \Pi_{\vec{n}}(z)}{1/n} \right| < 1,
\]

\[
\lim_{z \to 1} \lim_{m \to \infty} \left| \frac{g_2 - \Theta_{\vec{m}}(z)}{1/m} \right| = 1.
\]

$\Rightarrow$ there exists a neighborhood of 1 in $\mathbb{C} \setminus (0, 1)$ in which the Hermite–Padé approximants achieve a rate of convergence which is better than the rate of the Padé approximants.
Fixed denominator degree HP-approximants

- row sequences
  - for \( \Pi_{\vec{n}} \) (HP): \( \vec{n} = (n_0, n_1, n_1) \) such that \( n_0 \to \infty \) while \( n_1 \) remains constant, \( \rho_0 = 1, \rho_1 = \rho_2 = 0 \)
  - for \( \Theta_{\vec{m}} \) (Padé): \( \vec{m} = (n_0, -1, 2n_1 + 1) \)

**Theorem**

Assume that the measure \( d\tau(y) \) in the definition of the function \( u(x) \) is regular and that its support \([c, d] \subset (-\infty, 0)\). Let \( |z - 1| \leq 1/2 \). Then, for \( n_0 \) sufficiently large so that

\[
C \leq (n_0 - 2n_1 - 2)(1 - \Re(z)),
\]

we have

\[
\frac{|(g_2 - \Pi_{\vec{n}})(1/z)|}{|(g_2 - \Theta_{\vec{m}})(1/z)|} \leq \hat{C}|z - 1|^{2n_1 - 1},
\]

where \( C \) and \( \hat{C} \) are some constants that depend only on \( n_1 \).
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\[ g_2(z) = z \int_0^1 \frac{u(x)}{1-xz} \, dx, \quad u(x) = \log \left( \frac{x-c}{d-x} \right) = \int_c^d \frac{dy}{x-y}, \]

\[ g_1(z) = i \log(1 - z) \]

\[ [c, d] = [-2, -0.3] \]
\[ 16 \text{ coefficients} \]
\[ n_1 + n_2 + 2 = 6 \text{ unknowns} \]
\[ \text{partial sum } n = 16 \]
\[ \text{Padé approximant } \tilde{n} = (10, -1, 5) \]
\[ \text{linear HP } \tilde{n} = (10, 4, 0) \]
\[ \tilde{n} = (10, 3, 1) \]

"diagonal" approximant
\[ \tilde{n} = (10, 2, 2) \]

close to singularity

- from Padé to linear HP: we gain 4 digits
- from linear HP to "diagonal" approximants: we gain 3 or 4 digits
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\[ g_2(z) = z \int_0^1 \frac{u(x)}{1-xz} \, dx, \quad u(x) = \log \left( \frac{x-c}{d-x} \right) = \int_c^d \frac{dy}{x-y}, \]

\[ g_1(z) = i \log(1 - z) \]

16 coefficients

computed error curves versus theoretical error estimates
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\[ g_2(z) = z \int_0^1 \frac{u(x)}{1-xz} \, dx, \quad u(x) = \log \left( \frac{x-c}{d-x} \right) = \int_c^d \frac{dy}{x-y}, \]

\[ g_1(z) = i \log(1 - z) \]

increasing \( n_0 \) (\( n_1, n_2 \) fixed)

14 coefficients: \( n_0 = 14 \)

22 coefficients: \( n_0 = 22 \)

close to singularity from top to bottom: partial sum \( n_0 + 7 \), Padé app \( \vec{n} = (n_0, -1, 7) \), linear HP \( \vec{n} = (n_0, 6, 0) \) and diagonal HP \( \vec{n} = (n_0, 3, 3) \)

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HP approximants and the reduction of the Gibbs phenomenon
B. Beckermann, A. Matos, F. Wielonsky, Reduction of the Gibbs phenomenon for smooth functions with jumps by the $\epsilon$-algorithm, *JCAM* 219 (2008), 329-349.


