Error Estimates, Pade Approximants, and Pole Extraction from Power Series.

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The Power Series Expansion Method

1. Write dif. eqs. as sums of products.
2. Expand each function as a power series.
3. Treat each sum, product, or derivative as a separate step.
4. Equate powers of the independent variables.
5. Advance series until error reaches goal.

$$\left\|\mathbf{x}(t) - \sum_{j=0}^{k} \mathbf{x}_j t^j\right\| \leq ||c|| \left((1 - M|t|)^{-1/(m-1)} - \sum_{j=0}^{k} z_j t^j\right) \qquad (1)$$

where c are rescaled coefficients, $||c|| = c_{max}$, $m \geq 2$, $M = (m-1)||\mathbf{B}_N||$, and $||\mathbf{B}_N||$ is the largest row sum of the absolute value of coefficients of transformation $\mathbf{B}$.

Calculation of Error Limit: Rescaling.

P.G. Warne, D.A. Polignone Warne, J.S. Sochacki, G.E. Parker, and D.C. Carothers, "Explicit *A-Priori* Error Bounds and Adaptive Error Control for Approximation of Nonlinear Initial Value Differential Systems.", *Computers and Mathematics with Applications* **52** (2006), p.1695.

1.(Theorem 1)If $p = \prod_k u_k(t) = \sum_i p_i t^i$, $q = \prod_l v_l(t) = \sum_i q_i t^i$, and $k_{max} \leq l_{max}$ and $u_k = \sum_j u_{kj} t^j$ and $v_l = \sum_l v_{lj} t^j$ and $\forall k$, $|u_{kl}| \leq v_{kl}$, and $v_{k0} = 1$, then by induction, $p_{ik} \leq q_{ik}$.

2. Suppose $\exists$ a system of N differential equations $\mathbf{x}' = \mathbf{f}(\mathbf{x})$. Then rescale $\mathbf{x}$ to put initial conditions between 1 and -1:
If $x_i(0) = a_i$, then scaling $c_i \equiv a_i$ if $|a_i| > 1$, else $c_i \equiv 1$.
If $x_i \equiv c_i y_i$, then $y_i(0) = b_i$ with $|b_i| \leq 1$ and $\mathbf{y}' = \mathbf{f}(\mathbf{x})$.

3. For the power series method, $\mathbf{y}$ is written as

$$y_i' = \sum_{j_1=0}^{N} \sum_{j_2=0}^{N} \cdots \sum_{j_n=0}^{N} B_{i,j_1,j_2,\ldots,j_n} y_1^{j_1} y_2^{j_2} \cdots y_n^{j_n} \tag{2}$$

Calculation of Error Limit: Warne Transformation.

4. For Warne transformation $\mathbf{B}_N[\mathbf{y}] \equiv \mathbf{f} : \Re^n \to \Re^n$,

$$||\mathbf{B}_N|| \equiv \text{sup}\{||\mathbf{B}_N[\mathbf{u}]|| : \mathbf{u} \in \Re^n \text{where} ||\mathbf{u}|| = 1\} \tag{3}$$

$$||\mathbf{B}_N|| = \max_{1 \le i \le n} \left\{ \sum_{j_1=0}^{N} \sum_{j_2=0}^{N} \cdots \sum_{j_n=0}^{N} |B_{i,j_1,j_2,\ldots,j_n}| \right\} \tag{4}$$

5. Then on $||y - b|| < L$, $||\mathbf{f}|| \le ||\mathbf{B}_N||(L+1)^N$ and $||\partial f/\partial y_k|| \le m||\mathbf{B}_N||(L+1)^m$ where m is the largest degree of any nonzero term in $\mathbf{f}$.
Then $\exists$ a unique y in Eq. (2) for $t \in (-L/(||\mathbf{B}_N||(L+1)^m), L/((\mathbf{B}_N||(L+1)^m))$.
For $m > 1$, the interval is a maximum for $L = m - 1$, yielding

$$t \in \left(\frac{-1}{M} \left(\frac{m-1}{m} \right)^m, \frac{1}{M} \left(\frac{m-1}{m} \right)^m \right) \tag{5}$$

where $M = (m - 1)||\mathbf{B}_N||$.

Calculation of Error Limit: Majorizing Limit z on y.

6. Since $\mathbf{y}' = \mathbf{B}_N[\mathbf{y}]$, and $\mathbf{y}(0) = \mathbf{b}$, and $\mathbf{y} = \sum_j \mathbf{y}_j t^j$, $\mathbf{f} = \sum_j \mathbf{f}_j t^j$, we can iteratively generate terms:
$\mathbf{y}_0 = \mathbf{b}$, $\mathbf{f}_0 = \mathbf{f}(\mathbf{y}_0)$, $\mathbf{y}_{k+1} = \mathbf{f}_k/(k+1)$. So $||\mathbf{y}_{k+1}|| = ||\mathbf{f}||/(k+1)$.
7. Likewise, if $z' = ||\mathbf{B}_N||z^m$, and $z(0) = 1$, and $z = \sum_j z_j t^j$, then iteratively, $z_0 = 1$, $z_{k+1} = (z^m)_k||\mathbf{B}_N||/(k+1)$, yielding

$$z(t) = \begin{cases} e^{||\mathbf{B}_N||t} & \text{for } m = 1, \\ (1 - Mt)^{-1/(m-1)} & \text{for } m > 1. \end{cases} \tag{6}$$

8. We can use Theorem 1 on the limits of products:
Since $|y_{ij}| \leq ||\mathbf{y}_j|| \leq z_j$, then $|[y_1^{j_1} y_2^{j_2} \cdots y_n^{j_n}]_k| \leq (z^m)_k$.
9. Then $|f_{ik}| \leq \sum_{j_1=0}^N \sum_{j_2=0}^N \cdots \sum_{j_n=0}^N |B_{i,j_1,j_2,\ldots,j_n}|(z^m)_k \leq ||\mathbf{B}_N||(z^m)_k$.
$||\mathbf{f}_k|| \leq ||\mathbf{B}_N||(z^m)_k$ and $||\mathbf{y}_{k+1}|| \leq ||\mathbf{B}_N||(z^m)_k/(k+1) = z_{k+1}$.

Calculation of Error Limit: Transfer of Limit to x.

10. Since $||\mathbf{y}_{k+1}|| \leq z_{k+1}$ and

$$z(t) = \begin{cases} e^{||\mathbf{B}_N||t} & \text{for } m = 1, \\ (1 - Mt)^{-1/(m-1)} & \text{for } m > 1. \end{cases}$$

then the limit on $\mathbf{y}$ is

$$\left| y_i(t) - \sum_{j=0}^{k} y_{ij} t^j \right| \leq \begin{cases} e^{||\mathbf{B}_N||\;|t|} - \sum_{j=0}^{k} z_j |t|^j & \text{for } m = 1, \\ (1 - Mt)^{-1/(m-1)} - \sum_{j=0}^{k} z_j |t|^j & \text{for } m > 1. \end{cases} \tag{7}$$

Since $x_i = c_i y_i(t)$, then the limit on $\mathbf{x}$ is

$$\left\| \mathbf{x}(t) - \sum_{j=0}^{k} \mathbf{x}_j t^j \right\| \leq \begin{cases} ||c|| \left(e^{||\mathbf{B}_N||\;|t|} - \sum_{j=0}^{k} z_j |t|^j \right) & \text{for } m = 1, \\ ||c|| \left((1 - Mt)^{-1/(m-1)} - \sum_{j=0}^{k} z_j |t|^j \right) & \text{for } m > 1. \end{cases} \tag{8}$$

The coefficients z_j are easily calculated iteratively from $z_0 = 1$:

$$z_{k+1} = \left(\frac{(m-1)k + 1}{k + 1} \right) \frac{M}{m - 1} z_k \tag{9}$$

Calculation of Error Limit: A Simpler Bound.

Full error limit:

$$\left\|\mathbf{x}(t) - \sum_{j=0}^{k} \mathbf{x}_j t^j\right\| \le \begin{cases} ||c|| \left(e^{||\mathbf{B}_N||\ |t|} - \sum_{j=0}^{k} z_j |t|^j\right) & \text{for } m = 1, \\ ||c|| \left((1 - Mt)^{-1/(m-1)} - \sum_{j=0}^{k} z_j |t|^j\right) & \text{for } m > 1. \end{cases}$$

Since $((m-1)k+1)(k+1) \le m-1$, a simpler, less tight bound:

$$\left\|\mathbf{x}(t) - \sum_{j=0}^{k} \mathbf{x}_j t^j\right\| \le \frac{||c||\ |Mt|^{k+1}}{1 - |Mt|} \text{ for } m > 1. \tag{10}$$

This is an example of a Cauchy-Kovalevsky error limit.

Algebraic Maclaurin Padé. (P. G. Warne)

1.Get the power series to $O(t^{2N+1})$: $y(t) \approx \sum_{j=0}^{2N} k_j t^j$.
Then the Padé approximation for y is:

$$P_N(t) = \left(\sum_{j=0}^{N} a_j t^j\right) \Bigg/ \left(\sum_{j=0}^{N} b_j t^j\right) = \sum_{j=0}^{2N} k_j t^j \text{ with } b_0 = 1. \quad (11)$$

$$\sum_{j=0}^{2N} k_j t^j \sum_{j=0}^{N} b_j t^j = \sum_{j=0}^{N} a_j t^j = 0 \text{ to } O(t^{2N+1}). \quad (12)$$

2.Terms $N+1$ to $2N+1$ cancel, giving a matrix equation $k_{N+i-j} b_j = -k_{N+j}$.
Solve for b_j by Gaussian Elimination.
3.Cauchy products yield $a_i = \sum_{j=0}^{i} k_{i-j} b_j$.

Padé Error and Time Step. (P. G. Warne)

1.First Padé error term p_{2N+1} from power series

$$\sum_{j=0}^{2N+1} k_j t^j = \left(\sum_{j=0}^{N} a_j t^j\right) \Bigg/ \left(\sum_{j=0}^{N} b_j t^j\right) + p_{2N+1} t^{2N+1} + O(t^{2N+2}). \tag{13}$$

2.Next time step:

$$q \leq \left(\frac{\epsilon h}{|\tilde{w} - w|}\right)^{1/2N} = \left(\frac{\epsilon h}{|p_{2N+1}| h^{2N+1}}\right)^{1/2N}. \tag{14}$$

$$qh = \bar{h} \leq \left(\frac{\epsilon}{p_{2N+1}}\right)^{1/2N}. \tag{15}$$

Warne's Comparison of Errors for $y' = 1 + y^2$ ($\lambda = 1.5$).

Order	Step	Runge-Kutta	Taylor	Padé
4	10	0.0529	0.0761	0.474
	100	$0.106E-5$	$0.226E-6$	$0.182E-6$
	$1E5$	$0.104E-11$	$0.298E-12$	$0.163E-12$
8	10		0.128	0.177
	100		$0.240E-8$	$0.255E-14$
12	1		0.152	0.0902

Continued Fractions and Padé Approximants. Fractional Representation of π.

$$\pi = 3.14159265... \tag{16}$$

$$= 3 + 1/7.062513... \tag{17}$$

$$= 3 + 1/(7 + 1/15.9966...) \approx 3 + 1/(7 + 1/16) \tag{18}$$

$$= 3 + 1/(113/16) = 355/113 = 3.1415929... \tag{19}$$

$$3 + 1/7 = 22/7 = 3.143... \tag{20}$$

Unwinding of $f(x) = 3 - 5x + 7x^2 - 4x^3 + 11x^4$.

$$f(x) = 3\left(1 - \frac{5}{3}x + \frac{7}{3}x^2 - \frac{4}{3}x^3 + \frac{11}{3}x^4\right) = \tag{21}$$

$$= 3/\left(1 + \frac{5}{3}x + \frac{4}{9}x^2 - \frac{49}{27}x^3 - \frac{446}{81}x^4\right) = \tag{22}$$

$$= 3/\left(1 + \frac{5}{3}x\left(1 + \frac{4}{15}x - \frac{49}{45}x^2 - \frac{446}{135}x^3\right)\right) = \tag{23}$$

$$= 3/\left(1 + \frac{5}{3}x/\left(1 - \frac{4}{15}x - \frac{29}{25}x^2 - \frac{338}{125}x^3\right)\right) = \tag{24}$$

$$= 3/\left(1 + \frac{5}{3}x/\left(1 - \frac{4}{15}x\left(1 - \frac{87}{20}x - \frac{507}{50}x^2\right)\right)\right) = \tag{25}$$

$$= 3/\left(1 + \frac{5}{3}x/\left(1 - \frac{4}{15}x/\left(1 + \frac{87}{20}x + \frac{3513}{400}x^2\right)\right)\right) = \tag{26}$$

$$= 3/\left(1 + \frac{5}{3}x/\left(1 - \frac{4}{15}x/\left(1 + \frac{87}{20}x/\left(1 - \frac{1171}{580}x\right)\right)\right)\right) \tag{27}$$

Rewinding of a Polynomial.

When I rewind $f(x)$ I obtain $f(x) =$

$$= 3/\left(1+\frac{5}{3}x/\left(1-\frac{4}{15}x/\left(\left(1+\frac{338}{145}x\right)/\left(1-\frac{1171}{580}x\right)\right)\right)\right) = \tag{28}$$

$$= 3/\left(1+\frac{5}{3}x/\left(1+\left(-\frac{4}{15}x+\frac{1171}{2175}x^2\right)/\left(1+\frac{338}{145}x\right)\right)\right) = \tag{29}$$

$$= 3/\left(1+\frac{5}{3}x/\left(\left(1+\frac{898}{435}x+\frac{1171}{2175}x^2\right)/\left(1+\frac{338}{145}x\right)\right)\right) = \tag{30}$$

$$= 3/\left(1+\left(\frac{5}{3}x+\frac{338}{87}x^2\right)/\left(1+\frac{898}{435}x+\frac{1171}{2175}x^2\right)\right) = \tag{31}$$

$$= 3/\left(\left(1+\frac{541}{145}x+\frac{3207}{725}x^2\right)/\left(1+\frac{898}{435}x+\frac{1171}{2175}x^2\right)\right) = \tag{32}$$

$$= 3\left(1+\frac{898}{435}x+\frac{1171}{2175}x^2\right)/\left(1+\frac{541}{145}x+\frac{3207}{725}x^2\right) \tag{33}$$

Truncation of Original Series.

Suppose that I had applied the Padé Approximant to the first 3 terms of

$$f(x) = 3 - 5x + 7x^2 - 4x^3 + 11x^4. \tag{34}$$

Then the unwinding would have stopped at

$$g(x) = 3/\left(1 + \frac{5}{3}x/\left(1 - \frac{4}{15}x\right)\right). \tag{35}$$

Rewinding yields

$$g(x) = 3\left(1 - \frac{4}{15}x\right)/\left(1 + \frac{7}{5}x\right). \tag{36}$$

In unwinding above, the next term divides $\frac{-4}{15}x$ by $(1 + \frac{87}{20}x)$. Upon rewinding, every term is multiplied by $(1 + \frac{87}{20}x)$ except $\frac{-4}{15}$ of x. $g'(x) =$

$$= \frac{3\left(\left(1 + \frac{87}{20}x\right) - \frac{4}{15}x\right)}{\left(1 + \frac{87}{20}x\right) + \left(\frac{7}{5} + \frac{4}{15}\right)x\left(1 + \frac{87}{20}x\right) - \frac{4}{15}x} \tag{37}$$

$$= 3\left(1 + \frac{49}{12}x\right)/\left(1 + \frac{23}{4}x + \frac{29}{4}x^2\right) \tag{38}$$

Restoration of Padé Approximant.

$$g'(x) = 3\left(1 + \frac{49}{12}x\right) / \left(1 + \frac{23}{4}x + \frac{29}{4}x^2\right) \tag{39}$$

The next term multiplies every term by $(1 - \frac{1171}{580}x)$ except $\frac{87}{20}$ of x and $(\frac{5}{3})(\frac{87}{20})$ of x^2. $g''(x) =$

$$\frac{3\left(\left(1 - \frac{1171}{580}x\right) + \left(\frac{49}{12} - \frac{87}{20}\right)x\left(1 - \frac{1171}{580}x\right) + \frac{87}{20}x\right)}{\left(1 - \frac{1171}{580}x\right) + \left(\frac{23}{4} - \frac{87}{20}\right)x\left(1 - \frac{1171}{580}x\right) + \frac{87}{20}x + \frac{29}{4}x^2} \tag{40}$$

$$= 3\left(1 + \frac{898}{435}x + \frac{1171}{2175}x^2\right) / \left(1 + \frac{541}{145}x + \frac{3207}{725}x^2\right) \tag{41}$$

$$= f(x) \tag{42}$$

Small Terms.

$$1 + \epsilon/b = (b + \epsilon)/b \approx b/b \tag{43}$$

Separate terms by order of magnitude.
Separate different powers of parameters.

1)PS Expansions, Padé Approximants, and Poles.

PS Expansion: $e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{3!}x^3 + \frac{1}{4!}x^4 + \frac{1}{5!}x^5 + ...$
Padé Approximant: $e^x_{2/2} = (12 + 6x + x^2)/(12 - 6x + x^2)$

Pole: $z = \frac{1}{a}\left(\frac{1}{t/a-1}\right) = \frac{-1}{a}\left(1 + \frac{t}{a} + \left(\frac{t}{a}\right)^2 + ...\right)$

2)Preparation of a Test Case: Oscillation and Pole.

1) $y = t\sin\left(\frac{1}{t}\right) + \frac{1}{t}$.
2) $y = (t-a)\sin\left(\frac{1}{t-a}\right) + \frac{1}{t-a}$ to expand around $t = 0$.

3) $z = \frac{1}{t-a}$. $x = \sin(z)$. $x_{,t} = z_{,t}\cos(z)$.
4) $\left(\frac{x_{,t}}{z_{,t}}\right)^2 + x^2 = 1$. $(x_{,t})^2 + x^2(z_{,t})^2 = (z_{,t})^2$.
5) $y = (t-a)x + z$.

6) In MS Excel, I show $y = (t-2)\sin\left(\frac{20}{t-2}\right) + \frac{1}{(t-2)}$.

3)PS Expansions for $z = 1/(t-a)$ and $x = \sin(z)$.

1) $z = \frac{1}{a}\left(\frac{1}{t/a-1}\right) = \frac{-1}{a}\left(1 + \frac{t}{a} + \left(\frac{t}{a}\right)^2 + \left(\frac{t}{a}\right)^3 + \ldots\right) =$
$= \frac{-1}{a}\left(1 + \frac{t}{a}\right)\left(1 + \left(\frac{t}{a}\right)^2\right)\left(1 + \left(\frac{t}{a}\right)^4\right)\cdots$

2) $z_{,t} = \frac{-1}{a^2}\left(1 + 2\frac{t}{a} + 3\left(\frac{t}{a}\right)^2 + 4\left(\frac{t}{a}\right)^3 + \ldots\right)$.

3) $z_{,t}^2 = \frac{1}{a^4}\left(1 + 4\frac{t}{a} + 10\left(\frac{t}{a}\right)^2 + 20\left(\frac{t}{a}\right)^3 + \ldots\right)$.

4) $(x_{,t})^2 + x^2(z_{,t})^2 = (z_{,t})^2$.

5) $x = x_0 + x_1 t + x_2 t^2 + x_3 t^3 + x_4 t^4 + \ldots$

6) $x_{,t} = x_1 + 2x_2 t + 3x_3 t^2 + 4x_4 t^3 + \ldots$

7) $(x_{,t})^2 = x_1^2 + 4x_1x_2 + (6x_1x_3 + 4x_2^2)t^2 + (8x_1x_4 + 12x_2x_3)t^3 + \ldots$

8) $x^2 = x_0^2 + 2x_0x_tt + (2x_0x_2 + x_1^2)t^2 + (2x_0x_3 + 2x_1x_2)t^3 + \ldots$

9) $x^2(z_{,t})^2 = \frac{1}{a^4}\left(x_0^2 + \left(2x_0x_1 + \frac{4x_0}{a}\right)t + \left(2x_0x_2 + x_1^2 + \frac{8x_0x_1}{a} + \frac{10x_0}{a^2}\right)t^2 + \right.$
$\left. + \left(2x_0x_3 + 2x_1x_2 + \frac{8x_0x_2}{a} + \frac{x_1^2}{a^2} + \frac{20x_0x_1}{a^2} + \frac{20x_0}{a^3}\right)t^3 + \ldots\right)$

4)Change of Variable to Locate a Pole.

1) $z = 1/(t-a)$. $z,_t = -1/(t-a)^2 = -z^2$.
2) $x,_t = x,_z\, z,_t = -z^2 x,_z$.
3) $(x,_t)^2 + x^2(z,_t)^2 = (z,_t)^2$ becomes $x,_z^2 + x^2 = 1$.
4) $x = \sin(z - z_0)$ in $y = (t-a)x + z$ gives $y = \sin(z - z_0)/z + z$.

5)High Powers of Poles.

At high order any pole seems first power.

1) $(1-ax)^{-p} = 1 + pax + \frac{p(p+1)}{2!}a^2x^2 + \frac{p(p+1)(p+2)}{3!}a^3x^3 + ...$

Suppose b_n is the coefficient for term n.

Then $r \equiv b_n^2/(b_{(n-1)}b_{(n+1)})$ depends on power p and not a.

2) $\frac{b_n}{b_{n+1}} = \frac{n+1}{(p+n)a}$.

3) $r = \frac{b_n^2}{b_{(n-1)}b_{(n+1)}} = \frac{(p+n-1)(n+1)}{(p+n)n}$.

4) $p = \frac{n^2-1-n^2r}{-n-1+nr} = \frac{n^2(1-r)-1}{n(-1+r)-1}$.

5) $\lim_{n \to \infty} \frac{b_n}{b_{n+1}} = \lim_{n \to \infty} \frac{n+1}{(p+n)a} \approx \frac{1}{a}$.

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