Pade Approximant

Pade approximant (also known as **rational function approximation**) can be used to approximate both analytic function or empirical data. Pade approximant can often give better convergence than Taylor series. Sometimes, Taylor series is divergent, which will become convergent using Pade approximant. Lets firstly consider the approximation of analytic function, in most of the cases, N > M, and both of them are around 5 to 6.

$$\sum_{k=0}^{K} c_k x^k = f(x) \quad \text{where } c_k = \frac{1}{k!}\left.\frac{d^k f(x)}{dx^k}\right|_{x=0} \quad \text{Taylor series at } x=0$$

$$\frac{\sum_{n=0}^{N} a_n x^n}{\sum_{m=0}^{M} b_m x^m} = f(x) \quad \text{where } b_0 = 1 \quad \text{Pade approximant at } x=0$$

$$\frac{\sum_{n=0}^{N} a_n x^n}{\sum_{m=0}^{M} b_m x^m} = \sum_{k=0}^{K} c_k x^k \quad \text{where } K = N+M$$

$$\sum_{n=0}^{N} a_n x^n = \left(\sum_{k=0}^{K} c_k x^k\right)\left(\sum_{m=0}^{M} b_m x^m\right)$$

There are N+1 coefficients for a, M+1 coefficients for b (including $b_0 = 1$) and N+M+1 = K+1 coeficients for c. In order to find the Pade approximant's coefficients, we need to match the function value on both sides of equation 1 at x = 0, and the first K derivative values of both sides of equation 1 at x = 0.

Lets take derivative of LHS of equation 1, we have **property 1**.

$$\frac{d^1}{dx^1}\sum_{n=0}^{N} a_n x^n = \sum_{n=1}^{N} a_n n x^{n-1} \qquad \left.\frac{d^1}{dx^1}\sum_{n=0}^{N} a_n x^n\right|_{x=0} = a_1$$

$$\frac{d^2}{dx^2}\sum_{n=0}^{N} a_n x^n = \sum_{n=2}^{N} a_n n(n-1) x^{n-2} \qquad \left.\frac{d^2}{dx^2}\sum_{n=0}^{N} a_n x^n\right|_{x=0} = 2!a_2$$

$$\frac{d^3}{dx^3}\sum_{n=0}^{N} a_n x^n = \sum_{n=3}^{N} a_n n(n-1)(n-2) x^{n-3} \qquad \left.\frac{d^3}{dx^3}\sum_{n=0}^{N} a_n x^n\right|_{x=0} = 3!a_3$$

$$\ldots \qquad \ldots$$

$$\frac{d^L}{dx^L}\sum_{n=0}^{N} a_n x^n = \sum_{n=L}^{N} a_n \frac{n!}{(n-L)!} x^{n-L} \qquad \left.\frac{d^L}{dx^L}\sum_{n=0}^{N} a_n x^n\right|_{x=0} = L!a_L$$

$$\ldots \qquad \ldots$$

$$\frac{d^{N-1}}{dx^{N-1}}\sum_{n=0}^{N} a_n x^n = a_{N-1}(N-1)! + a_N N! x \qquad \left.\frac{d^{N-1}}{dx^{N-1}}\sum_{n=0}^{N} a_n x^n\right|_{x=0} = a_{N-1}(N-1)!$$

$$\frac{d^N}{dx^N}\sum_{n=0}^{N} a_n x^n = a_N N! \qquad \left.\frac{d^N}{dx^N}\sum_{n=0}^{N} a_n x^n\right|_{x=0} = a_N N!$$

$$\frac{d^{N+1}}{dx^{N+1}}\sum_{n=0}^{N} a_n x^n = 0 \qquad \left.\frac{d^{N+1}}{dx^{N+1}}\sum_{n=0}^{N} a_n x^n\right|_{x=0} = 0$$

Lets take derivative of RHS of equation 1, we have **property 2**.

$$\frac{d^1}{dx^1}(fg) = \frac{d^1 f}{dx^1} g + f \frac{d^1 g}{dx^1}$$

$$\frac{d^2}{dx^2}(fg) = \frac{d^2 f}{dx^2} g + \frac{d^1 f}{dx^1}\frac{d^1 g}{dx^1} + \frac{d^1 f}{dx^1}\frac{d^1 g}{dx^1} + f\frac{d^2 g}{dx^2} = \frac{d^2 f}{dx^2} g + 2\frac{d^1 f}{dx^1}\frac{d^1 g}{dx^1} + f\frac{d^2 g}{dx^2}$$

$$\frac{d^3}{dx^3}(fg) = \frac{d^3 f}{dx^3} g + \frac{d^2 f}{dx^2}\frac{d^1 g}{dx^1} + 2\frac{d^2 f}{dx^2}\frac{d^1 g}{dx^1} + 2\frac{d^1 f}{dx^1}\frac{d^2 g}{dx^2} + \frac{d^1 f}{dx^1}\frac{d^2 g}{dx^2} + f\frac{d^3 g}{dx^3} = \frac{d^3 f}{dx^3} g + 3\frac{d^2 f}{dx^2}\frac{d^1 g}{dx^1} + 3\frac{d^1 f}{dx^1}\frac{d^2 g}{dx^2} + f\frac{d^3 g}{dx^3}$$

$$\frac{d^L}{dx^L}(fg) = \sum_{l=0}^{L} C_l^L \frac{d^{L-l} f}{dx^{L-l}}\frac{d^l g}{dx^l}$$

$$\frac{d^L}{dx^L}(\textstyle\sum_{k=0}^{K} c_k x^k)(\sum_{m=0}^{M} b_m x^m)\Big|_{x=0}$$

$$= \sum_{l=0}^{L}\left[C_l^L \times \frac{d^{L-l}(\sum_{k=0}^{K} c_k x^k)}{dx^{L-l}}\bigg|_{x=0} \times \frac{d^{l}(\sum_{m=0}^{M} b_m x^m)}{dx^{l}}\bigg|_{x=0}\right]$$

where $K > M, K = M + N$

$$= \sum_{l=0}^{L}\Big[C_l^L \times \big[(L-l)!c_{L-l}\, boxcar(0,K;L-l)\big]\times\big[l!b_l\, boxcar(0,M;l)\big]\Big]$$

where $boxcar(x_0,x_1,x) = \begin{bmatrix} 1 & if & x_0 \le x \le x_1 \\ 0 & if & (x < x_0)\cup(x > x_1) \end{bmatrix}$

$$= \sum_{l=0}^{L}\big[L!c_{L-l}b_l \times boxcar(\max(0,L-K),\min(M,L);l)\big]$$

see remark 1 and remark 2

$$= \sum_{l=\max(0,L-K)}^{\min(M,L)}\big[L!c_{L-l}b_l\big]$$

This is property 2.

Remark 1	$boxcar(0,K;L-l)\times boxcar(0,M;l)$	$\Leftrightarrow$	$(L-l\ge 0)\cap(L-l\le K)\cap(l\ge 0)\cap(l\le M)$
		$\Leftrightarrow$	$(L\ge l)\cap(L-K\le l)\cap(l\ge 0)\cap(l\le M)$
		$\Leftrightarrow$	$(l\ge 0)\cap(l\ge L-K)\cap(l\le M)\cap(l\le L)$
		$\Leftrightarrow$	$(l\ge \max(0,L-K))\cap(l\le \min(M,L))$
		$\Leftrightarrow$	$boxcar(\max(0,L-K),\min(M,L))$
Remark 2	$C_l^L\times(L-l)!l! \;=\; \frac{L!}{(L-l)!l!}\times(L-l)!l! \;=\; L!$		

<u>Suppose N > M</u>, we have :

	LHS		RHS				
0th	a_0	=	$\sum_{l=\max(0,0-K)}^{\min(M,0)}[0!c_{0-l}b_l]$	=	$\sum_{l=0}^{0}[0!c_{0-l}b_l]$	=	c_0b_0
1st	$1!a_1$	=	$\sum_{l=\max(0,1-K)}^{\min(M,1)}[1!c_{1-l}b_l]$	=	$\sum_{l=0}^{1}[1!c_{1-l}b_l]$	=	$1!(c_1b_0+c_0b_1)$
2nd	$2!a_2$	=	$\sum_{l=\max(0,2-K)}^{\min(M,2)}[2!c_{2-l}b_l]$	=	$\sum_{l=0}^{2}[2!c_{2-l}b_l]$	=	$2!(c_2b_0+c_1b_1+c_0b_2)$
3rd	$3!a_3$	=	$\sum_{l=\max(0,3-K)}^{\min(M,3)}[3!c_{3-l}b_l]$	=	$\sum_{l=0}^{3}[3!c_{3-l}b_l]$	=	$3!(c_3b_0+c_2b_1+c_1b_2+c_0b_3)$
…	…		…				
M-1th	$(M-1)!a_{M-1}$	=	$\sum_{l=\max(0,M-1-K)}^{\min(M,M-1)}[(M-1)!c_{M-1-l}b_l]$			=	$\sum_{l=0}^{M-1}[(M-1)!c_{M-1-l}b_l]$
Mth	$M!a_M$	=	$\sum_{l=\max(0,M-K)}^{\min(M,M)}[M!c_{M-l}b_l]$			=	$\sum_{l=0}^{M}[M!c_{M-l}b_l]$
M+1th	$(M+1)!a_{M+1}$	=	$\sum_{l=\max(0,M+1-K)}^{\min(M,M+1)}[(M+1)!c_{M+1-l}b_l]$			=	$\sum_{l=0}^{M}[(M+1)!c_{M+1-l}b_l]$
M+2th	$(M+2)!a_{M+2}$	=	$\sum_{l=\max(0,M+2-K)}^{\min(M,M+2)}[(M+2)!c_{M+2-l}b_l]$			=	$\sum_{l=0}^{M}[(M+2)!c_{M+2-l}b_l]$
…	…		…				
N-1th	$(N-1)!a_{N-1}$	=	$\sum_{l=\max(0,N-1-K)}^{\min(M,N-1)}[(N-1)!c_{N-1-l}b_l]$			=	$\sum_{l=0}^{M}[(N-1)!c_{N-1-l}b_l]$
Nth	$N!a_N$	=	$\sum_{l=\max(0,N-K)}^{\min(M,N)}[N!c_{N-l}b_l]$			=	$\sum_{l=0}^{M}[N!c_{N-l}b_l]$
N+1th	0	=	$\sum_{l=\max(0,N+1-K)}^{\min(M,N+1)}[(N+1)!c_{N+1-l}b_l]$			=	$\sum_{l=0}^{M}[(N+1)!c_{N+1-l}b_l]$
N+2th	0	=	$\sum_{l=\max(0,N+2-K)}^{\min(M,N+2)}[(N+2)!c_{N+2-l}b_l]$			=	$\sum_{l=0}^{M}[(N+2)!c_{N+2-l}b_l]$
…	…		…				
N+M -1th	0	=	$\sum_{l=\max(0,N+M-1)}^{\min(M,N+M-1)}[(N+M-1)!c_{N+M-1-l}b_l]$			=	$\sum_{l=0}^{M}[(N+M-1)!c_{N+M+1-l}b_l]$
N+Mth	0	=	$\sum_{l=\max(0,N+M)}^{\min(M,N+M)}[(N+M)!c_{N+M-l}b_l]$			=	$\sum_{l=0}^{M}[(N+M)!c_{N+M-l}b_l]$

There are N+M+1 = K+1 equations in total. N+1 of them on LHS are non zero (i.e. M of them on LHS are zero), M of them on RHS are sums of less than M+1 terms, N+1 of them on RHS are sums of exactly M+1 terms. By dividing both sides of all the above equations by the corresponding factorials, we have the matrix in the next page. The solution for Pade approximant is then a 2 steps approach : (1) solve the lower M equations for all M 'b' coefficients (note : there are M+1 b coefficients, including **b_0 = 1**), then (2) solve the upper N+1 equations for all N+1 'a' coefficients (note : all c coefficients are known, they are different derivatives of the analytic function that we want to approximate).

0th	a_0	=	$c_0 b_0$
1st	a_1	=	$c_1 b_0 + c_0 b_1$
2nd	a_2	=	$c_2 b_0 + c_1 b_1 + c_0 b_2$
3rd	a_3	=	$c_3 b_0 + c_2 b_1 + c_1 b_2 + c_0 b_3$
…	…		…
M-1th	a_{M-1}	=	$\sum_{l=0}^{M-1} c_{M-1-l} b_l$
Mth	a_M	=	$\sum_{l=0}^{M} c_{M-l} b_l$
M+1th	a_{M+1}	=	$\sum_{l=0}^{M} c_{M+1-l} b_l$
M+2th	a_{M+2}	=	$\sum_{l=0}^{M} c_{M+2-l} b_l$
…	…		…
N-1th	a_{N-1}	=	$\sum_{l=0}^{M} c_{N-1-l} b_l$
Nth	a_N	=	$\sum_{l=0}^{M} c_{N-l} b_l$
N+1th	0	=	$\sum_{l=0}^{M} c_{N+1-l} b_l$
N+2th	0	=	$\sum_{l=0}^{M} c_{N+2-l} b_l$
…	…		…
N+M-1th	0	=	$\sum_{l=0}^{M} c_{N+M+1-l} b_l$
N+Mth	0	=	$\sum_{l=0}^{M} c_{N+M-l} b_l$

In matrix form :

$$A = CB$$

$$A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}_{(N+M+1)\times 1} \qquad C = \begin{bmatrix} C_1 \\ C_2 \end{bmatrix}_{(N+M+1)\times(M+1)} \qquad B = \begin{bmatrix} b_0 \\ b_1 \\ \dots \\ b_M \end{bmatrix}_{(M+1)\times 1}$$

$$A_1 = \begin{bmatrix} a_0 \\ a_1 \\ \dots \\ a_N \end{bmatrix}_{(N+1)\times 1} \qquad C_1 = \begin{bmatrix} C_{11} \\ C_{12} \end{bmatrix}_{(N+1)\times(M+1)}$$

$$A_2 = \begin{bmatrix} 0 \\ 0 \\ \dots \\ 0 \end{bmatrix}_{M\times 1} \qquad C_{11} = \begin{bmatrix} c_0 & 0 & 0 & \dots & 0 \\ c_1 & c_0 & & \dots & \\ c_2 & c_1 & c_0 & \dots & \\ \dots & \dots & \dots & \dots & \dots \\ c_M & c_{M-1} & c_{M-2} & \dots & c_0 \end{bmatrix}_{(M+1)\times(M+1)}$$

$$C_{12} = \begin{bmatrix} c_{M+1} & c_M & c_{M-1} & \dots & c_1 \\ c_{M+2} & c_{M+1} & c_M & \dots & c_2 \\ c_{M+3} & c_{M+2} & c_{M+1} & \dots & c_3 \\ \dots & \dots & \dots & \dots & \dots \\ c_N & c_{N-1} & c_{N-2} & \dots & c_{N-M} \end{bmatrix}_{(N-M)\times(M+1)}$$

$$C_2 = \begin{bmatrix} c_{N+1} & c_N & c_{N-1} & \dots & c_{N-M+1} \\ c_{N+2} & c_{N+1} & c_N & \dots & c_{N-M+2} \\ c_{N+3} & c_{N+2} & c_{N+1} & \dots & c_{N-M+3} \\ \dots & \dots & \dots & \dots & \dots \\ c_{N+M} & c_{N+M-1} & c_{N+M-2} & \dots & c_N \end{bmatrix}_{M\times(M+1)}$$

The solution is :

$$B = C_2^{-1} A_2$$ (using either LU decomposition or Cholesky decomposition)

$$A_1 = C_1 B$$

We have derive the solution for the case when N < M. The result is very similar.