PADE APPROXIMANTS, STJELTJES FUNCTIONS AND VARIATIONAL PROPERTIES

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Dedicated to my friend Maciej Pindor

1 Definition and algorithms

Linear systems

Given a formal power series $f(z) = \sum_{n=0}^{\infty} f_n z^n$ the $[M/N]$ P.A. are rational functions

$$[M/N]_f(z) = \frac{P_M(z)}{Q_N(z)} \qquad Q_N(z) = \sum_{k=0}^{N} q_k\, z^k \qquad P_M(z) = \sum_{k=0}^{M} p_k\, z^k$$

defined by

$$\frac{P_M(z}{Q_N(z}) - f(z)) = O(z^{N+M+1})$$

The Taylor expansion of P.A. agrees with $f(z)$ up to order $N+M$ and the polynomials. If $q_0 = Q(0) \neq 0$ then the above definition is equivalent to

$$Q_N(z)\, f(z) - P_M(z) = O(z^{N+M+1})$$

which provides a linear system for q_i/q_0 and p_i/q_0 . The system is solvable if

$$D_{M/N} = \begin{vmatrix} f_M & \dots & f_{M+1-N} \\ \vdots & & \vdots \\ f_{M+1-N} & \dots & f_M \end{vmatrix} \neq 0 \qquad N \geq 1$$

and $D_{M/N}$ can be identified with with q_0 . We define $f_k = 0$ if $k < 0$. If $N = 0$ we set $q_0 = 1$ and $[M/0]$ are partial sums of $f(z)$.

Explicit formulae

The denominator polynomial $Q_N(z)$ is given by

$$Q_N(z) = D_{M/N}^{-1} \begin{vmatrix} f_{M+1} & f_M & \dots & f_{M+1-j} & \dots & f_{M+1-N} \\ \vdots & \vdots & & & \vdots & \vdots \\ f_{M+N} & f_{M+N-1} & \dots & f_{M+N-j} & \dots & f_M \\ & & & & & \\ 1 & x & \dots & x^j & \dots & x^N \end{vmatrix}$$

The numerator polynomial is given by

$$Q_N(z) = D_{M/N}^{-1} \begin{vmatrix} f_{M+1} & f_M & \dots & f_{M+1-j} & \dots & f_{M+1-N} \\ \vdots & \vdots & & & \vdots & \vdots \\ f_{M+N} & f_{M+N-1} & \dots & f_{M+N-j} & \dots & f_M \\ & & & & & \\ \sum_{k=0}^{M} f_k x^k & \sum_{j=k}^{M} f_k x^k & \dots & \sum_{k=j}^{M} f_k x^k & \dots & \sum_{k=N}^{M} f_k x^k \end{vmatrix}$$

Nuttal's formula we quote another compact formula to compute P.A. we shall prove later, by considering approximations to the resolvent of a symmetric operator.

$$[N-1/N]_f(z) = (f_0 \; \dots f_{N-1}) \begin{pmatrix} f_0 - xf_1 & \dots & f_{N-1} - xf_N \\ \vdots & & \vdots \\ f_-N - 1xf_N & \dots & f_{2N-2} - xf_{2N-1} \end{pmatrix} \begin{pmatrix} f_0 \\ \vdots \\ f_{N-1} \end{pmatrix}$$

The Padé table has entries are $[M/N]$. It is normal if $D_[M/N] \neq 0$ for any $N \geq 0, \; M \geq 0$: its elements are ratios of irreducible polynomials P_M and Q_N (no common divisors).

If $D_[M/N] = 0$ then the entry $[M/N]$ is given by the ratio of two reducible polinomials $P_M = R_k \, P_{M-k}$ and $Q_N = R_k \, Q_{N-k}$ where R_k is a polynomial of degree $< \max(M, N)$, whose coefficents are arbitrary. The Pad/'e table whose entries are ratios of irreducible polynomials has blocks of equal entries.

Examples The Padé table has blocks if f is a rational function or a function of z^q for $q > 1$. Take fon instance $f(z) = (1-z)^{-1}$ with $f_n = 1$. Then $D_{[0/N]=1}$ but $D_{[M/N]} = 0$ for $M \geq 1, N \geq 1$

$$D_{[1/2]} = \begin{vmatrix} 1 & 1 \\ 1 & 1 \end{vmatrix} = 0 \qquad [1/2] = \frac{1 + (1+q_1)z}{1 + q_1 z - (1+q_1)z^2} = \frac{1 \times (1 + (1+q_1)z)}{(1-z) \times (1 + (1+q_1)z)}$$

Algebraic properties We list a few properties follwoing from defnition

1) If the $[M/N]$ P.A. exists ($D_{[M/N]} \neq 0$) exists it is unique.

2) $[M+J/N]_f(z) = \sum_{k=0}^{J-1} f_k\, z^k + z^J [M/N]_{\hat{f}}(z)$ $\qquad \hat{f}(z) = \sum_{k=0}^{\infty} f_{k+J} z^k$

3) $[M-J/N]_f(z) = z^{-J}\, [M-J/N]_{\hat{f}}(z)$ $\qquad \hat{f}(z) = z^J f(z)$

4) $[M/N]_{f+R_n}(z) = R_n + [M-J/N]_f(z)$ $\qquad$ degree $(R_n) \leq M-n$

5) $[M/N]_{1/f}(z) = \Big(\, [M/N]_f(z)\, \Big)^{-1}$

6) The diagonal $[N/N]_f(z)$ P.A. are invariant for omographic tranformations of f namely $\mathsf{T}f = (\alpha+\beta f)/(\gamma+\delta f)$ and of z preserving the origin $T(z) = az/(b+cz)$

Continued fractions

Are defined by

$$S = b_0 + \cfrac{a_0}{b_1 + \cfrac{a_1}{b_2 + \cfrac{a_2}{\ddots + \cfrac{a_{n-1}}{b_n + r_n}}}} \qquad\qquad r_n = \frac{a_n}{b_{n+1} + r_n}$$

The following recurrence holds

$$S = \frac{A_n + r_n\, A_{n-1}}{B_n + r_n\, B_{n-1}} \qquad\qquad \begin{cases} A_n = b_n\, A_{n-1} + a_{n-1}\, A_{n-2} \\ B_n = b_n\, B_{n-1} + a_{n-1}\, B_{n-2} \end{cases}$$

initialized by

$$A_{-1} = 1 \qquad A_0 = b_0 \qquad\qquad B_{-1} = 0 \qquad B_0 = 1$$

The ratios A_n / B_n are the truncations of the continued fractions with $r_n = 0$.

Theorem For positive continues fractions $a_n > 0,\ b_n > 0$ the even and odd sequences are monotonic

$$\frac{A_0}{B_0} \le \dots \frac{A_{2n}}{B_{2n}} \le \frac{A_{2n+2}}{B_{2n+2}} \le S \le \frac{A_{2n+1}}{B_{2n+1}} \le \frac{A_{2n-1}}{B_{2n-1}} \le \dots \le \frac{A_1}{B_1}$$

Analytic continued fractions

Given a power series $f(z) = \sum_{n=0}^{\infty} f_n z^n$ where $f_0 = 1$ we consider the recurrence

$$f(z) \equiv \frac{f_1(z)}{f_0} = \frac{1}{1 - \alpha_0 z - \beta_1 z^2 \frac{f_2(z)}{f_1(z)}} \quad \cdots \quad \frac{f_n(z)}{f_{n-1}} = \frac{1}{1 - \alpha_{n-1} z - \beta_n z^2 \frac{f_{n+1}(z)}{f_n(z)}}$$

Letting

$$f_n(z) = 1 + \sum_{k\geq 1} f_k^{(n)} \, z^k \qquad\qquad f_0^{(n)} = 1$$

and $f_k^{(1)} = f_k$ we start from the first relation and after multiplying both sides by the denominator of the left side we determine α_0, β_1 and f_2 according to

$$\alpha_0 = f_1 \qquad \beta_1 = f_2 - \alpha_0 f_1 \qquad f_k^{(2)} = \frac{1}{\beta_1}(f_{k+2} - \alpha_0 f_{k+1})$$

At the next orders the recurrence reads

$$\alpha_{n-1} = f_1^{(n)} - f_1^{(n-1)} \qquad \beta_n = f_2^{(n)} - \alpha_{n-1} f_1^{(n)} - f_2^{(n-1)}$$

$$f_k^{(n+1)} = \frac{1}{\beta_k}\left(f_{k+2}^{(n)} - \alpha_{n-1} f_{k+1}^{(n)} - f_{k+2}^{(n-1)}\right)$$

Truncations and P.A.

The even and odd truncations of the countinues fraction give two diagonal sequences of P.A. Let

$$F(z) = \frac{1}{z} f\left(\frac{1}{z}\right) = \cfrac{1}{z - \alpha_0 - \cfrac{\beta_1}{z - \alpha_1 + \cfrac{\beta_2}{\ddots + \cfrac{\beta_n}{z - \alpha_n + r_n}}}}$$

Identifying $a_n = -\beta_n,\ b_n = z - \alpha_{n-1}$ the truncations A_n/B_n satisfy

$$\begin{cases} A_n = (z - \alpha_{n-1})\, A_{n-1} - \beta_{n-1}\, A_{n-2} \\ B_n = (z - \alpha_{n-1})\, B_{n-1} - \beta_{n-1}\, B_{n-2} \end{cases} \qquad \begin{cases} A_0 = 0 & A_1 = 1 \\ B_0 = 1 & B_1 = z - \alpha_0 \end{cases}$$

Hence $A_n = \hat{Q}_{n-1}(z)$ and $B_n = \hat{Q}_n(z)$ are polynomials of order $n-1$ and n
Letting $P_n = z^n \hat{P}_n(z^{-1})$ and $Q_n = z^n \hat{Q}_n(z^{-1})$ it can be shown that

$$f(z) = \frac{P_{N-1}(z)}{Q_N(z)} + O(z^{2N}) \qquad \boxed{\frac{P_{N-1}(z)}{Q_N(z)} = [N-1/N]_f(z)}$$

Positive measures

Orthogonal polynomials Let $\mu(t)$ be a positive measure on $\mathbb{R}$ and let

$$\mathcal{F}(g) = \int_{-\infty}^{+\infty} g(t)\, d\mu(t)$$

The moments and their generating function are

$$f_n = \mathcal{F}(t^n) \qquad\qquad f(z) = \mathcal{F}\left(\frac{1}{1-tz}\right) = \sum_{n=0}^{\infty} f_n\, z^n$$

We define the orthogonal polynomials $\hat{Q}_n(z)$ and their associates by $\hat{P}_n(z)$ by

$$\mathcal{F}\Big(t^k \hat{Q}_N(t)\Big) = 0 \quad \text{for} \quad 0 \le k \le N-1 \qquad\qquad \hat{P}_{N-1}(z) = \mathcal{F}\left(\frac{\hat{Q}_N(x) - \hat{Q}_N(t)}{z-t}\right)$$

The normalization is $z^{-n}\hat{Q}_N(z) \to 1$ for $z \to \infty$. The linear systems saisfies by the coefficients of $\hat{Q}_N(z)$ are the same as the ones for the denominator $Q_n(z)$ of the $[N-/N]$ P.A. and the same relation holds between $\hat{P}_{n-1}(z)$ and $P_{n-1}(z)$.

$$[N-1/N]_f(z) = \frac{z^{N-1}\hat{P}_{N-1}(z^{-1})}{z^N \hat{Q}_N(z^{-1})} = \frac{P_{N-1}(z)}{Q_N(z)}$$

Approximate measures

The zeroes $z = r_k^{(N)}$ of the orthogonal polynomial $\hat{Q}_N(z)$ are all real and belong to the support of μ . ince $Q_N(0) = 1$ we can write

$$\frac{P_{N-1}(z)}{Q_N(z)} = \frac{P_{N-1}(z)}{(1 - zr_1^{(N)}) \cdots (1 - zr_N^{(N)})} = \sum_{k=1}^{N} \frac{\gamma_k}{1 - zr_k}$$

We introduce an atomic measure $\mu_n(t)$ such that

$$\mathcal{F}_N(g) = \int_{-\infty}^{+\infty} g(t)\, d\mu_N(t) \qquad \mu_N(t) = \sum_{k=1}^{n} \gamma_k^{(N)} \vartheta(t - r_k^{(N)})$$

The approximate functional satisfies

$$\mathcal{F}\left(\frac{1}{1 - tz}\right) = \mathcal{F}_N\left(\frac{1}{1 - tz}\right) + (z^{2N})$$

so that consequence

$$\mathcal{F}_N(t^k) = \mathcal{F}(t^k) \qquad \text{for} \qquad 0 \le k \le 2N - 1$$

Quadrature formulae

The approximate functional $\mathcal{F}_N$ allows an analytic extrapolation of the first $2N-1$ moments of the measure, i.e. of the first $2N-1$ coefficients of $f(z)$

$$f_n^{(N)} = \mathcal{F}_N(t^n) = \sum_{k=1}^{N} \gamma_k^{(N)} \left(r_k^{(N)}\right)^n \qquad f_n^{(N)} = f_n \ \text{ for } \quad 0 \le n \le 2N-1$$

The transform of a function $g(t)$, which is a quadrature with respect to $\mu(t)$.

Theorem The transform $\mathcal{F}_N(g)$ is the Gauss quadrature of $\mathcal{F}(g)$ since it is exact if math g(t) for any polynomial of order $m \le 2N-1$

$$\mathcal{F}_N(g) = \sum_{n=1}^{N} g(r_n^{(N)})\, \gamma_n^{(N)}$$

Le T polynomial of order $m \le 2N-1$

$$\mathcal{F}_N(T) = \sum_{k=1}^{m} T_k\, \mathcal{F}_N(t^k) = \sum_{k=1}^{m} T_k\, \mathcal{F}(t^k) = \mathcal{F}_N(T)$$

If $\mu(t) = t$ with support on $[-1, 1]$ then $Q_N(z)$ are Legendre polynomial, their zeroes $r_n^{(N)}$ are the quadrature ponts and $\gamma_n^{(N)}$ the weights.

Stjeltjes functions

If the support of $\mu(t)$ is $\mathbb{R}_+$ then its Hilbert transform

$$f(z) = \mathcal{F}\left(\frac{1}{1-tz}\right) = \int_0^\infty \frac{d\mu(t)}{1-zt}$$

is a Stjeltjes function. It is analytic on the the complex z cut along $\mathbb{R}_+$

i) The coefficients α_n, β_n of the continued fraction expansion are positive.

ii) The zeroes of $Q_N(z)$, orthogonal polynomials with respect to $\mu(t)$, are on $\mathbb{R}_+$ and interlace with the zeroes of $Q_{N-1}(z)$.

iii) If $x \in \mathbb{R}_-$ then $f(x) > 0$ and the following bounds hold

$$[0/1]_f(x) \leq \cdots \leq [N-1/N]_f(x) \leq f(x) \leq [N/N]_f(x) \leq \cdots \leq [1/1]_f(x)$$

iv) The sequences $[N-1/N]_f(z),\ [N/N]_f(z)$ converge uniformly to $f(z)$ in any compact domain of the cut plane $\mathbb{C} - \mathbb{R}_+$ provided that

$$\sum_{n=0}^{\infty} f_n^{-1/2n} = +\infty \qquad \text{satisfied if} \quad f_n < a\, c^n\, (2n)!$$

Self adjoint operators

The spectral decomposition of a self adjoint operator A in a Hilbert space $\mathcal{H}$ establishes a precise relation with positive measures

$$\mathsf{A} = \int_{-\infty}^{+\infty} t \, dP(t)$$

Letting $\phi \in \mathcal{H}$ we have

$$\mu(t) = \langle \phi | P(t) | \rangle \qquad\qquad f(z) = \langle \phi | (I - z\mathsf{A})^{-1} | \phi \rangle$$

Galerkin' method Letting $\phi, \phi_1, \ldots, \phi_n \in \mathcal{E}_N \subset \mathcal{H}$ we consider the projector P_N defined by

$$\mathsf{P}_N = \sum_{i,k=0}^{N-1} (G^{-1})_{ik} \; |\phi_i\rangle\langle\phi_k| \qquad\qquad G_{ik} = \langle \phi_i | \phi_k \rangle$$

We solve the approximate equation for the the restriction $\mathsf{A}_N = \mathsf{P}_N \mathsf{A} \mathsf{P}_N$

$$\psi_N = \phi + z\mathsf{A}_N \psi_N \qquad\qquad \langle \phi | \psi_N \rangle = \langle \phi | (I - z\mathsf{A}_N)^{-1} | \phi \rangle$$

Letting $\psi_N = c_0 \phi_0 + \ldots + c_{N-1} \phi_{N-1}$ we obtain

$$\boxed{\langle \phi | \psi_N \rangle = \mathbf{b}^* \cdot M^{-1} \mathbf{b}} \qquad b_k = \langle \phi_k | \phi \rangle \qquad M_{ik} = \langle \phi_i | (I - z\mathsf{A}) | \phi_k \rangle$$

Perturbative anzsatz Choosing the base $\phi_k = \mathsf{A}^k \phi$ it is immediate to show that

$$\langle \phi | (I - z\mathsf{A}_N)^{-1} | \phi \rangle = \phi | (I - z\mathsf{A})^{-1} | \phi \rangle + O(z^{2N})$$

The approximate resolvent is a ratio of two polynominals $P_{N-1}(z)/Q_N(z)$, hence it agrees with $[N-1/N]$ P.A. to $f(z)$ and coincides with Nuttal's formula.

$$\langle \phi | (I - z\mathsf{A}_N)^{-1} | \phi \rangle = [N-1/N]_{\langle \phi | (I - zA)^{-1} | \phi \rangle}$$

Variational methods

The quadratic functional defined on $\mathcal{H}$

$$\mathcal{L}(\chi) = \langle \chi | \phi \rangle + \langle \phi | \chi \rangle - \langle \chi | (1 - z\mathsf{A}) | \chi \rangle$$

is stationary for for $\chi = \psi$ where $\psi = (1 - z\mathsf{A})^{-1} \phi$. Indeed

$$\delta \mathcal{L}(\chi) = \mathcal{L}(\chi + \delta\chi) - \mathcal{S}(\chi) = \langle \delta\chi | \phi - (1 - z\mathsf{A})\chi \rangle + \langle \phi - (1 - z\mathsf{A})\chi | \delta\chi \rangle$$

Choosing $\chi \in \mathcal{E}_N$ the variational solution agrees with Galerkin's method.

$$\{\delta \mathcal{L}(\chi)\}_{\chi \in \mathcal{E}_N} = 0 \qquad \chi = \psi_N \equiv (1 - z\mathsf{A})^{-1} \phi \qquad \mathcal{L}(\psi_N) = \langle \phi | \psi_N \rangle$$

Variational bounds

With the perturbative ansatz the variational solution is the $[N-1/N]$ P.A. If A is positive then $(I - x\mathsf{A})$ for $x \in \mathbb{R}_-$ is positive and

$$\mathcal{L}(\psi) - \mathcal{L}(\chi) = \|(I - xA)^{-1/2}\,\phi - (I - xA)^{1/2}\,\chi\|^2 \geq 0$$

Lower bounds

From previous inequality we obtain

$$\mathcal{L}(\chi) \leq f(x) \equiv \langle\phi|(I - x(\mathsf{A})^{-1}|\phi\rangle \qquad \boxed{[N-1/N]_f(x) \leq f(x) \qquad x \in \mathbb{R}_-}$$

and the sequence $[N-1/N]_f(x)$ is monotonically increasing .

Upper bounds

We consider the functional $\mathcal{U}$ defined by

$$\mathcal{U}(\chi) = \langle\phi|\phi\rangle + z\langle\chi|A|\phi\rangle + z\langle\phi|A|\chi\rangle - z\langle\chi|A(1 - z\mathsf{A})|\chi\rangle$$

It is easy to check that it is stationary for $\chi = \psi \equiv (1 - z\mathsf{A})^{-1}\phi$ and $\phi = f(z)$. In the subspace given by the perturbative ansatz the stationary soution is $[N/N]_f(x)$

$$\mathcal{U}(\chi) \geq f(x) \equiv \langle\phi|(I - x(\mathsf{A})^{-1}|\phi\rangle \qquad \boxed{f(x) \leq [N/N]_f(x) \qquad x \in \mathbb{R}_-}$$

Generalizations

Matrix P.A. They are defined for an analytic $L \times L$ matrix $F_{ik}(z)$ of order . Explicit formulae of Nuttal's type are obtained if the matrix is given by

$$F_{ik}(z) = \langle \phi_i | (I - z\mathsf{A})^{-1} | \phi_k \rangle \qquad i, j = 0, \ldots, L-1$$

by the Galerking or variational method in a subspace

$$\mathcal{E}_{LN} = \{\phi, \phi_1, \ldots, \phi_{L-1}, \mathsf{A}\,\phi, \mathsf{A}\,\phi_1, \ldots, \mathsf{A}\,\phi_{L-1}, \ldots, \mathsf{A}^{N-1}\,\phi, \mathsf{A}\,\mathsf{A}^{N-1}\phi_1, \ldots, \mathsf{A}^{N-1}\,\phi_{L-1}\}$$

The P.A. to a stjeltjes matrix $F(x)$ have bounding properties on $\mathbb{R}_-$

$$[N-1/N]_(x) \leq F(x) \leq [N/N]F(x) \qquad\qquad x \in \mathbb{R}_-$$

Generalized P.A. Consider a sequence of polynomials $L_n(z)$ and their generating function $K(z,t) = \sum t^z L_n(z)$. For instance $K(z,t) = e^{-zt}$ and $L_n(z)$ Laguerre polynomials. Letting

$$f(z) = \mathcal{F}(K(z,t)) = \int_{-\infty}^{+\infty} K(z,t) d\mu(t) = \sum_n f_n L_n(z)$$

the generalized P.A. are defined by the corresponding quadrature formula

$$[N-1/N]_f^{\mathrm{gen}}(z) = \mathcal{F}_N(K(z,t)) = \sum \gamma_n^{(N)} K\Big(z, r_n^{(N)}\Big)$$

Conclusions

Algebraic properties The P.A. are obtained by solving linear systems. If the ratio of polynomials is irreducible the Pad/'e table is normal, otherwise there are blocks. The diagonal P.A. are invariant by omographic transformations.

Continued fractions This algorithm has optimal computational complexity. It provides the diagonal sequence of $[n-1/n]$, $[n/n]$ for $1 \leq n \leq N$ given a Taylor series up to order $2N$. To be used with extended precision, necessary to counteract noise effects.

Stjeltjes functions The denominators of diagonal sequences of P.A. are orthogonal polynomials, with respect to a positive measure, their zeroes being on its support. This implies convergence of P.A. in the cut plane and bounding properties on the real axis excluding the cut.

Resolvents of symmetric operators The mean value of the resolvent is a Stielties function. The Galerkin method in a subspace $\mathcal{E}_N$ defined by the perturbative ansatz gives the diagonal P.A. They are stationary values of quadratic functionals in the subspace $\mathcal{E}_N$. For positive operators the P.A. give bounds.