Supplements to Mathematical Methods in Science and Engineering
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CHAPTER 15: INFINITE SERIES

Frequently we encounter integrals that can not be evaluated exactly. Even though nowadays modern computers can be used to evaluate almost any integral numerically, methods for obtaining approximate expressions of various types of integrals remain extremely useful. Having an approximate yet an analytic expression for a given integral, not only allows us to push further with the analytic approach, but also helps us to understand and interpret the results better. In this regard, in Bayin (2006) we have introduced the asymptotic series. We now introduce two more useful methods for obtaining approximate values of integrals, that is, the method of steepest descent and the saddle-point integrals. They are both closely related to the asymptotic series.

I. Method of Steepest Descent

Consider the integral

$$I = \int_{x_1}^{x_2} dx\; F(x), \tag{0.1}$$

where the range could be infinite. We now write I as

$$I = \int_{x_1}^{x_2} dx\; e^{f(x)}, \tag{0.2}$$

where $f(x)$ is defined as

$$f(x) = \ln[F(x)]. \tag{0.3}$$

If $f(x)$ has a steep maximum at x_0, where

$$f'(x_0) = \frac{1}{F(x_0)} F'(x_0) = 0 \tag{0.4}$$

and

$$F''(x_0) < 0, \tag{0.5}$$

we can approximate $f(x)$ in the neighborhood of x_0 by taking only the first two nonzero terms of the Taylor series:

$$f(x) = f(x_0) + \ f'(x_0)(x - x_0) + \frac{1}{2!}\ f''(x_0)(x - x_0)^2 + \cdots , \tag{0.6}$$

as

$$f(x) \simeq f(x_0) + \frac{1}{2!}\ f''(x_0)(x - x_0)^2. \tag{0.7}$$

If the range includes the point x_0, we can write I as

$$\begin{aligned} I &= \int_{x_1}^{x_2} dx\ F(x) && (0.8) \\ &= \int_{x_1}^{x_2} dx\ e^{f(x)} && (0.9) \\ &\simeq \int_{x_1}^{x_2} dx\ \exp\left[f(x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2\right] && (0.10) \\ &\simeq F(x_0) \int_{x_1}^{x_2} dx\ e^{-\frac{1}{2}\left|f''(x_0)\right|(x-x_0)^2}. && (0.11) \end{aligned}$$

If the end points do not contribute to the integral significantly, we can replace I with

$$I \simeq F(x_0) \int_{-\infty}^{\infty} dx\ e^{-\frac{1}{2}\left|f''(x_0)\right|(x-x_0)^2}, \tag{0.12}$$

where the integrand,

$$e^{-\frac{1}{2}\left|f''(x_0)\right|(x-x_0)^2}, \tag{0.13}$$

is a Gaussian as shown in Figure (0.1). We can now evaluate the integral in Equation (0.12) to obtain the approximate expression

$$I \simeq \sqrt{\frac{2\pi}{|f''(x_0)|}}\ F(x_0). \tag{0.14}$$

1. Evaluate the integral

$$\Gamma(x + 1) = \int_0^{\infty} t^x e^{-t} dt \tag{0.15}$$

for large x.

Solution:

We first rewrite the integrand as

$$\begin{aligned} F(x;t) &= e^{f(x;t)} && (0.16) \\ &= t^x e^{-t} = e^{x \ln t - t}, && (0.17) \end{aligned}$$

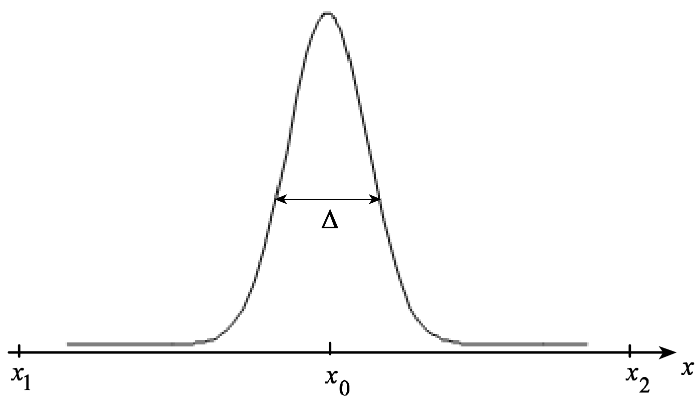

Fig. 0.1 In one dimension the method of steepest descent allows us to approximate the integrand in Equation (0.1), $F(x)$, that has a high maximum at x_0, with a Gaussian, $F(x_0)e^{-\frac{1}{2}|f''(x_0)|(x-x_0)^2}$, where the width, Δ, is $\Delta \propto 1/\sqrt{|f'(x_0)|}$ and $f(x) = \ln[F(x)]$.

hence determine $f(x,t)$ as

$$f(x;t) = x \ln t - t. \tag{0.18}$$

Evaluating the first two derivatives with respect to t:

$$f'(x;t) = \frac{x}{t} - 1, \tag{0.19}$$

$$f''(x;t) = -\frac{x}{t^2}, \tag{0.20}$$

we see that the maximum of $f(x;t)$ is located at $t = x$. Finally, using Equation (0.14) we obtain the approximate value of $\Gamma(x+1)$ as

$$\Gamma(x+1) \simeq \sqrt{2\pi x}x^x e^{-x}, \tag{0.21}$$

which is good for large x. When x is an integer, n, this is nothing but the Stirling's approximation of the factorial $n!$.

Important:

ii) Note that the large x condition assures us that the coefficient of the third order term in the Taylor series expansion about $t = x$:

$$f(x;t) = f(x;x) + \frac{1}{2!}\, f''(x;x)(t-x)^2 + \frac{1}{3!} f'''(x;x)(t-x)^3 + \cdots, \tag{0.22}$$

is negligible for t values near x. That is,

$$\left| \frac{1}{3!} f'''(x;x)(t-x)^3 / \frac{1}{2!} f''(x;x)(t-x)^2 \right| = \frac{2}{3} \left| \frac{t-x}{x} \right| \ll 1. \tag{0.23}$$

ii) The approximate formula we have obtained in Equation (0.21) is nothing but the first term in the asymptotic expansion of $\Gamma(x+1)$:

$$n! = \sqrt{2\pi n}\, n^n e^{-n} \left(1 + \frac{1}{12n} + \frac{1}{288n^2} + \cdots \right). \tag{0.24}$$

iii) A Series expansion of the integrand in Equation (0.15) would not be useful.

II. Saddle-Point Integrals

In general, the method of steepest descent is applicable to contour integrals of the form

$$I(\alpha) = \int_C F(z)\, dz \tag{0.25}$$

$$= \int_C e^{\alpha f(z)}\, dz, \tag{0.26}$$

where α is large and positive and C is a path in the complex plane where the end points do not contribute significantly to the integral. The method of steepest descent works if the function, $f(z)$, has a maximum at some point z_0 on the contour. However, if the function is analytic, we can always deform the contour so that it passes through the point z_0 without altering the value of the integral.

From the theory of complex functions (Chapter 12) we know that the real and the imaginary parts, u and v, of an analytic function,

$$f(z) = u(x,y) + iv(x,y), \tag{0.27}$$

satisfy the Laplace's equation. That is,

$$\nabla^2 u(x,y) = 0 \tag{0.28}$$

and

$$\nabla^2 v(x,y) = 0. \tag{0.29}$$

From Equation (0.28) it is seen that if

$$\frac{\partial^2 u}{\partial x^2} < 0, \tag{0.30}$$

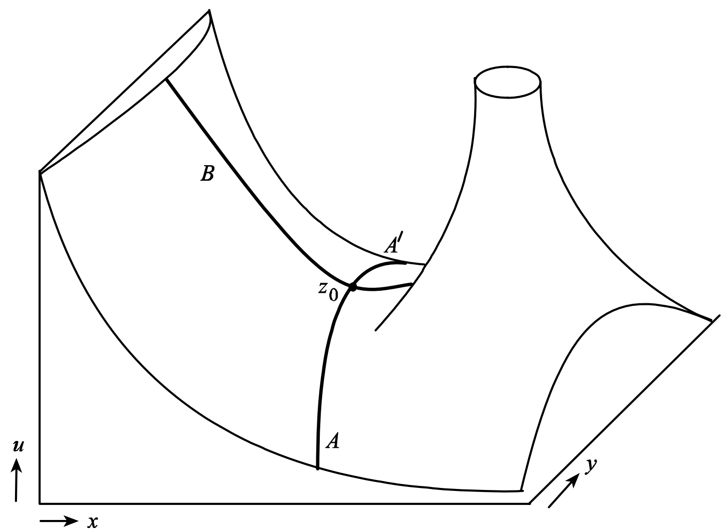

Fig. 0.2 The path AA' is the path that follows the steepest descent. The path B is perpendicular to AA', hence it follows the ridges.

then

$$\frac{\partial^2 u}{\partial y^2} > 0. \tag{0.31}$$

Same conclusion also holds for $v(x, y)$. Using Theorem (1.4) in pg.18 of Bayin (2008), we conclude that the point z_0 that satisfies

$$\left.\frac{\partial u}{\partial x}\right|_{z_0} = \left.\frac{\partial u}{\partial y}\right|_{z_0} = 0 \tag{0.32}$$

must be a saddle point of the surface $u(x, y)$, where the surface looks like a saddle or a mountain pass (Fig. 0.2). By the Cauchy-Riemann conditions we also infer that at z_0

$$\left.\frac{\partial v}{\partial x}\right|_{z_0} = \left.\frac{\partial v}{\partial y}\right|_{z_0} = 0, \tag{0.33}$$

hence

$$\frac{df(z_0)}{dz} = 0. \tag{0.34}$$

In other words, a saddle point of $u(x, y)$ is also a saddle point of $v(x, y)$.

About the saddle point we can write the Taylor series

$$f(z) = f(z_0) + \frac{1}{2!}f''(z_0)(z - z_0)^2 + \frac{1}{3!}f'''(z_0)(z - z_0)^2 + \cdots$$

and for points on the contour near the saddle point we can use the approximation

$$f(z) \simeq f(z_0) + \frac{1}{2} f''(z_0)(z - z_0)^2. \tag{0.35}$$

Using polar representations of $f''(z_0)$ and $(z - z_0)$:

$$f''(z_0) = \rho_0 e^{i\phi_0}, \tag{0.36}$$

$$(z - z_0) = re^{i\theta}, \tag{0.37}$$

where z is a point on the contour, we can approximate the integral $I(\alpha)$ [Eq. (0.25)]by

$$I(\alpha) \simeq \int_{C'} dz\ e^{\alpha[f(z_0)+\frac{1}{2}f''(z_0)(z-z_0)^2]} \tag{0.38}$$

$$\simeq \int_{C'} dr\ e^{i\theta} e^{\alpha[f(z_0)+\frac{1}{2}\rho_0 e^{i\phi_0} r^2 e^{i2\theta}]} \tag{0.39}$$

$$\simeq e^{\alpha f(z_0)} \int_{C'} dr\ e^{i\theta} e^{\alpha \frac{1}{2}\rho_0 r^2 e^{i(\phi_0+2\theta)}} \tag{0.40}$$

$$\simeq e^{\alpha f(z_0)} \int_{C'} dr\ e^{i\theta} e^{\alpha \frac{1}{2}\rho_0 r^2 [\cos(\phi_0+2\theta)+i\sin(\phi_0+2\theta)]}, \tag{0.41}$$

where C' is now a contour that passes through the saddle point z_0. We are now looking for directions, θ values, that allow us to approximate the value of this integral only by using the values of $f(z)$ in the neighborhood of z_0. Note that for points near the saddle point the surface is nearly flat, hence θ varies very slowly, hence we have written

$$dz \simeq dr\ e^{i\theta}. \tag{0.42}$$

We can also take $e^{i\theta}$ outside the integral sign to write

$$I(\alpha) \simeq e^{\alpha f(z_0)}\ e^{i\theta} \int_{C'} dr\ e^{\alpha \frac{1}{2}\rho_0 r^2 [\cos(\phi_0+2\theta)+i\sin(\phi_0+2\theta)]}. \tag{0.43}$$

The integrand has two factors:

$$e^{\alpha \frac{1}{2}\rho_0 r^2 [\cos(\phi_0+2\theta)\ ]} \tag{0.44}$$

and

$$e^{i\alpha \frac{1}{2}\rho_0 r^2 [\sin(\phi_0+2\theta)\ ]}. \tag{0.45}$$

The first factor is an exponential, which could be decaying or growing depending on the sign of the cosine, while the second factor oscillates wildly for large α. For this method to work effectively, we have to pick a direction that makes the exponential decay in the fastest possible way, thus justifying the name steepest-descent, while suppressing the effect the wildly fluctuating second factor. From the following table, we see that the paths that follow the steepest descent from the saddle point, z_0, are the ones that follow the directions that make $\cos(\phi_0 + 2\theta) = -1$. Since for these paths $\sin(\phi_0 + 2\theta) = 0$, they also eliminate the concerns caused by the wildly fluctuating second factor. If we take $(\phi_0 + 2\theta) = \pi$, the direction that we have to follow becomes

$$\theta = -\frac{\phi_0}{2} + \frac{\pi}{2}, \tag{0.46}$$

where ϕ_0 is determined from Equation (0.36).

Choice of angles in the saddle-point method:

$(\phi_0 + 2\theta)$	$[\cos(\phi_0 + 2\theta) + i\sin(\phi_0 + 2\theta)]$	θ
0	$+1$	$-\frac{\phi_0}{2}$
π	-1	$-\frac{\phi_0}{2} + \frac{\pi}{2}$
2π	$+1$	$-\frac{\phi_0}{2} + +\pi$
3π	-1	$-\frac{\phi_0}{2} + \frac{3\pi}{2}$
4π	$+1$	$-\frac{\phi_0}{2} + +2\pi$

Every time we change θ, that is, the direction that we start moving at z_0, by $\pi/2$, the quantity

$$[\cos(\phi_0 + 2\theta) + i\sin(\phi_0 + 2\theta)] \tag{0.47}$$

changes its value from $+1$ to -1. Depending on which direction we are passing through the saddle point, the directions that correspond to the steepest descent are given as

$$\theta = -\frac{\phi_0}{2} \pm \frac{\pi}{2}. \tag{0.48}$$

For these directions the integrand in Equation (0.43) is a Gaussian, hence for large positive α only the points very close to z_0 contribute to the integral. The directions perpendicular to these follow the ridges and give rise to exponentially increasing functions in Equation (0.43). Any direction in between will compromise the advantages of this method. Keep in mind that usually this method gives the first term in the asymptotic expansion of $I(\alpha)$ for large α. To chose the correct sign in Equation (0.48) we need to look at the topography more carefully and see which way to deform the contour. For example, for $\phi_0 = \pi/2$, in Figure (0.3) we show two possible topographies that require

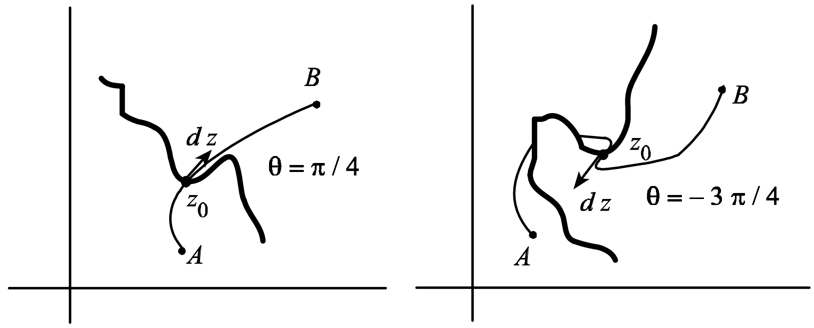

Fig. 0.3 To possible 'mountain ranges': For the one on the left we use + and for the one on the right we use − in Equation (0.48).

the + and the − signs, respectively. In these figures dz is a tangent vector to the path at z_0 pointing in the direction we move.

In the light of these, we now write an approximate expression for $I(\alpha)$ as

$$I(\alpha) \simeq e^{\alpha f(z_0)} \int_{-\infty}^{\infty} e^{-\alpha \frac{1}{2}\rho_0 r^2} e^{i\theta}\, dr \tag{0.49}$$

$$\simeq \sqrt{\frac{2\pi}{\alpha\rho_0}}\, e^{\alpha f(z_0)} e^{i\theta}, \tag{0.50}$$

where θ takes one of the values

$$\theta = -\frac{\phi_0}{2} \pm \frac{\pi}{2} \tag{0.51}$$

and

$$\phi_0 = \tan^{-1}\left[\frac{\operatorname{Im} f''(z_0)}{\operatorname{Re} f''(z_0)}\right]. \tag{0.52}$$

Note that since for large α only points near z_0 contribute to the integral, we have taken the limits in Equation (0.49) as $\pm\infty$.

2. Evaluate $\Gamma(z+1)$ using the definition

$$\Gamma(z) = \int_0^{\infty} e^{-t} t^{z-1}\, dt, \;\; \operatorname{Re} z > 0, \tag{0.53}$$

via the saddle-point method.

Solution:

Using the definition of $\Gamma(z)$ [Eq. (0.53)] we write

$$\Gamma(z+1) = \int_0^{\infty} e^{-t} t^{z}\, dt \tag{0.54}$$

$$= \int_0^{\infty} e^{-t+z\ln t}\, dt. \tag{0.55}$$

Using the polar representation $z = \alpha e^{i\beta}$, we write

$$\Gamma(z+1) = \int_0^\infty \exp\left[\alpha\left(\ln t - \frac{t}{z}\right)e^{i\beta}\right]\ dt \tag{0.56}$$

and compare it with

$$\Gamma(z+1) = \int_0^\infty e^{\alpha f(t)} dt \tag{0.57}$$

to obtain

$$f(t) = \left(\ln t - \frac{t}{z}\right)e^{i\beta}, \tag{0.58}$$

the first two derivatives of which are given as

$$f'(t) = \left(\frac{1}{t} - \frac{1}{z}\right)e^{i\beta} \tag{0.59}$$

and

$$f''(t) = -\frac{1}{t^2}e^{i\beta}. \tag{0.60}$$

Setting the first derivative to zero we obtain the saddle point, t_0, as

$$f'(t_0) = 0 \Rightarrow t_0 = z. \tag{0.61}$$

This gives

$$f(t_0) = (\ln z - 1)e^{i\beta} \tag{0.62}$$

and

$$f''(t_0) = -\frac{e^{i\beta}}{z^2} \tag{0.63}$$

$$= -\frac{1}{\alpha^2}e^{-i\beta}. \tag{0.64}$$

Using the polar representation $f''(t_0) = \rho e^{i\phi_0}$, we obtain

$$\rho = \frac{1}{\alpha^2},\ \phi_0 = \pi - \beta. \tag{0.65}$$

We now have to decide between the two possibilities for θ :

$$\theta = -\frac{\pi - \beta}{2} + \frac{\pi}{2} = \frac{\beta}{2} \tag{0.66}$$

and

$$\theta = -\frac{\pi - \beta}{2} - \frac{\pi}{2} = -\pi + \frac{\beta}{2}. \tag{0.67}$$

In our previous example, where z was real, $\beta = 0$ and $\theta = 0$, it seems that

$$\theta = \frac{\beta}{2} \tag{0.68}$$

is the right choice. This gives the steepest descent approximation of $\Gamma(z+1)$ as

$$\begin{aligned} \Gamma(z+1) &\simeq \sqrt{2\pi\alpha}\; e^{z\ln z - z}\; e^{i\beta/2} && (0.69) \\ &\simeq \sqrt{2\pi}\; z^{z+\frac{1}{2}} e^{-z}. && (0.70) \end{aligned}$$

Even though the integral definition [Eq. (0.54)] is valid for $\operatorname{Re} z > 0$, the above result is good for $|z| \gg 1$, provided that we stay away from the negative real axis where we have a branch cut.

3. Show that the approximate expression for $\Gamma(z+1)$ obtained via the saddle-point method:

$$\Gamma(z+1) = \sqrt{2\pi}\; z^{z+\frac{1}{2}} e^{-z}, \tag{0.71}$$

is only the first term in the asymptotic expansion of $\Gamma(z+1)$.

Solution:

We first write equation (0.70) as

$$\begin{aligned} \Gamma(z) &\simeq \sqrt{2\pi}\; (z-1)^{z-\frac{1}{2}} e^{-(z-1)} && (0.72) \\ &\simeq \sqrt{2\pi} z^{z-\frac{1}{2}} \left(1 - \frac{1}{z}\right)^{z-\frac{1}{2}} e^{-(z-1)} && (0.73) \\ &\simeq \sqrt{2\pi} z^{z-\frac{1}{2}} e^{-z}. && (0.74) \end{aligned}$$

Next we return to

$$\Gamma(z+1) = \int_0^\infty dt\; e^{f(t)}, \tag{0.75}$$

where

$$f(t) = -t + z\ln t. \tag{0.76}$$

The saddle point, $f'(t_0) = 0$, of $f(t)$ is located at $t_0 = z$. We now expand $f(t)$ about the saddle point to write

$$f(t) = f(z) + A_1(t-z) + A_2(t-z)^2 + A_3(t-z)^3 + \cdots, \tag{0.77}$$

where

$$A_k = \frac{1}{k!}\frac{d^k f(z)}{dt^k}. \tag{0.78}$$

Substituting $f(t)$ [Eq. (0.76)] into Equation (0.77) we obtain

$$f(t) = [-z + z\ln z] - \frac{(t-z)^2}{2z} + \frac{(t-z)^3}{3z^2} - \frac{(t-z)^4}{4z^3} + \cdots, \tag{0.79}$$

which when substituted into Equation (0.75) gives

$$\Gamma(z+1) = z^z e^{-z} \int_0^\infty dt \exp\left[\frac{(t-z)^2}{2z} + \frac{(t-z)^3}{3z^2} - \frac{(t-z)^4}{4z^3} + \cdots\right]. \tag{0.80}$$

To simplify, we use the substitution

$$s = \frac{t-z}{\sqrt{2z}} \tag{0.81}$$

to get

$$\Gamma(z+1) = \sqrt{2z}\ z^z e^{-z} \int_{-\sqrt{z/2}}^\infty ds \exp\left[-s^2 + \frac{s^3}{3}\sqrt{\frac{8}{z}} - \frac{s^4}{z} + \cdots\right]. \tag{0.82}$$

We now write this as

$$\Gamma(z+1) \simeq \sqrt{2z}\ z^z e^{-z} \int_{-\sqrt{z/2}}^\infty ds\ e^{-s^2} \exp\left(\frac{s^3}{3}\sqrt{\frac{8}{z}} - \frac{s^4}{z}\right) \tag{0.83}$$

and then expand the exponential to get

$$\begin{aligned}\Gamma(z+1) \simeq \sqrt{2z}\ z^z e^{-z} \int_{-\sqrt{z/2}}^\infty ds\ e^{-s^2} &\left[1 + \left(\frac{s^3}{3}\sqrt{\frac{8}{z}} - \frac{s^4}{z}\right)\right.\\ &\left.+\frac{1}{2!}\left(\frac{s^3}{3}\sqrt{\frac{8}{z}} - \frac{s^4}{z}\right)^2 + \cdots\right],\end{aligned} \tag{0.84}$$

which when the integrals are evaluated yields the series

$$\Gamma(z+1) \simeq \sqrt{2\pi}\ z^{z+\frac{1}{2}} e^{-z}\left[1 + \frac{1}{12z} + \frac{1}{288z^2} + \cdots\right]. \tag{0.85}$$

For integers, $z = n$, this gives the asymptotic expansion of the factorial,

$$n! \simeq \sqrt{2\pi}\ n^{n+\frac{1}{2}} e^{-n}\left[1 + \frac{1}{12n} + \frac{1}{288n^2} + \cdots\right], \tag{0.86}$$

the first term of which is the well known Stirling's formula valid for large n:

$$n! \simeq \sqrt{2\pi}\ n^{n+\frac{1}{2}} e^{-n}. \tag{0.87}$$

Keep in mind that the several steps of this derivation lacks the desired rigor, but nevertheless produces the right answer [Eq. (0.24)].

II. Padé Approximants

In Bayin (2006) we have seen how to use contour integrals and Euler Maclaurin sum formula to sum series. Both techniques required that the general term of the series be known. In applications we frequently encounter situations where only the first few terms of the series can be determined. Furthermore, these terms may not be sufficient to reveal the general term of the series. We are know going to introduce an intriguing technique that will allow us to evaluate series sums to very high level of accuracy.

As an example we will consider the series

$$f(x) = 1 + x - \frac{5}{2}x^2 + \frac{13}{2}x^3 - \frac{141}{8}x^4 + \cdots , \tag{0.88}$$

where only the first five terms are known. Let us first introduce the general method. Consider a series whose first M terms are given :

$$f(x;M) = \sum_{i=0}^{M} a_i x^i. \tag{0.89}$$

We write $f(x;M)$ as the ratio of two polynomials:

$$f(x;M) = \frac{P(x;N)}{Q(x;L)}, \tag{0.90}$$

where

$$P(x;N) = \sum_{j=0}^{N} p_j x^j, \tag{0.91}$$

$$Q(x;L) = \sum_{k=0}^{L} q_k x^k \tag{0.92}$$

and

$$M = N + L. \tag{0.93}$$

We have $(N + L + 2) = M + 2$ unknowns, where $(N + 1)$ p_j's and $(L + 1)$ q_k's, are to be determined from the known $M + 1$ values of a_i. We now write

Equation (0.90) as

$$f(x;M)\left(\sum_{k=0}^{L} q_k x^k\right) = \left(\sum_{j=0}^{N} p_j x^j\right), \tag{0.94}$$

$$\left(\sum_{i=0}^{M} a_i x^i\right)\left(\sum_{k=0}^{L} q_k x^k\right) = \left(\sum_{j=0}^{N} p_j x^j\right), \tag{0.95}$$

$$\left(a_0 + a_1 x + \cdots + a_M x^M\right)\left(q_0 + q_1 x + \cdots + q_L x^L\right) = \left(p_0 + p_1 x + \cdots + a_N x^N\right) . \tag{0.96}$$

Since when $P(x;N)$ and $Q(x;L)$ are multiplied with the same constant, $f(x;M)$ does not change, hence we can set

$$q_0 = 1, \tag{0.97}$$

thus obtaining

$$\left(a_0 + a_1 x + \cdots + a_M x^M\right)\left(1 + q_1 x + \cdots + q_L x^L\right) = \left(p_0 + p_1 x + \cdots + p_N x^N\right) . \tag{0.98}$$

We now have $N+L+1 = M+1$ unknowns, $p_0, p_1, \ldots, p_N; q_1, \ldots, q_L$, to be determined from the $N+1$ values of a_i, $i = 0, 1, \ldots, M$. Expanding Equation (0.98) and equating the coefficients of the equal powers of x gives the following $M+1$ equations:

$$\begin{aligned}
a_0 &= p_0, \\
a_1 + a_0 q_1 &= p_1, \\
a_2 + a_1 q_1 + a_0 q_2 &= p_2, \\
&\vdots \\
a_N + a_{N-1} q_1 + \cdots + a_0 q_N &= p_N, \\
a_{N+1} + a_N q_1 + \cdots + a_{N-L+1} q_L &= 0, \\
&\vdots \\
a_{N+L} + a_{N+L-1} q_1 + \cdots + a_N q_L &= 0,
\end{aligned} \tag{0.99}$$

for the $M+1$ unknowns, where we have taken

$$a_i = 0 \text{ when } i > M, \tag{0.100}$$

$$p_j = 0 \text{ when } j > N, \tag{0.101}$$

$$q_k = 0 \text{ when } k > L. \tag{0.102}$$

The first $N+1$ equations can be written as

$$\begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_N \end{pmatrix} = \begin{pmatrix} a_0 & 0 & \cdots & 0 \\ a_1 & a_0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ a_N & a_{N-1} & \cdots & a_0 \end{pmatrix} \begin{pmatrix} 1 \\ q_1 \\ \vdots \\ q_N \end{pmatrix}, \tag{0.103}$$

while the remaining equations become

$$\begin{pmatrix} a_N & a_{N-1} & \cdots & a_{N-L+1} \\ a_{N+1} & a_N & \cdots & a_{N-L+2} \\ \vdots & \vdots & \vdots & \vdots \\ a_M & a_{M-1} & \cdots & a_N \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_L \end{pmatrix} = - \begin{pmatrix} a_{N+1} \\ a_{N+2} \\ \vdots \\ a_M \end{pmatrix}. \tag{0.104}$$

These are two sets of linear equations. Since a_i's are known, we can solve the second set for the q_k values, which when substituted into the first set will yield the p_j values. For a review of linear algebra and techniques on solving systems of linear equations we recommend Bayin (2008).

Let us now return to the series in Equation (0.88), where $M=4$ and choose

$$N = L = 2. \tag{0.105}$$

Using the values

$$a_0 = 1,\ a_1 = 1,\ a_2 = -\frac{5}{2},\ a_3 = \frac{13}{2},\ a_4 = -\frac{141}{8}, \tag{0.106}$$

the two linear systems to be solved becomes

$$\begin{pmatrix} a_2 & a_1 \\ a_3 & a_2 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = - \begin{pmatrix} a_3 \\ a_4 \end{pmatrix}, \tag{0.107}$$

$$\begin{pmatrix} -\frac{5}{2} & 1 \\ \frac{13}{2} & -\frac{5}{2} \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = - \begin{pmatrix} \frac{13}{2} \\ -\frac{141}{8} \end{pmatrix} \tag{0.108}$$

and

$$\begin{pmatrix} p_0 \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} a_0 & 0 & \cdots \\ a_1 & a_0 & \cdots \\ a_2 & a_1 & a_0 \end{pmatrix} \begin{pmatrix} 1 \\ q_1 \\ q_2 \end{pmatrix}, \tag{0.109}$$

$$\begin{pmatrix} p_0 \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & \cdots \\ 1 & 1 & \cdots \\ -\frac{5}{2} & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ q_1 \\ q_2 \end{pmatrix}. \tag{0.110}$$

The first set yields the values of q_k as

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} \frac{11}{2} \\ \frac{29}{4} \end{pmatrix}. \tag{0.111}$$

Using these values in the second set we obtain

$$\begin{pmatrix} p_0 \\ \\ p_1 \\ \\ p_2 \end{pmatrix} = \begin{pmatrix} 1 \\ \\ \frac{13}{2} \\ \\ \frac{41}{4} \end{pmatrix}. \tag{0.112}$$

Thus, we obtain the **Padé approximant** $f^{(2,2)}(x)$ as

$$f^{(2,2)}(x) = \frac{1 + \frac{13}{2}x + \frac{41}{4}x^2}{1 + \frac{11}{2}x + \frac{29}{4}x^2}. \tag{0.113}$$

To interpret this result, it is time to reveal the truth about the five terms we have in Equation (0.88). They are just the first five terms of the Taylor series expansion of

$$F(x) = \sqrt{\frac{1+4x}{1+2x}}. \tag{0.114}$$

This function has a pole at

$$x = -\frac{1}{2} \tag{0.115}$$

and a branch point at

$$x = -\frac{1}{4}. \tag{0.116}$$

In other words, the Taylor series:

$$f(x) = 1 + x - \frac{5}{2}x^2 + \frac{13}{2}x^3 - \frac{141}{8}x^4 + \cdots , \tag{0.117}$$

converges only for

$$|x| \leq \frac{1}{4}. \tag{0.118}$$

We now construct the following table to compare $F(x)$, $f(x)$, $f^{(2,2)}(x)$ for various values of x :

x	0	1/4	1/2	1	3.0	7.0
$F(x)$	1	1.1547	1.22474	1.29099	1.36277	1.39044
$f(x)$	1	1.12646	0.585938	-11.625	-1270.63	-40202.6
$f^{(2,2)}(x)$	1	1.1547	1.22472	1.29091	1.36254	1.39012
$f^{(1,3)}(x)$	1	1.15426	1.2196	1.24966	0.89702	0.316838
$f^{(3,1)}(x)$	1	1.15428	1.2199	1.2513	0.712632	-2.91771

The last two rows are the other two Padé approximants corresponding to the choices $(N,L) = (1,3)$ and $(N,L) = (3,1)$, respectively:

$$f^{(1,3)}(x) = \frac{1 + \frac{363}{100}x}{1 + \frac{263}{100}x - \frac{13}{100}x^2 + \frac{41}{200}x^3} \tag{0.119}$$

and

$$f^{(3,1)}(x) = \frac{1 + \frac{193}{52}x + \frac{11}{52}x^2 - \frac{29}{104}x^3}{1 + \frac{141}{52}x}. \tag{0.120}$$

From this table it is seen that the Padé approximant, $f^{(2,2)}(x)$, approximates the function $F(x)$ much better than the Taylor series, $f(x)$, truncated after the fifth term. It is also interesting that $f^{(2,2)}(x)$ remains to be an excellent approximation even outside the domain, $|x| > 1/4$, where the Taylor series ceases to be valid. In this case, the symmetric Padé approximant; $f^{(2,2)}(x)$, gives a much better approximation than its antisymmetric counterparts.

Definition: For a given function, $f(x)$, the Padé approximant, $R_{N/L}(x) \equiv [N,L]$, of order (N,L) is defined as the rational function

$$R_{N/L}(x) = \frac{p_0 + p_1 x + p_2 x^2 + \cdots + p_N x^N}{1 + q_1 x + q_2 x^2 + \cdots + q_L x^L}. \tag{0.121}$$

$R_{N/L}(x)$ agrees with $f(x)$ to the highest possible order, that is,

$$f(x) - R_{N/L}(x) = c_{N+L+1}x^{N+L+1} + c_{N+L+2}x^{N+L+2} + \cdots \tag{0.122}$$

In other words, the first $(N+L)$ terms of the Taylor series expansion of $R_{N/L}(x)$ exactly cancel the first $(N+L+1)$ terms of the Taylor series of $f(x)$. For a given (N,L) the Padé approximant is unique. Padé approximants will often be a superior approximation to a function, compared to the one obtained by truncating the Taylor series. As in the above example, it may even work where the Taylor series do not .

III. Interesting Sites and additional References

In the following sites we can find encyclopedic information about the Padé approximants and also find other references and links:
`http://en.wikipedia.org/wiki/Pade_approximant`
`http://mathworld.wolfram.com/PadeApproximant.html`.
The following sites can be used for computer codes and simulations:
`http://www.mathworks.com/matlabcentral/fileexchange/4388`,
`http://demonstrations.wolfram.com/PadeApproximants/`.

For additional references we give

Antia, H.M., *Numerical Methods for Scientists and Engineers*, Birkhauser, Basel, 2002.

Baker, G.A, Jr., *Essentials of Padé Approximants*, Academic, 1975.

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