INTRODUCTION TO PADÉ APPROXIMANTS

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H. Padé
(1863-1953)
Student of Hermite
His thesis won
French Academy of
Sciences Prize

C. Hermite
(1822-1901)
Used Padé
approximants
to prove that e
is trancendental

But origins of subject go back to Cauchy, Jacobi, Frobenius.

Historical Reference: C. Brezinski, *History of Continued Fractions and Padé Approximants*, Springer-Verlag, (Berlin, 1991)

Why Padé?

1) Convergence Acceleration [e.g. ϵ-algorithm]

2) Numerical Solutions to Partial Differential Equations [$\exp(\mathbf{A}t) \approx Q(\mathbf{A}t)^{-1} P(\mathbf{A}t)$]

3) Analytic Continuation of Power Series [regions of convergence beyond a disk]

4) Includes Study of Orthogonal Polys on Interval [Padé denominators for Markov functions are orthogonal]

5) Finding Zeros/Roots, Poles/Singularities [use zeros and poles of Padé approximants to predict - e.g. QD algorithm]

Padé Approximants (PA) generalize Taylor Polynomials

Given $f(z) = \sum_{k=0}^{\infty} c_k z^k$

Taylor poly $P_m(z) = \sum_{k=0}^{m} c_k z^k$

Then

$$f(z) - P_m(z) = \sum_{k=m+1}^{\infty} c_k z^k$$

$$f(z) - P_m(z) = \mathcal{O}\left(z^{m+1}\right)$$

Equivalently,

$$\begin{aligned} P_m(0) &= f(0) \\ P_m'(0) &= f'(0) \\ &\vdots \\ P^{(m)}(0) &= f^{(m)}(0) \,. \end{aligned}$$

Idea of PA: Given m, n

$$\text{Rational function } R = P/Q$$

$$\deg P \leq m\,, \quad \deg Q \leq n$$

Choose P, Q so that

$$(f - R)(z) = \mathcal{O}\left(z^l\right)\,,$$

l as large as possible.

How large can we expect l to be?

	P	has	$m+1$	parameters
	Q	has	$n+1$	parameters
	P/Q	has	-1	parameter
So	total	of	$m+n+1$	parameters

Expect: $\left(f - \dfrac{P}{Q}\right)(z) = \mathcal{O}\left(z^{m+n+1}\right).$

NOT ALWAYS POSSIBLE

Ex: $m = n = 1, \quad f(z) = 1 + z^2 + z^4 + \cdots .$

$$R(z) = \frac{P(z)}{Q(z)} = \frac{az+b}{cz+d}.$$

Want

$$R(z) = 1 + z^2 + \mathcal{O}\left(z^3\right) . \tag{1}$$

But R is either identically constant or one-to-one.

From (1), neither is possible $[R'(0) = 0]$.

Idea: Linearize by requiring

$$Qf - P = \mathcal{O}\left(z^{m+n+1}\right)$$

$\mathcal{P}_k :=$ all polynomials of degree $\leq k$.

DEF Let $f(z) = \sum_0^\infty c_k z^k$ be a formal power series, and m, n nonnegative integers. A **Padé form** (PF) **of type** (m, n) is a pair (P, Q) such that $P = \sum_{k=0}^{m} p_k z^k \in \mathcal{P}_m$, $Q = \sum_{k=0}^{n} q_k z^k \in \mathcal{P}_n$, $Q \not\equiv 0$ and

(2) $$Qf - P = \mathcal{O}\left(z^{m+n+1}\right) \quad \text{as } z \to 0 .$$

Proposition Padé forms of type (m, n) always exist.

Proof. (2) is a system of $m+n+1$ homogeneous equations in $m+n+2$ unknowns:

(3) $$\sum_{j=0}^{n} c_{k-j} q_j - p_k = 0 , \quad 0 \le k \le m$$

(4) $$\sum_{j=0}^{n} c_{k-j} q_j = 0 , \quad k = m+1, \ldots, m+n .$$

$$c_{m,n} := \left(c_{m+i-j}\right)_{i,j=1}^{n} \quad \text{Toeplitz matrix}$$

THM Every PF of type (m,n) for $f(z)$ yields the same rational function.

Proof. (P,Q) and $\left(\hat{P},\hat{Q}\right)$ are PF's.

$$\begin{aligned} Qf - P &= \mathcal{O}\left(z^{m+n+1}\right) \\ \hat{Q}f - \hat{P} &= \mathcal{O}\left(z^{m+n+1}\right) \end{aligned}$$

so

$$-\hat{Q}P + \hat{P}Q = \mathcal{O}\left(z^{m+n+1}\right) \in \mathcal{P}_{m+n}\,.$$

Thus $\hat{P}Q \equiv \hat{Q}P \Rightarrow \hat{P}/\hat{Q} \equiv P/Q\,.$ □

DEF The uniquely determined rational P/Q is called the **Padé Approximant** (PA) of type (m,n) for $f(z)$, and is denoted by

$$[m/n]_f(z) \quad \text{or} \quad r_{m,n}(f;z)\,.$$

Remark In reduced form

$$[m/n]_f(z) = p_{m,n}(z)/q_{m,n}(z)\,,$$

where we (often) normalize so that

$$q_{m,n}(0) = 1\,, \qquad p_{m,n}(0) = c_0\,,$$

$p_{m,n}$ and $q_{m,n}$ relatively prime.

Padé Table for f

Taylor polys

[0/0]	[0/1]	[0/2]	$\cdots$
[1/0]	[1/1]	[1/2]	$\cdots$
[2/0]	[2/1]	[2/2]	$\cdots$
$\vdots$	$\vdots$	$\vdots$	

Equal entries occur in “square” blocks.

Ex: $f(z) = 1 + z^2 + z^4 + z^6 + \cdots \quad \left(= \dfrac{1}{1 - z^2} \right)$

Block structure

$$
\begin{array}{|cccccccc}
\hline
[0/0] & = & [0/1] & [0/2] & = & \cdot & \cdot & \cdot \\
\parallel & & \parallel & \parallel & & & & \\
[1/0] & = & [1/1] & [1/2] & = & \cdot & \cdot & \cdot \\
 & & & \parallel & & & & \\
[2/0] & = & [2/1] & [\quad] & = & \cdot & \cdot & \cdot \\
\parallel & & \parallel & \parallel & & & & \\
[3/0] & = & [3/1] & [\quad] & = & \cdot & \cdot & \cdot \\
 & & & \parallel & & & & \\
[4/0] & = & [4/1] & [\quad] & = & \cdot & \cdot & \cdot
\end{array}
$$

THM Let p/q be a reduced PA for $f(z)$, with $c_0 \neq 0$. Suppose

$$
\begin{aligned}
m &= \text{exact deg of } p \\
n &= \text{exact deg of } q
\end{aligned}
$$

and

$$qf - p = \mathcal{O}\left(z^{m+n+k+1}\right) \quad \textbf{exactly}\,.$$

Then

(a) $k \geq 0$

(b) $[\mu/\nu]_f = p/q$ iff

$$m \leq \mu \leq m + k\,, \quad n \leq \nu \leq n + k\,.$$

See: W. B. Gragg, *The Padé Table and its Relation to Certain Algorithms of Numerical Analysis*, SIAM Review (1972), 1-62.

DEF A Padé approximant is said to be **normal** if it appears exactly once in table. We say "f is normal" if every entry in its Padé table is normal.

Ex: $f(z) = e^z$ is normal.

Determinant Representations and Frobenius Identities.

$f(z) = \sum_{k=0}^{\infty} c_k z^k, \quad f_m(z) := \sum_{k=0}^{m} c_k z^k \in \mathcal{P}_m$

$$u_{m,n}(z) := \begin{vmatrix} f_m(z) & z f_{m-1}(z) & \cdots & z^n f_{m-n}(z) \\ c_{m+1} & c_m & \cdots & c_{m-n+1} \\ c_{m+2} & c_{m+1} & & c_{m-n+2} \\ \vdots & \vdots & & \vdots \\ c_{m+n} & c_{m+n-1} & \cdots & c_m \end{vmatrix}$$

$$v_{m,n}(z) := \begin{vmatrix} 1 & z & \cdots & z^n \\ c_{m+1} & c_m & \cdots & c_{m-n+1} \\ c_{m+2} & c_{m+1} & & c_{m-n+2} \\ \vdots & \vdots & & \vdots \\ c_{m+n} & c_{m+n-1} & \cdots & c_m \end{vmatrix}$$

Note: $u_{m,n}(z) \in \mathcal{P}_m, \; v_{m,n}(z) \in \mathcal{P}_n.$

THM $f(z) v_{m,n}(z) - u_{m,n}(z) = \mathcal{O}\left(z^{m+n+1}\right).$

DEF For arbitrary, but fixed polys g, h, let

$$w_{m,n}(z) := g(z)u_{m,n}(z) + h(z)v_{m,n}(z)$$

$$c_{m,n} := \det \left(c_{m+i-j}\right)_{i,j=1}^{n}$$

THM Between any 3 entries in the table of $w_{m,n}$ functions, there is a homogeneous linear relation with poly coefficients which can be computed from the coefficients c_k of f.

$$c_{m,n+1}w_{m+1,n} - c_{m+1,n}w_{m,n+1} = c_{m+1,n+1}zw_{m,n}$$

$$c_{m+1,n}w_{m-1,n} + c_{m,n+1}w_{m,n-1} = c_{m,n}w_{m,n}$$

$$c_{m,n}c_{m+1,n}w_{m,n+1} - c_{m,n+1}c_{m+1,n+1}zw_{m,n-1}$$

$$= (c_{m+1,n}c_{m,n+1} - c_{m,n}c_{m+1,n+1}z)w_{m,n}$$

. . .

Proof. Use *Sylvester's identity* on determinant representation for Padé denominator $v_{m,n}$.

$$\det A \det A_{i,j;k,l} = \det A_{i;k} \det A_{j;l} - \det A_{i;l} \det A_{j;k}$$

Padé Approximants for the Exponential

$$f(z) = e^z = \sum_{k=0}^{\infty} \frac{z^k}{k!}$$

Want to find $p_{m,n} \in \mathcal{P}_m$, $q_{m,n} \in \mathcal{P}_n$ such that

$$q_{m,n}(z)e^z - p_{m,n}(z) = \mathcal{O}\left(z^{m+n+1}\right) . \tag{5}$$

Let $D := d/dz$. Then

$$D\left[qe^z\right] = qe^z + q'e^z = e^z\,(I+D)\,q$$

Apply D^{m+1} to (5)

$$e^z\,(I+D)^{m+1}\,q_{m,n} + 0 = \mathcal{O}\left(z^n\right)$$
$$\Rightarrow (I+D)^{m+1}\,q_{m,n} = k_{m,n}z^n$$
$$\Rightarrow q_{m,n} = k_{m,n}(I+D)^{-(m+1)}z^n .$$

Recall

$$(1+x)^{-(m+1)} = \sum_{j=0}^{\infty} (-1)^j \binom{m+j}{m} x^j .$$

So

$$q_{m,n}(z) = k_{m,n} \sum_{j=0}^{n} (-1)^j \binom{m+j}{m} D^j z^n$$
$$= k_{m,n} \sum_{j=0}^{n} (-1)^j \binom{m+j}{m} \frac{n!}{(n-j)!} z^{n-j} .$$

$$q_{m,n}(z) = \sum_{k=0}^{n} \frac{(m+n-k)!n!}{(m+n)!(n-k)!} \frac{(-z)^k}{k!}$$

$$q_{m,n}e^z - p_{m,n} = \mathcal{O}\left(z^{m+n+1}\right) ,$$
$$q_{m,n} - p_{m,n}e^{-z} = \mathcal{O}\left(z^{m+n+1}\right) .$$

So $p_{m,n}(-z) = q_{n,m}(z)$,

$$p_{m,n}(z) = \sum_{k=0}^{m} \frac{(m+n-k)!m!}{(m+n)!(m-k)!} \frac{z^k}{k!} .$$

Also from

$$D^{m+1}[q_{m,n}e^z - p_{m,n}] = k_{m,n}z^n e^z ,$$

and integration by-parts we get

$$q_{m,n}(z)e^z - p_{m,n}(z)$$

$$= \frac{(-1)^n}{(m+n)!} z^{m+n+1} \int_0^1 s^n (1-s)^m e^{sz} ds \,.$$

Remark For $|z| \leq \rho$,

$$|q_{m,n}(z)| \leq 1 + \rho + \frac{\rho^2}{2!} + \frac{\rho^3}{3!} + \cdots = e^\rho \,.$$

So $q_{m,n}$ form a **normal family** in $\mathbb{C}$. Further, if $m+n \to \infty$, $m/n \to \lambda$,

$$\text{coeff of } z^k \to \frac{(-1)^k}{(1+\lambda)^k k!} \,.$$

Hence . . .

THM (Padé) Let $m_j,\, n_j \in \mathbb{Z}^+$ satisfy

$$m_j + n_j \to \infty\,, \qquad m_j/n_j \to \lambda \qquad \text{as } j \to \infty.$$

Then

$$\lim_{j\to\infty} q_{m_j,n_j}(z) = e^{-z/(1+\lambda)}\,,$$

$$\lim_{j\to\infty} p_{m_j,n_j}(z) = e^{\lambda z/(1+\lambda)}\,,$$

and

$$\lim_{j\to\infty} [m_j/n_j](z) = e^{z}\,,$$

locally uniformly in $\mathbb{C}$. More precisely $(m = m_j,\, n = n_j)$

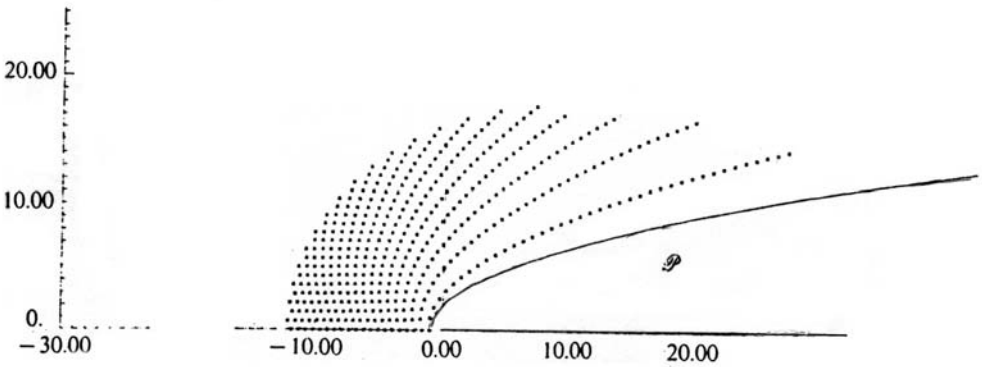
$$|[m/n](z) - e^z|$$

$$= \frac{m!n!\,|z|^{m+n+1} e^{2\mathfrak{Re}(z)/(1+\lambda)}}{(m+n)!(m+n+1)!}(1+o(1))\,.$$

COR All zeros and poles of PA's to e^z go to infinity as $m+n\to\infty$.

But where are they located?

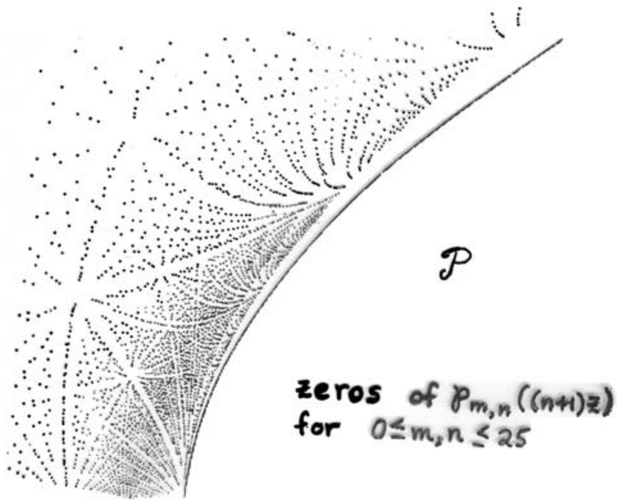
Zeros of $p_{m,0}(z) = \sum_{k=0}^{m} z^k/k!\,,\ m = 1, 2, \ldots, 40$



THM (S+Varga) For every $m,\ n \geq 0$, the normalized Padé numerator $p_{m,n}((n+1)z)$ for e^z is zero-free in the parabolic region

$$\mathcal{P} : y^2 \leq 4(x+1)\,, \quad x > -1\,.$$

Result is sharp!



THM (S+Varga) Consider any **ray sequence** $[m_j/n_j](z)$ where $n_j/m_j \to \sigma$ $(0 \le \sigma < \infty)$.

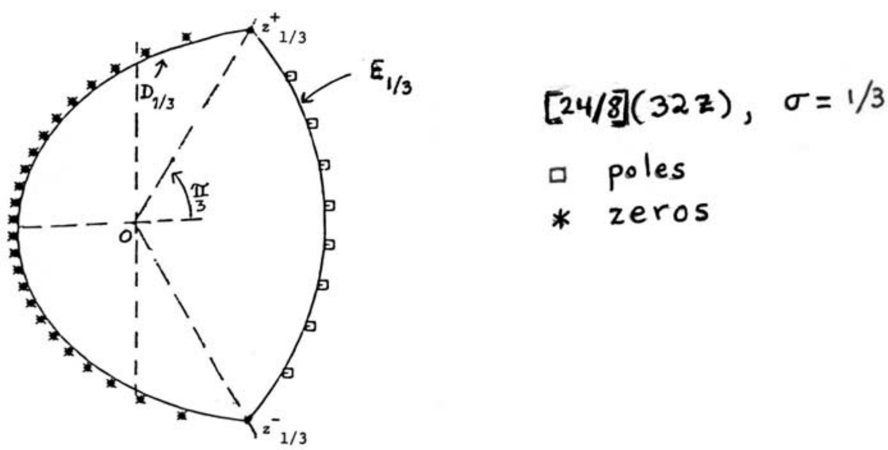
$$S_\sigma := \left\{ z \,:\, |\arg z| > \cos^{-1}[(1-\sigma)/(1+\sigma)] \right\}$$

$$w_\sigma(z) = \frac{C_\sigma\, z\, e^{g(z)}}{[1+z+g(z)]^{\frac{2}{(1+\sigma)}}[1-z+g(z)]^{\frac{2\sigma}{(1+\sigma)}}},$$

where $g(z) := \sqrt{1+z^2-2z\left(\frac{1-\sigma}{1+\sigma}\right)}$. Then

(i) $\hat{z}$ is a lim. pt. of **zeros** of $[m_j/n_j]\,((m_j+n_j)z)$ iff $\hat{z} \in D_\sigma := \left\{ z \in \overline{S}_\sigma : |w_\sigma(z)| = 1,\ |z| \le 1 \right\}$.

(ii) $\hat{z}$ is a lim. pt. of **poles** of $[m_j/n_j]\,((m_j+n_j)z)$ iff $\hat{z} \in E_\sigma := \left\{ z \in \overline{\mathbb{C} \setminus S_\sigma} : |w_\sigma(z)| = 1,\ |z| \le 1 \right\}$.



More recent variations:

Multi-point Padé Approx.

Let $B^{(m+n)} = \left\{ x_k^{(m+n)} \right\}_{k=0}^{m+n} \subset \mathbb{R}$,

$R_{m,n} = P_{m,n}/Q_{m,n}$, $\deg P_{m,n} = m$, $\deg Q_{m,n} = n$, interpolates e^z in $B^{(m+n)}$.

THM (Baratchart+S+Wielonsky) If $B^{(m+n)} \subset [-\rho, \rho]$, $m = m_\nu$, $n = n_\nu$ $(m + n \to \infty)$, then

$$R_{m,n}(z) \to e^z \qquad \forall\, z \in \mathbb{C}\,.$$

Moreover, the zeros and poles of $R_{m,n}$ lie within ρ of the zeros and poles, respectively, of the Padé approximants $[m/n](z)$ to e^z.

COR Conclusion holds for best *uniform* rational approx. to e^x on any compact subinterval of $\mathbb{R}$.

Analogous results for best L_2-rational approximants to e^z on unit circle.

Introduction to Convergence Theory

$f(z) = \sum_{k=0}^{\infty} c_k z^k$

$[m/0]_f(z) = \sum_{k=0}^{m} c_k z^k$ converges in largest open disk centered at $z = 0$ in which f is analytic:

$$|z| < R\,, \quad \text{where} \quad \frac{1}{R} = \limsup_{m\to\infty} |c_m|^{1/m}\,.$$

Next simplest case: $[m/1]_f$.

$$v_{m,1}(z) = \det \begin{pmatrix} 1 & z \\ c_{m+1} & c_m \end{pmatrix} = c_m - z c_{m+1}\,.$$

Assume $c_{m+1} \neq 0$. Then $v_{m,1}$ has zero at c_m/c_{m+1}.

$$\liminf_{m\to\infty} \left|\frac{c_{m+1}}{c_m}\right| \leq \frac{1}{R} \leq \limsup_{m\to\infty} \left|\frac{c_{m+1}}{c_m}\right|\,.$$

It's possible for ratios to have *many* limit points different from $1/R$.

ALL IS NOT ROSES - There can be "spurious" poles.

Perron's Example: $\exists\, f$ entire $(R = \infty)$ such that every point in $\mathbb{C}$ is a limit point of poles of some subsequence of $[m/1]_f$.

THM (de Montessus de Ballore, 1902) Let f be meromorphic with precisely ν poles (counting multiplicity) in the disk $\Delta : |z| < \rho$, with no poles at $z = 0$. Then

$$\lim_{m\to\infty}[m/\nu]_f(z) = f(z)$$

uniformly on compact subsets of $\Delta\backslash\{\nu$ poles of $f\}$. Furthermore, as $m \to \infty$, the poles of $[m/\nu]_f$ tend, respectively, to the ν poles of f in Δ.

Ex: $f(z) = z\Gamma(z)$ has poles at $z = -1, -2, \ldots$.

The n-th column of Padé table will converge to $z\Gamma(z)$ in $\{|z| < n + 1\} \setminus \{-1, \ldots, -n\}$.

Proof of de Montessus de Ballore Theorem:

Hermite's Formula Suppose g is analytic inside and on Γ, a simple closed contour. Let $z_1, z_2, \ldots, z_\mu$ be points interior to Γ, regarded with multiplicities $n_1, n_2, \ldots, n_\mu$. Set

$$N := n_1 + n_2 + \cdots + n_\mu \,.$$

Then ∃ a unique poly $p \in \mathcal{P}_{N-1}$ such that

$$p^{(j)}(z_k) = g^{(j)}(z_k)\,, \qquad \begin{array}{l} j = 0, 1, \ldots, n_k - 1\,, \\ k = 1, \ldots, \mu\,. \end{array}$$

Moreover,

$$p(z) = \frac{1}{2\pi i}\int_\Gamma \frac{\omega(\zeta) - \omega(z)}{\omega(\zeta)(\zeta - z)}\, g(\zeta)\, d\zeta \qquad z \in \mathbb{C}\,,$$

$$g(z) - p(z) = \frac{1}{2\pi i}\int_\Gamma \frac{\omega(z) g(\zeta)}{\omega(\zeta)(\zeta - z)}\, d\zeta \qquad z \text{ inside } \Gamma\,,$$

where

$$\omega(z) := \prod_{j=1}^{\mu} (z - z_j)^{n_j}\,.$$

Idea of Proof of de M. de Ballore Thm

f meromorphic with ν poles in $|z| < \rho$.

$u_{m,\nu}$, $v_{m,\nu}$ PF of type (m, ν) for f .

(6) $$f v_{m,\nu} - u_{m,\nu} = \mathcal{O}\left(z^{m+\nu+1}\right) .$$

Let $Q_\nu \in \mathcal{P}_\nu$ have zeros at poles of f with same multiplicity.

$$Q_\nu f v_{m,\nu} - Q_\nu u_{m,\nu} = \mathcal{O}\left(z^{m+\nu+1}\right)$$

$$= \frac{1}{2\pi i} \int_{|\zeta|=\rho-\epsilon} \frac{z^{m+\nu+1} \left(Q_\nu f v_{m,\nu}\right)(\zeta)}{\zeta^{m+\nu+1}(\zeta - z)} \, d\zeta \, ,$$

for $|z| < \rho - \epsilon$.

For $v_{m,\nu}$ suitably normalized, integral $\to 0$ for $|z| < \rho - \epsilon$.

Method extends to multi-point Padé .

What about other sequences from Padé Table, such as rows, diagonals, ray sequences?

THM (Wallin) There exists f entire such that the diagonal sequence $[n/n]_f(z)$, $n = 0, 1, 2, \ldots,$ is unbounded at every point in $\mathbb{C}$ except $z = 0$.

Baker-Gammel-Wills Conjecture: If f is analytic in $|z| < 1$ except for m poles ($\neq 0$), then there exists a **subsequence** of diagonal PAs $[n/n]_f(z)$ that converges to f locally uniformly in $\{|z| < 1\} \setminus \{m \text{ poles of } f\}$.

Conjecture is FALSE!

D. S. Lubinsky, "Rogers-Ramanujan and . . . ", *Annals of Math*, **157** (2003), 847-889.

Next step: Consider a weaker form of convergence, such as convergence in measure or convergence in capacity.

Nuttall-Pommerenke

Near-diagonal PAs will be inaccurate approximations to f only on sets of small capacity (transfinite diameter).

THM f analytic at ∞ and in a domain $D \subset \overline{\mathbb{C}}$ with $\mathrm{cap}(\overline{\mathbb{C}} \setminus D) = 0$. Let $R_{m,n}(z)$ denote the PA to f at ∞. Fix $r > 1$, $\lambda > 1$. Then for $\epsilon,\ \eta > 0$ there exists an m_0 such that

$$|R_{m,n}(z) - f(z)| < \epsilon^m$$

for all $m > m_0$, $1/\lambda \leq m/n \leq \lambda$, and for all z in $|z| < r$, $z \notin E_{m,n}$, $\mathrm{cap}(E_{m,n}) < \eta$.

THM (Stahl) Let $f(z)$ be analytic at infinity. There exists a unique compact set $\mathcal{K}_0 \subset \mathbb{C}$ such that

(i) $\mathcal{D}_0 := \overline{\mathbb{C}} \setminus \mathcal{K}_0$ is a domain in which $f(z)$ has a single-valued analytic continuation,

(ii) $\mathrm{cap}(\mathcal{K}_0) = \inf_{\mathcal{K}} \mathrm{cap}(\mathcal{K})$, where the infimum is over all compact sets $\mathcal{K} \subset \mathbb{C}$ satisfying (i),

(iii) $\mathcal{K}_0 \subset \mathcal{K}$ for all compact sets $\mathcal{K} \subset \mathbb{C}$ satisfying (i) and (ii).

The set $\mathcal{K}_0$ is called minimal set (for single-valued analytical continuation of $f(z)$) and the domain $\mathcal{D}_0 \subset \overline{\mathbb{C}}$ is called extremal domain.

THM (Stahl) Let the function $f(z)$ be defined by

$$f(z) = \sum_{j=0}^{\infty} f_j z^{-j}$$

and have all its singularities in a compact set $E \subset \overline{\mathbb{C}}$ of capacity zero. Then any close to diagonal sequence of Padé approximants $[m/n](z)$ to the function $f(z)$ converges in capacity to $f(z)$ in the extremal domain $\mathcal{D}_0$.