An important generalization of Taylor series that is permissible in the complex plane is the **Laurent series**. Every function that is analytic within an *annulus* $R_1 < |z - z_0| < R_2$ has a unique power series expansion

$$f(z) \;=\; \sum_{n=-\infty}^{\infty} c_n \, (z - z_0)^n \quad , \quad c_n \;=\; \frac{1}{2\pi i} \oint_C \frac{f(\zeta)\, d\zeta}{(\zeta - z_0)^{n+1}} \quad , \tag{33}$$

where C is a circle of radius r such that $R_1 < r < R_2$.

• If $f(z)$ is analytic in a *neighborhood* of $z = z_0$, but not at $z = z_0$, then this point is called an **isolated singularity**. If the Laurent series is truncated to a finite range of terms with $n < 0$, i.e.

$$f(z) \;=\; \sum_{n=-m}^{\infty} c_n \, (z - z_0)^n \quad , \tag{34}$$

then $z = z_0$ is a **pole of order** m. A pole of order unity is designated as a **simple pole**. If the series about the singularity at $z = z_0$ is not so truncated, then this point is called an **essential singularity**. For example, for $f(z) = \exp(-1/z)$, the origin $z = 0$ is an essential singularity.

• **Example 5:** Consider Laurent series for the function

$$f(z) \;=\; \frac{1}{z\,(z - a)^2} \quad , \quad |a| \;>\; 0 \quad . \tag{35}$$

This has a <u>simple pole at $z = 0$</u> and <u>a pole of order two at $z = a$</u>, as becomes obvious when expressing it via partial fractions:

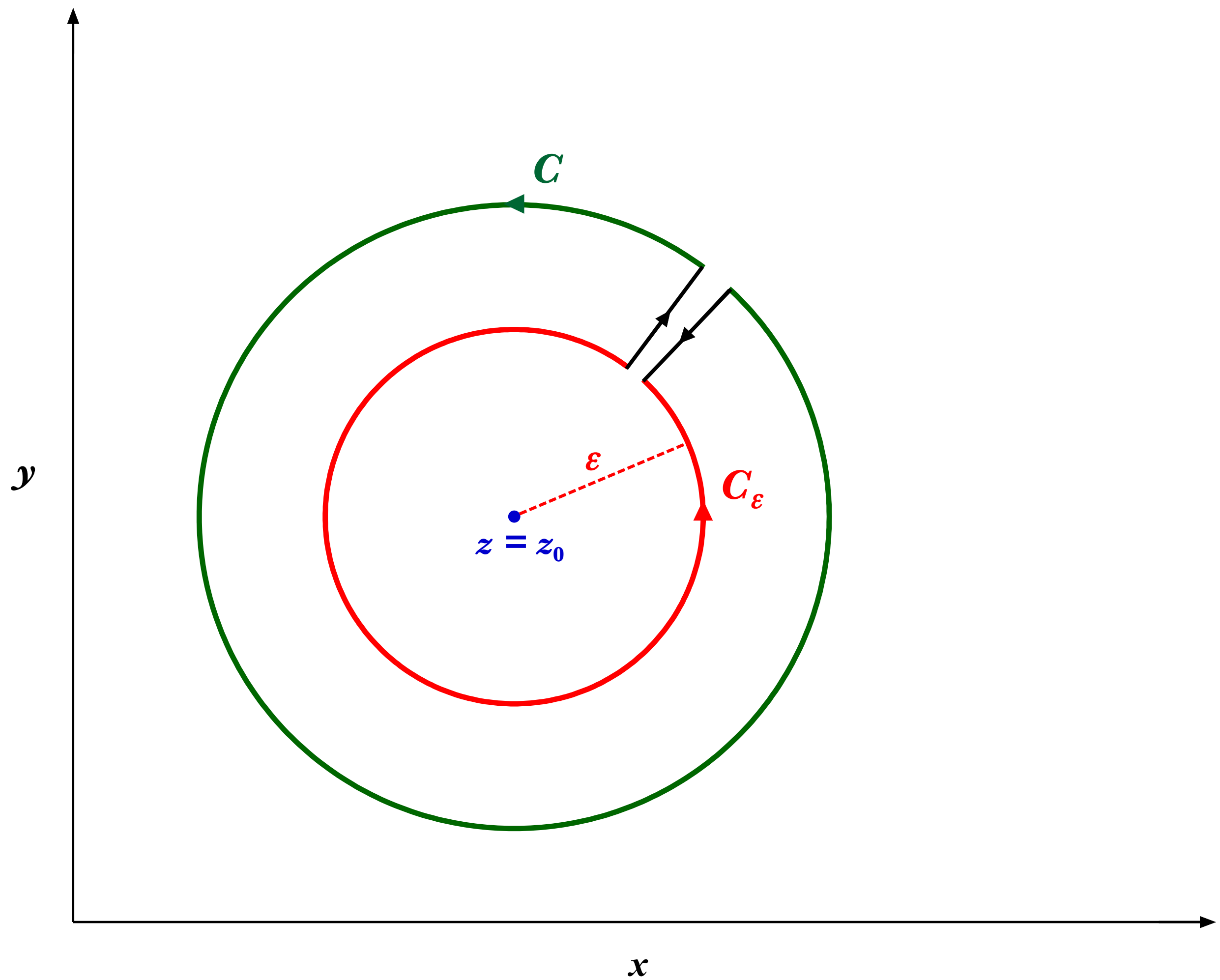
$$f(z) \;=\; \frac{1}{a^2 z} - \frac{1}{a^2(z - a)} + \frac{1}{a(z - a)^2} \quad . \tag{36}$$

One can then form a Laurent series about $z = 0$ that has convergence within the annulus $a_1 \leq |z| \leq a_2$ for any $0 < a_1 < a_2 < a$. Thus,

$$\begin{aligned} f(z) \;&=\; \frac{1}{z\,(a - z)^2} \;=\; \frac{1}{a^2 z} \, \frac{1}{(1 - z/a)^2} \\ &=\; \frac{1}{a^2 z} \left(1 + \frac{2z}{a} + \frac{3z^2}{a^2} + \frac{4z^3}{a^3} + \frac{5z^4}{a^4} + \dots \right) \quad . \end{aligned} \tag{37}$$

The second factor is expanded using a **binomial series** form.

Contour Geometry for Cauchy Integral Formula



6 The Theorem of Residues

To conclude this brief exposition of complex analysis, our focus will turn to a powerful tool of use in the evaluation of integrals. If $f(z)$ is analytic within and on a closed contour C, except for a finite number of isolated singularities inside C (at $z = z_0,\, z_1 \ldots$), then the **Residue Theorem** states that **A & W, Sec. 7.1**

$$\boxed{\oint_C f(z)\, dz \;=\; 2\pi i \sum_n \mathrm{Res}\,[f(z_n)] \;=\; \sum_n \oint_{C_n} f(z)\, dz \quad .} \tag{38}$$

Here, C_n is a contour that specifically surrounds $z = z_n$ but no other singularities. Accordingly, $\mathrm{Res}[f(z_n)]$ (or $\mathrm{Res}[z_n]$) is called the **Residue of** f **at** $z = z_n$, and it is precisely c_{-1}, the coefficient of $1/(z - z_n)$ in the Laurent series expansion of $f(z)$ around $z = z_n$.

- *Proof:* Using the Laurent series expansion, for the z_n pole we have

$$\oint_{C_n} f(z)\, dz \;=\; \sum_{k=-\infty}^{\infty} c_k \oint_{C_n} (z - z_n)^k\, dz \quad , \tag{39}$$

Clearly, if $k \geq 0$, then as $(z - z_n)^k$ is analytic, the contour integrals of these terms contribute zero each. If $k \leq -2$, zero also results, since the integrals are just higher-order derivatives of a constant function. [This is alternatively demonstrated in Problem 6.4.1 of Arfken & Weber.] Only the $k = -1$ term is retained, and

$$\oint_{C_n} f(z)\, dz \;=\; c_{-1} \oint_{C_n} \frac{dz}{z - z_n} \;=\; 2\pi i\, c_{-1} \quad , \tag{40}$$

as desired. Selecting the contours C_n so that they successively surround each of the poles z_n then proves the Residue Theorem.

$*$ The ability to isolate each of the poles and surround them by quasi-circular portions of an extended contour is the reason why the result is constrained to a finite number of singularities.

• Recipes for calculating residues include:

$$\begin{aligned} \text{Simple pole:} \qquad & \text{Res}[f(a)] \;=\; \lim_{z\to a} (z-a)\, f(z) \quad , \\ m^{th}\text{order pole:} \qquad & \text{Res}[f(a)] \;=\; \frac{1}{(m-1)!} \lim_{z\to a} \frac{d^{m-1}}{dz^{m-1}} \Big[(z-a)^m\, f(z) \Big] \quad . \end{aligned} \tag{41}$$

Also, if $f(z) = P(z)/Q(z)$, with $Q(a) = 0$ but $P(a) \neq 0$, then for a simple pole, $\text{Res} f(a) = P(a)/Q'(a)$.

• **Example 6:** Consider again the Laurent series for the function

$$f(z) \;=\; \frac{1}{z\,(z-a)^2} \quad , \quad |a| \;>\; 0 \quad , \tag{42}$$

about $z = 0$. The Residue Theorem can be employed to evaluate the series coefficients:

$$c_n \;=\; \frac{1}{2\pi i} \oint_C \frac{d\zeta}{\zeta^{n+2} (\zeta - a)^2} \;=\; \text{Res} \left[\frac{1}{\zeta^{n+2} (\zeta - a)^2} \right]_{\zeta = 0} \quad . \tag{43}$$

Thus,

$$c_n \;=\; \begin{cases} 0 \quad , & n \;\leq\; -2 \;, \\ \dfrac{1}{a^2} \quad , & n \;=\; -1 \;, \\ \dfrac{n+2}{a^{n+3}} \quad , & n \;\geq\; 0 \quad , \end{cases} \tag{44}$$

and the Laurent series is (for $k = n + 1$)

$$f(z) \;=\; \sum_{n=-\infty}^{\infty} c_n z^n \;=\; \sum_{k=0}^{\infty} \frac{k+1}{a^2\, z} \left(\frac{z}{a} \right)^k \tag{45}$$

as before.

• The power of the Residue Theorem will become apparent when techniques for integral evaluation will be explored later in the course.

2. INTERPOLATION, FITTING AND ROOT SOLVING

Matthew Baring — Lecture Notes for PHYS 516, Fall 2022

1 Lagrange Interpolation

• A common technique for interpolation using polynomials. We start with a set of $n+1$ data points $(x_k,\, f(x_k))$, $0 \leq k \leq n$. Consider the fit

$$f(x) \;\approx\; P_n(x) \;=\; \sum_{k=0}^{n} w_k(x)\, f(x_k) \tag{1}$$

where $P_n(x)$ is an $n^{\rm th}$ degree polynomial. We require equality at all the $x = x_j$, so that

$$f(x_j) \;=\; \sum_{k=0}^{n} w_k(x_j)\, f(x_k) \quad . \tag{2}$$

The simplest (but not necessarily unique) way to achieve these equalities is to demand that the weighting functions $w_k(x)$ assume following form

$$w_k(x) \;=\; \frac{1}{\beta_k} \prod_{m=0}^{k-1} (x - x_m) \prod_{m=k+1}^{n} (x - x_m) \quad , \tag{3}$$

i.e., n^{th} degree polynomials. With the definition

$$\boxed{\alpha_n(x) \;\equiv\; \prod_{m=0}^{n} (x - x_m) \;\; ,} \tag{4}$$

the weighting function becomes $w_k(x) = \alpha_n(x)/[\beta_k(x - x_k)]$.

• This form, substituted into Eq.(2) yields non-zero contributions only for $k = j$, implying $w_j(x_j) = 1$ and

$$\beta_j \;=\; \prod_{m=0}^{j-1}(x_j - x_m) \prod_{m=j+1}^{n}(x_j - x_m) \;\equiv\; \alpha'_n(x_j) \quad . \tag{5}$$

The equivalence to $\alpha'_n(x_j)$ is perhaps most easily established by taking logarithms of each side of Eq. (4). It follows that

$$\boxed{P_n(x) \;=\; \sum_{k=0}^{n} \frac{\alpha_n(x)}{(x - x_k)\,\alpha'_n(x_k)}\; f(x_k) \quad .} \tag{6}$$

This is the principal equation of **Lagrange Interpolation**.

$*$ It is a good technique for functions of modest dynamic range.

$*$ **Example 1:** Consider

$$f(x) \;=\; \frac{\log_e(1+x)}{x} \quad , \quad 0 < x \le 1 \quad . \tag{7}$$

Take exact values/limits at $x = 0,\ 1/2,\ 1$. Then

$$\alpha_2(x) \;=\; x\left(x - \frac{1}{2}\right)(x-1) \tag{8}$$

and

$$\alpha'_2(0) \;=\; \frac{1}{2}\ ,\ \ \alpha'_2(1/2) \;=\; -\frac{1}{4}\ ,\ \ \alpha'_2(1) \;=\; \frac{1}{2}\ , \tag{9}$$

so that the Lagrange interpolating function is

$$P_2(x) \;=\; 2.0\left(x - \frac{1}{2}\right)(x-1) - 3.2437\,x(x-1) + 1.3863\,x\left(x - \frac{1}{2}\right) \ , \tag{10}$$

with less than 0.5% error on $(0,1]$.

N.B. Interpolations of a polynomial reduce to the polynomial itself when they are of equal or higher order.

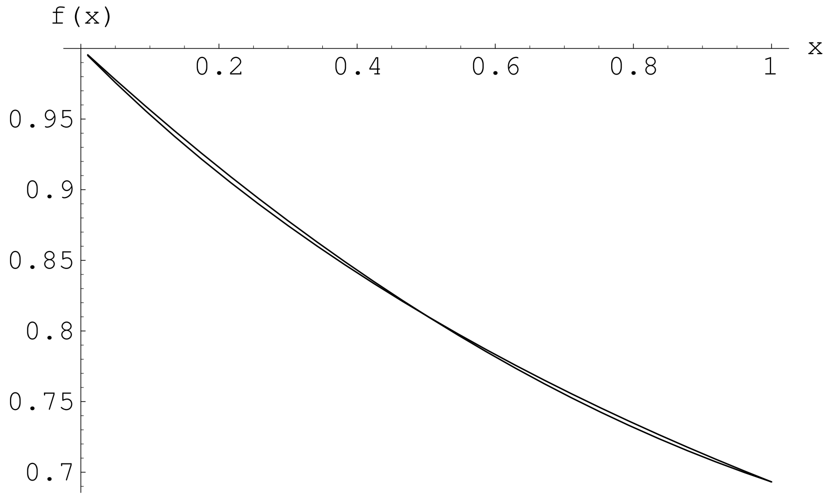


Figure 1: A comparison of $\log_e(1+x)/x$ and the Lagrange interpolating function of Example 1.

• *Increasing order does not necessarily imply increasing accuracy.*

Examples of this can be seen in bumpy or discontinuous functions, such as step functions. Then piecewise lower-order (e.g. linear) interpolations may prove superior to higher order polynomials.

$*$ Hence *careful consideration of the construction of an interpolation* on a case-by-case basis is warranted.

• A semi-formal (and case-specific) analysis of accuracy is provided in Mathews & Walker (p. 348). Without reproducing the details, the accuracy of the Lagrange interpolation is of third-order, i.e.

$$\Big|P_n(x) - f(x)\Big| \;\sim\; \frac{(x_n - x_0)^3}{n^3}\,\Big|f'''(x)\Big| \quad . \tag{11}$$

This can be established using Taylor series expansions.

$*$ Hence, discontinuities, singularities and cusp points are prime locations for where accuracy is rapidly degraded.

2 Cubic Splines

• Splines are interpolations that are generally a sequence of functions that span sequential data intervals, demanding continuity and differentiability at the boundaries between intervals. It is usual to require continuity in the second derivative also, forcing consideration of cubic polynomials $f_i(x)$. Such **cubic splines**, are the most popular choice of splines and interpolative techniques, being common in image enhancement and graphics applications.

∗ Hence, we seek a fit to a set of points (x_i, y_i) with cubic functions $f_i(x)$ defined on $n-1$ intervals $x_i \leq x \leq x_{i+1}$, $i = 1, 2, \ldots n-1$. Obviously,

$$\begin{aligned} f_{i-1}(x_i) &= f_i(x_i) = y_i \quad , \quad i = 2, \ldots, n-1 \ , \\ f'_{i-1}(x_i) &= f'_i(x_i) \equiv y'_i \quad , \quad i = 2, \ldots, n-1 \ , \\ f''_{i-1}(x_i) &= f''_i(x_i) \equiv y''_i \quad , \quad i = 2, \ldots, n-1 \ . \end{aligned} \tag{12}$$

The derivatives y'_i and y''_i are clearly unknowns, and byproducts of the spline fit, *i.e., they do not necessarily match the derivative of* $y = f(x)$.

∗ Considering the second derivative of the cubic splines leads to linear interpolations in f''_i. Setting

$$r_i = \frac{x - x_i}{\delta_i} \quad , \quad \delta_i = x_{i+1} - x_i \ , \tag{13}$$

so that $0 \leq r_i \leq 1$. It is trivial to determine the interpolation

$$f''_i(x) = y''_i(1 - r_i) + y''_{i+1} r_i \quad , \quad i = 1, \ldots, n-1 \ . \tag{14}$$

Twice integrating this with respect to x and selecting constants to guarantee continuity of the f_i yields cubics with only y''_i as unknowns:

$$f_i(x) = y_i(1 - r_i) + y_{i+1} r_i - \frac{\delta_i^2}{6} r_i(1 - r_i) \Big[(2 - r_i) y''_i + (1 + r_i) y''_{i+1} \Big] \ , \tag{15}$$

for $i = 1, \ldots, n-1$. Hence, we have satisfied continuity of the spline and its second derivative at the data points, but not that of the first derivatives.

This is easily done by differentiating Eq. (15) and imposing $f'_{i-1}(x_i) = f'_i(x_i)$. The result is a sequence of recurrence relations:

$$
\begin{aligned}
(x_i - x_{i-1})y''_{i-1} + 2(x_{i+1} - x_{i-1})y''_i + (x_{i+1} - x_i)y''_{i+1} \\
= 6\left[\frac{y_{i+1} - y_i}{x_{i+1} - x_i} - \frac{y_i - y_{i-1}}{x_i - x_{i-1}}\right] \quad .
\end{aligned}
\tag{16}
$$

• This set of $n - 2$ simultaneous equations can be solved for the y''_i by matrix techniques, or by using Mathematica's `Solve[]` function.

∗ It should be noted that <u>we are short two equations</u>, and these pertain to arbitrary choices of endpoint conditions at x_1 and x_n. One common choice is setting $y''_1 = 0 = y''_n$, generating the so-called *natural spline*. The choice can be tailored to the problem at hand.