Applied Analysis

Topics to be covered:

1. Dimensional analysis
2. Euler-Maclaurin formula
3. Formal power series & Lagrange inversion formula
4. Fundamentals of asymptotic analysis
   - Asymptotic sequence and series
   - Asymptotic root finding
5. Asymptotic analysis of exponential integrals
   - Watson's lemma
   - Laplace's method
   - Method of steepest descents
   - Method of stationary phase
   - Analysis of integral transformation: Fourier, Laplace, Mellin transforms
6. Asymptotic analysis of differential equations
   - Majorant series, Cauchy theorem
   - Asymptotic behavior near ordinary and regular singular points
   - Asymptotic behavior near irregular singular points, Stokes phenomenon
7. Asymptotic solutions of ODE with respect to parameters
   - Poincaré-Lighthill-Kuo (PLK) method (i.e., method of strained coordinates)
   - Method of multiple scales
   - WKBJ method
8. Asymptotic solutions of linear boundary-value problem (BVP)
   - Outer and inner asymptotics
   - Boundary layers and internal layers

Textbooks:

- Peter D. Miller, *Applied Asymptotic Analysis*
- James D. Murray, *Asymptotic Analysis*
- Wolfgang Wasow, *Asymptotic Expansions for Ordinary Differential Equations*

Introduction

- Examples of asymptotic analysis

Taylor expansion

Consider a smooth function $f \in C^\infty(a,b)$, for any $n \in \mathbb{N}$ we have

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x-x_0)^k + o((x-x_0)^n)$$

If the Taylor series is convergent in $B(x_0, r)$, for any $x \in B(x_0, r)$ we have

$$\lim_{N\to\infty} S_N(x) = f(x), \qquad S_N(x) = \sum_{k=0}^{N} \frac{f^{(k)}(x_0)}{k!}(x-x_0)^k$$

On the other hand, the Peano form of the remainder states that

$$\lim_{x\to x_0} \frac{f(x) - S_n(x)}{(x-x_0)^n} = 0$$

Note that there are two limits considering $N \to \infty$ and $x \to x_0$, respectively. The convergence of Taylor series studies the limit of $N \to \infty$. However, for asymptotic analysis, we consider one fixed n and study the behavior as $x \to x_0$.

Stirling formula

$$n! = \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \left(1 + \frac{1}{12n} + \frac{1}{288n^2} + o\left(\frac{1}{n^2}\right)\right), \qquad n \to \infty$$

Note that the power series usually does not converge in asymptotic analysis. It needs to be **truncated** in order to compute the values.

Exponential integral

Keep using integration by parts, the exponential integral has the following expansion

$$E_i(x) = \int_x^\infty \frac{e^{-t}}{t}\,\mathrm{d}t = \left[-\frac{e^{-t}}{t}\right]_x^\infty + \int_x^\infty \frac{e^{-t}}{t^2}\,\mathrm{d}t = \frac{e^{-x}}{x} + \int_x^\infty \frac{e^{-t}}{t^2}\,\mathrm{d}t$$

$$= e^{-x}\left(\frac{1}{x} - \frac{1}{x^2} + \frac{2}{x^3} - \cdots + (-1)^N \frac{N!}{x^{N+1}}\right) + C\int_x^\infty \frac{e^{-t}}{t^{N+2}}\,\mathrm{d}t$$

Sum of powers

$$\sum_{k=1}^{n} k^2 = \frac{1}{6}n(n+1)(2n+1), \qquad \sum_{k=1}^{n} k^3 = \frac{1}{4}n^2(n+1)^2$$

The sum of powers can be calculated based on the Faulhaber's formula, in which the Bernoulli numbers B_r are used.

$$\sum_{k=1}^{n} k^p = \frac{n^{s+1}}{s+1} + \frac{1}{2}n^s + \frac{s}{12}n^{s-1} - \frac{s(s-1)(s-2)}{720}n^{s-2} - \cdots$$

$$= \frac{1}{s+1}\sum_{r=0}^{s} \binom{s+1}{r} B_r\, n^{s+1-r}$$

Prime number theorem (PNT)

The prime-counting function $\pi(x)$ is defined to be the number of primes less than or equal to x, for any real number x. The asymptotic expansion of $\pi(x)$ is

$$\pi(x) = \frac{x}{\ln x} + o\left(\frac{x}{\ln x}\right), \qquad x \to \infty$$

The Riemann hypothesis is equivalent to proving the remainder as $o\left(\sqrt{x}\ln x\right)$.

- Focus of asymptotic analysis

Series

$$f(n) = \sum_{k=1}^{n} a_k\,, \qquad f_n(x) = \sum_{k=1}^{n} a_k(x)\,, \qquad k \to \infty$$

Integral

$$f(x) = \int_{I(x)} g(x,t)\,\mathrm{d}t\,, \qquad f(x) = \int_{S(x)} \omega(x)$$

Limiting behaviors

$$x - x_0 \to 0, \qquad x \to +\infty, -\infty, \pm\infty, \qquad z \to \infty \text{ for } z \in \mathbb{C}$$

Dimensional Analysis

- Example: Pendulum

Consider the following physical quantities

$$M = m\ [\mathrm{kg}], \qquad L = l\ [\mathrm{m}], \qquad g = g_0\ [\mathrm{m/s^2}], \qquad \theta = \theta_0, \qquad T = t\ [\mathrm{s}]$$

Now we define another unit system

$$[\mathrm{kg}] = \lambda_1\ [\mathrm{u}_1], \qquad [\mathrm{m}] = \lambda_2\ [\mathrm{u}_2], \qquad [\mathrm{s}] = \lambda_3\ [\mathrm{u}_3]$$

Under this unit system, we have

$$M = \lambda_1 m\ [\mathrm{u}_1], \qquad L = \lambda_2 l\ [\mathrm{u}_2], \qquad g = \frac{\lambda_2}{\lambda_3^2} g_0\ [\mathrm{u}_2/\mathrm{u}_3^2]$$

The period of the pendulum should be consistent under different unit systems, which gives

$$T = \lambda_3 f(m, l, g_0, \theta_0) = f\left(\lambda_1 m, \lambda_2 l, \frac{\lambda_2}{\lambda_3^2} g_0, \theta_0\right)$$

Note that λ_1 does not show up in the LHS, so mass M does not influence period T. We choose

$$\lambda_2 = \frac{1}{l}, \qquad \lambda_3 = \sqrt{\frac{g_0}{l}}$$

The dimensional analysis gives the formula of period t [s] as

$$\sqrt{\frac{g_0}{l}} f(\cdot, l, g, \theta_0) = f(\cdot, 1, 1, \theta_0) = K(\theta_0), \qquad t = f(\cdot, l, g, \theta_0) = K(\theta_0)\sqrt{\frac{l}{g_0}}$$

- International System of Units (SI)

The SI units are obtained from the SI defining constants, instead of directly defining the units. Some SI defining constants include

$$\Delta\nu_{\mathrm{Cs}} = 9\ 192\ 631\ 770\ \ [\mathrm{s^{-1}}], \qquad c = 299\ 792\ 458\ \ [\mathrm{m/s}]$$

$$h = 6.626\ 070\ 15 \times 10^{-34}\ \ [\mathrm{kg \cdot m^2/s}], \qquad e = 1.602\ 176\ 634 \times 10^{-19}\ \ [\mathrm{A \cdot s}]$$

$$k = 1.380\ 649 \times 10^{-23}\ \ [\mathrm{kg \cdot m^2/(s^2 \cdot K)}], \qquad N_A = 6.022\ 140\ 76 \times 10^{23}\ \ [\mathrm{mol^{-1}}]$$

- Buckingham π theorem

Consider a problem that involves basic units $[\mathrm{u}_i]$ for $i = 1,2,\cdots,n$. The physical quantities are denoted as A_j for $j = 1,2,\cdots,m$. We want to study another quantity $B = f(A_1,\cdots,A_m)$. Let

$$A_i = a_i[\mathrm{u}_1]^{x_{i1}}[\mathrm{u}_2]^{x_{i2}}\cdots[\mathrm{u}_n]^{x_{in}}, \qquad B = b[\mathrm{u}_1]^{y_1}[\mathrm{u}_2]^{y_2}\cdots[\mathrm{u}_n]^{y_n}$$

Denote $\alpha_i = (x_{i1}, x_{i2},\cdots,x_{in})^T, \beta = (y_1, y_2,\cdots,y_n)^T$ are vectors in $\mathbb{R}^n$. Consider a basis of the space $V = \mathrm{span}(\alpha_1,\cdots,\alpha_m)$ as $\{\alpha_1,\cdots,\alpha_k\}$. Therefore, we have

$$\alpha_j = z_{j1}\alpha_1 + \cdots z_{jk}\alpha_k, \qquad \text{for } j > k, \qquad \beta = w_1\alpha_1 + \cdots + w_k\alpha_k$$

Now consider a new set of units $[\tilde{\mathrm{u}}_i]$ given as

$$[\mathrm{u}_i] = \lambda_i[\tilde{\mathrm{u}}_i], \qquad i = 1,2,\cdots,n, \qquad \lambda_i \in \mathbb{R}_{>0}$$

Then we obtain

$$A_i = a_i \lambda_1^{x_{i1}} \cdots \lambda_n^{x_{in}} [\tilde{\mathrm{u}}_1]^{x_{i1}} \cdots [\tilde{\mathrm{u}}_n]^{x_{in}}, \qquad B = b \lambda_1^{y_1} \cdots \lambda_n^{y_n} [\tilde{\mathrm{u}}_1]^{y_1} \cdots [\tilde{\mathrm{u}}_n]^{y_n}$$

The consistency of B under the two unit systems leads to

$$\lambda_1^{y_1} \cdots \lambda_n^{y_n} f(a_1, \cdots, a_m) = f\left(a_1 \lambda_1^{x_{11}} \cdots \lambda_n^{x_{1n}}, \cdots, a_m \lambda_1^{x_{m1}} \cdots \lambda_n^{x_{mn}}\right)$$

Choose $\lambda_1, \cdots, \lambda_n$ such that

$$a_i \lambda_1^{x_{i1}} \cdots \lambda_n^{x_{in}} = 1, \qquad \text{for } 1 \le i \le k, \qquad k = \dim(V)$$

This is equivalent to

$$x_{i1} \ln \lambda_1 + \cdots + x_{in} \ln \lambda_n = -\ln a_i, \qquad \text{for } 1 \le i \le k$$

There are k equations for n unknowns λ_i, which implies that we can successfully choose them. Now the equation becomes

$$\lambda_1^{y_1} \cdots \lambda_n^{y_n} f(a_1, \cdots, a_m) = f\left(1, \cdots, 1, a_{k+1} \lambda_1^{x_{(k+1)1}} \cdots \lambda_n^{x_{(k+1)n}}, \cdots, a_m \lambda_1^{x_{m1}} \cdots \lambda_n^{x_{mn}}\right)$$

Note that for $j > k$, we have $\alpha_j = z_{j1}\alpha_1 + \cdots z_{jk}\alpha_k$, which implies that

$$\lambda_1^{x_{j1}} \cdots \lambda_n^{x_{jn}} = \left(\lambda_1^{x_{11}} \cdots \lambda_n^{x_{1n}}\right)^{z_{j1}} \cdots \left(\lambda_1^{x_{k1}} \cdots \lambda_n^{x_{kn}}\right)^{z_{jk}} = \left(\frac{1}{a_1}\right)^{z_{j1}} \cdots \left(\frac{1}{a_k}\right)^{z_{jk}}, \qquad \text{for } j > k$$

The equation further becomes

$$\frac{f(a_1, \cdots, a_m)}{a_1^{w_1} \cdots a_k^{w_k}} = f\left(1, \cdots, 1, a_{k+1}\left(\frac{1}{a_1}\right)^{z_{(k+1)1}} \cdots \left(\frac{1}{a_k}\right)^{z_{(k+1)k}}, \cdots, a_m \left(\frac{1}{a_1}\right)^{z_{m1}} \cdots \left(\frac{1}{a_k}\right)^{z_{mk}}\right)$$

There are $m - k$ additional parameters left, assuming that we have k independent parameters. This non-dimensional procedure is important.

Example: Quantum states of neutrons in the Earth's gravitational field

This is an experiment from Nesvizhevsky et al. (2002, Nature). We want to find the discrete energy state from dimensional analysis. Given the following physical quantities

Mass of neutron m	Earth's gravity g	Planck constant $\hbar$
1.675×10^{-27}	9.8	1.0545×10^{-34}
[kg]	[m·s^{-2}]	[kg·m^{2}·s^{-1}]

The energy E has a unit of [kg·m^{2}·s^{-2}]. The dimensional analysis gives

$$E_g \propto m^{\frac{1}{3}} g^{\frac{2}{3}} \hbar^{\frac{2}{3}} \propto 1 \text{ peV}$$

This shows that the quantum states of neutrons in the Earth's gravitational field is observable. The constants are related to the zeros of the Airy function. However, if for the gravitational effect between two neutrons, we need to replace g by gravitational constant G as our relevant physical quantity, which is 6.674×10^{-11} [kg^{-1}·m^{3}·s^{-2}]. In this case, we have

$$E_G \propto m^5 G^2 \hbar^{-2} \propto 10^{-58}\ \mathrm{peV}$$

The gravitational effect between two neutrons cannot be observed as expected.

Example: QED fine-structure constant

The relevant physical quantities are listed below

e	ε_0	h	c
1.602×10^{-19}	8.854×10^{-12}	6.676×10^{-34}	2.99×10^{8}
[A·s]	[$A^2 \cdot s^4 \cdot kg^{-1} \cdot m^{-3}$]	[$kg \cdot m^2 \cdot s^{-1}$]	[$m \cdot s^{-1}$]

We want to obtain a dimensionless number α that quantifies the strength of the electromagnetic interaction between elementary charged particles. Based on the units, we have

$$\alpha \propto \frac{e^2}{\varepsilon_0 hc}, \qquad \alpha = \frac{e^2}{2\varepsilon_0 hc} \approx \frac{1}{137}$$

Example: KdV equation

$$au_t + bu_x + cuu_x + du_{xxx} = 0$$

The non-dimensional version can be obtained by considering

$$x = \lambda_1 \tilde{x}, \qquad t = \lambda_2 \tilde{t}, \qquad u = \lambda_3 \tilde{u}$$

Then we have

$$a\frac{\lambda_3}{\lambda_2}\tilde{u}_{\tilde{t}} + b\frac{\lambda_3}{\lambda_1}\tilde{u}_{\tilde{x}} + c\frac{\lambda_3^2}{\lambda_1}\tilde{u}\tilde{u}_{\tilde{x}} + d\frac{\lambda_3}{\lambda_1^3}\tilde{u}_{\tilde{x}\tilde{x}\tilde{x}} = 0$$

We choose λ_i satisfying

$$a\frac{\lambda_3}{\lambda_2} = 1, \qquad c\frac{\lambda_3^2}{\lambda_1} = 6, \qquad d\frac{\lambda_3}{\lambda_1^3} = 1, \qquad u_t + \gamma u_x + 6uu_x + u_{xxx} = 0$$

Furthermore, with the Galileo transform $\tilde{x} = x - \gamma t$, we have

$$u_t + 6uu_x + u_{xxx} = 0$$

Example: Lorenz equation

$$\dot{x} = a_1 y - a_2 x, \qquad \dot{y} = a_3 x - a_4 y - a_5 xz, \qquad \dot{z} = a_6 xy - a_7 z$$

Consider

$$x \to \lambda_1 x, \qquad y \to \lambda_2 y, \qquad z \to \lambda_3 z, \qquad t \to \lambda_4 t$$

We can reduce the number of parameters from 7 to 3 as

$$\dot{x} = \sigma(y - x), \qquad \dot{y} = x(\rho - z) - y, \qquad \dot{z} = xy - \beta z$$

Typically, we choose $\sigma = 10$, $\beta = 8/3$. At $\rho = 28$, the Lorenz system has chaotic solutions.

➢ Dimensional analysis as differential equation

Consider a simple version with only one parameter

$$f(\lambda^{x_1}a_1,\cdots,\lambda^{x_m}a_m)=\lambda^y f(a_1,\cdots,a_m)$$

The derivative with respect to λ gives

$$\sum_{i=1}^{m} x_i\lambda^{x_i-1}a_i\frac{\partial f}{\partial a_i}(\lambda^{x_1}a_1,\cdots,\lambda^{x_m}a_m)=y\lambda^{y-1}f(a_1,\cdots,a_m)$$

Let $\lambda=1$, we obtain a differential equation

$$\sum_{i=1}^{m} x_i a_i\frac{\partial f}{\partial a_i}=yf,\qquad f=f(a_1,\cdots,a_m)$$

We can choose the following solution form

$$f=a_1^{y/x_1}\cdot g\left(\frac{a_2}{a_1^{x_2/x_1}},\cdots,\frac{a_m}{a_1^{x_m/x_1}}\right)$$

The trick of first taking the derivative and then setting a special value to the parameter is useful.

➢ Exercise

Navier-Stokes equation

$$\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}=-\frac{1}{\rho}\nabla p+\nu\nabla^2\boldsymbol{u}-g\hat{\mathbf{z}}$$

With the scales ρ, P, U, L, we have

$$\frac{U^2}{L}\left(\frac{\partial\tilde{\boldsymbol{u}}}{\partial\tilde{t}}+\tilde{\boldsymbol{u}}\cdot\tilde{\nabla}\tilde{\boldsymbol{u}}\right)=-\frac{P}{\rho L}\tilde{\nabla}\tilde{p}+\frac{\nu U}{L^2}\tilde{\nabla}^2\tilde{\boldsymbol{u}}-g\hat{\mathbf{z}}$$

The non-dimensional N-S equation becomes

$$\frac{\partial\tilde{\boldsymbol{u}}}{\partial\tilde{t}}+\tilde{\boldsymbol{u}}\cdot\tilde{\nabla}\tilde{\boldsymbol{u}}=-\frac{P}{\rho U^2}\tilde{\nabla}\tilde{p}+\frac{1}{\mathrm{Re}}\tilde{\nabla}^2\tilde{\boldsymbol{u}}-\frac{1}{\mathrm{Fr}^2}\hat{\mathbf{z}},\qquad \mathrm{Re}=\frac{UL}{\nu},\qquad \mathrm{Fr}=\frac{U}{\sqrt{gL}}$$

The Reynolds number Re denotes the ratio of inertia to viscous dissipation. The Froude number Fr denotes the ratio of inertia to the external force.

Planck units

With $c, G, \hbar, \varepsilon_0, k_B$ all considered as 1, we have the Planck units $[\tilde{u}_i]$. From the SI units of these physical constants, we have

$$[\tilde{L}][\tilde{T}]^{-1}=c\ [\mathrm{m}\cdot\mathrm{s}^{-1}],\qquad [\tilde{M}]^{-1}[\tilde{L}]^3[\tilde{T}]^{-2}=G\ [\mathrm{kg}^{-1}\cdot\mathrm{m}^3\cdot\mathrm{s}^{-2}]$$

$$[\tilde{M}][\tilde{L}]^2[\tilde{T}]^{-1}=\hbar\ [\mathrm{kg}\cdot\mathrm{m}^2\cdot\mathrm{s}^{-1}],\qquad [\tilde{I}]^2[\tilde{M}]^{-1}[\tilde{L}]^{-3}[\tilde{T}]^4=\varepsilon_0\ [\mathrm{A}^2\cdot\mathrm{kg}^{-1}\cdot\mathrm{m}^{-3}\cdot\mathrm{s}^4]$$

$$[\tilde{M}][\tilde{L}]^2[\tilde{T}]^{-2}[\tilde{\theta}]^{-1}=k_B\ [\mathrm{kg}\cdot\mathrm{m}^2\cdot\mathrm{s}^{-2}\cdot\mathrm{K}^{-1}]$$

There are 5 independent units to be determined by these 5 physical constants. We thus have

$$[\tilde{L}] = \sqrt{\hbar G/c^3}\ [\mathrm{m}], \qquad [\tilde{T}] = \sqrt{\hbar G/c^5}\ [\mathrm{s}]\,, \qquad [\tilde{M}] = \sqrt{\hbar c/G}\ [\mathrm{kg}]$$

$$[\tilde{I}] = c^3\sqrt{\frac{\varepsilon_0}{G}}\ [\mathrm{A}], \qquad [\tilde{\theta}] = \frac{c^2}{k_B}\sqrt{\frac{\hbar c}{G}}\ [\mathrm{K}]$$

Volterra (predator-prey) equation

$$\dot{x} = x(\alpha - \beta y), \qquad \dot{y} = -y(\gamma - \delta x), \qquad x(0) = x_0, \qquad y(0) = y_0$$

We want to analyze the period $T(\alpha, \beta, \gamma, \delta, x_0, y_0)$. The unit of each parameter is

$$[\alpha] = [\gamma] = [\mathrm{s}^{-1}], \qquad [\beta] = [\delta] = [\mathrm{m}^{-1} \cdot \mathrm{s}^{-1}], \qquad [x_0] = [y_0] = [\mathrm{m}], \qquad [T] = [\mathrm{s}]$$

With another unit system

$$[\mathrm{m}] = \lambda_1\ [\mathrm{u}_1], \qquad [\mathrm{s}] = \lambda_2\ [\mathrm{u}_2]$$

The consistency of period T gives

$$T = \lambda_2 f(\alpha, \beta, \gamma, \delta, x_0, y_0) = f\left(\frac{\alpha}{\lambda_2}, \frac{\beta}{\lambda_1\lambda_2}, \frac{\gamma}{\lambda_2}, \frac{\delta}{\lambda_1\lambda_2}, \lambda_1 x_0, \lambda_1 y_0\right)$$

Since the LHS does not involve λ_1, we conclude that β, δ, x_0, y_0 do not influence the period. Now we choose $\lambda_2 = \alpha$, and we obtain

$$T = f(\alpha, \gamma) = \frac{1}{\alpha} f\left(1, \frac{\gamma}{\alpha}\right)$$

The period of the system only depends on α and γ, and under the non-dimensional sense, the function form only depends on the ratio γ/α.

Euler-Maclaurin Formula

Consider approximating an integral over $I = [a, b]$ by separating into n intervals as

$$\int_a^b f(x)\,\mathrm{d}x \approx T_n = \sum_{i=1}^{n} \frac{f(x_{i-1}) + f(x_i)}{2} \cdot \frac{b-a}{n}$$

Another perspective is to approximate the sum of a series by an integral

$$S_n = \sum_{k=1}^{n} f(k) \approx \int_1^n f(x)\,\mathrm{d}x$$

We want to analyze the difference between the integral and the sum. The Euler-Maclaurin formula originates from these two applications.

Example: Power function

Consider $\mu \in \mathbb{N}$ and $f(x) = x^\mu$. Denote the interval step as $h = (b-a)/n$.

$$S_n = h\sum_{i=0}^{n-1} f(x_i) = h\sum_{i=0}^{n-1} (a+ih)^\mu = h\sum_{i=0}^{n-1}\sum_{j=0}^{\mu}\binom{\mu}{j} a^{\mu-j}(ih)^j = \sum_{j=0}^{\mu}\binom{\mu}{j} a^{\mu-j}h^{j+1}\sum_{i=0}^{n-1} i^j$$

The sum of powers can be calculated from the exponential generating function

$$g(z) = \sum_{j=0}^{\infty}\frac{z^j}{j!}\sum_{i=0}^{n-1} i^j = \sum_{i=0}^{n-1}\sum_{j=0}^{\infty}\frac{(iz)^j}{j!} = \sum_{i=0}^{n-1} e^{iz} = \frac{e^{nz}-1}{e^z-1}$$

Note that the Bernoulli numbers satisfy

$$\frac{z}{e^z-1} = \sum_{p=0}^{\infty}\frac{B_p}{p!}z^p$$

We thus have

$$g(z) = \frac{z}{e^z-1}\cdot\frac{e^{nz}-1}{z} = \sum_{p=0}^{\infty}\frac{B_p}{p!}z^p \cdot \sum_{q=0}^{\infty}\frac{n^{q+1}}{(q+1)!}z^q = \sum_{j=0}^{\infty} a_j \frac{z^j}{j!}$$

The sum of powers is then obtained as

$$a_j = \sum_{i=0}^{n-1} i^j = \frac{1}{j+1}\sum_{p=0}^{j}\binom{j+1}{p} B_p\, n^{j+1-p}$$

Finally, we have

$$\begin{aligned} S_n &= \sum_{j=0}^{\mu}\binom{\mu}{j} a^{\mu-j}h^{j+1}\frac{1}{j+1}\sum_{k=0}^{j}\binom{j+1}{k} B_k\, n^{j+1-k} \\ &= \sum_{k=0}^{\mu}\frac{B_k}{n^{k-1}}\sum_{j=k}^{\mu}\binom{\mu}{j} a^{\mu-j}h^{j+1}\frac{1}{j+1}\binom{j+1}{k}\, n^j \end{aligned}$$

The combinatorial numbers can be simplified to

$$
\begin{aligned}
S_n &= \sum_{k=0}^{\mu} \frac{B_k}{n^{k-1}} a^\mu h \frac{\mu!}{k!\,(\mu+1-k)!}\left[\left(1+\frac{nh}{a}\right)^{\mu+1-k}-1\right]\left(\frac{nh}{a}\right)^{k-1} \\
&= \sum_{k=0}^{\mu} \frac{B_k}{n^{k-1}} a^\mu h \frac{\mu!}{k!\,(\mu+1-k)!}\left(\frac{b^{\mu+1-k}-a^{\mu+1-k}}{a^{\mu+1-k}}\right)\left(\frac{b-a}{a}\right)^{k-1} \\
&= \sum_{k=0}^{\mu} B_k \binom{\mu}{k} h^k \cdot \frac{b^{\mu+1-k}-a^{\mu+1-k}}{\mu+1-k} \\
&= \frac{1}{\mu+1}\left(b^{\mu+1}-a^{\mu+1}\right) + \sum_{k=1}^{\mu} \frac{B_k}{k!} h^k \left[\frac{\mu!\cdot b^{\mu+1-k}}{(\mu+1-k)!} - \frac{\mu!\cdot a^{\mu+1-k}}{(\mu+1-k)!}\right]
\end{aligned}
$$

Recall that $f(x) = x^\mu$, and we obtain

$$
S_n = \int_a^b f(x)\,\mathrm{d}x + \sum_{k=1}^{\infty} \frac{B_k}{k!} h^k \left[f^{(k-1)}(b) - f^{(k-1)}(a)\right]
$$

Note that the Bernoulli numbers are

$$
B_0 = 1, \qquad B_1 = -\frac{1}{2}, \qquad B_{2k+1} = 0 \text{ for } k \geq 1
$$

We can thus write

$$
S_n = \int_a^b f(x)\,\mathrm{d}x - \frac{h}{2}[f(b) - f(a)] + \sum_{l=1}^{\infty} \frac{B_{2l}}{(2l)!} h^{2l} \left[f^{(2l-1)}(b) - f^{(2l-1)}(a)\right]
$$

In fact, the trapezoidal rule approximate the integral as

$$
T_n = S_n + \frac{h}{2}[f(b) - f(a)]
$$

Finally, we have

$$
T_n = \int_a^b f(x)\,\mathrm{d}x + \sum_{l=1}^{\infty} \frac{B_{2l}}{(2l)!} h^{2l} \left[f^{(2l-1)}(b) - f^{(2l-1)}(a)\right]
$$

Usually, we can write it as

$$
\int_a^b f(x)\,\mathrm{d}x = T_n - \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!} h^{2l} \left[f^{(2l-1)}(b) - f^{(2l-1)}(a)\right] + R_{mn}
$$

- Euler-Maclaurin formula

Consider a function $f \in C^m[a,b]$. For $n \in \mathbb{N}^+$ we have

$$
\int_a^b f(x)\,\mathrm{d}x = T_n - \sum_{k=2}^{m} \frac{B_k}{k!} h^k \left[f^{(k-1)}(b) - f^{(k-1)}(a)\right] + R_{mn}
$$

The remainder term R_{mn} is given by

$$R_{mn} = \frac{(-1)^m}{m!} h^m \int_a^b B_m\left(\left\{\frac{x-a}{b-a} n\right\}\right) f^{(m)}(x)\,\mathrm{d}x$$

Note that $\{y\} = y - [y]$ and the Bernoulli polynomial $B_m(t)$ is

$$B_m(t) = \sum_{k=0}^{m} \binom{m}{k} B_k t^{m-k}$$

Proof. First consider $n = 1$ case with $h = b - a$. We need to prove

$$\int_a^b f(x)\,\mathrm{d}x = \frac{b-a}{2}[f(a) + f(b)] - \sum_{k=2}^{m} \frac{B_k}{k!}(b-a)^k \left[f^{(k-1)}(b) - f^{(k-1)}(a)\right] + R_{m1}$$

Denote $F(x)$ as the integral function

$$F(x) = \int_a^x f(x)\,\mathrm{d}x, \qquad F(a) = 0$$

Now we need to prove

$$F(b) = \frac{b-a}{2}[F'(a) + F'(b)] - \sum_{k=2}^{m} \frac{B_k}{k!}(b-a)^k \left[F^{(k)}(b) - F^{(k)}(a)\right] + R_{m1}$$

As a comparison, the Taylor expansion is

$$F(b) = F'(a)(b-a) + \sum_{k=2}^{m} \frac{1}{k!}(b-a)^k F^{(k)}(a) + \tilde{R}_m$$

Consider two functions $f, g \in C^m[a,b]$. The formula of integration by parts is

$$\int_a^b f(x) g^{(m)}(x)\,\mathrm{d}x = \left[\sum_{k=0}^{m-1} (-1)^k f^{(k)}(x) g^{(m-1-k)}(x)\right]_a^b + (-1)^m \int_a^b f^{(m)}(x) g(x)\,\mathrm{d}x$$

With a change of variable, we have

$$\int_a^b f(x) g^{(m)}(a+b-x)\,\mathrm{d}x = \sum_{k=0}^{m-1} \left[f^{(k)}(a) g^{(m-1-k)}(b) - f^{(k)}(b) g^{(m-1-k)}(a)\right]$$
$$+ \int_a^b f^{(m)}(x) g(a+b-x)\,\mathrm{d}x \qquad (*)$$

We need to choose $g(x)$ properly. To prove the Taylor expansion, we require

$$g^{(m)}(x) \equiv 1, \qquad g^{(k)}(a) = 0, \qquad k = 0,1,\cdots,m-1$$

This sets the function $g(x)$ as

$$g(x) = \frac{(x-a)^m}{m!}$$

To prove the E-M formula, we also require that $g(x)$ is a polynomial, in order to obtain $F(b)$ on the LHS of the formula.

$$g^{(m)}(x) \equiv 1 \qquad \Longrightarrow \qquad g(x) = \sum_{p=0}^{m} b_p \frac{(x-a)^{m-p}}{(m-p)!}, \qquad b_0 = 1$$

The derivative becomes

$$g^{(k)}(x) = \sum_{p=0}^{m-k} b_p \frac{(x-a)^{m-k-p}}{(m-k-p)!}$$

Furthermore, the $k = 0$ term requires

$$g^{(m-1)}(b) = \frac{b-a}{2}, \qquad g^{(m-1)}(a) = \frac{a-b}{2} \qquad \Longrightarrow \qquad b_1 = \frac{a-b}{2}$$

Similarly, for other terms we require

$$g^{(k)}(a) = g^{(k)}(b), \qquad \text{for } k = 0,1,\cdots,m-2$$

This leads to a linear system

$$\sum_{p=0}^{m-k-1} b_p \frac{(b-a)^{m-k-p}}{(m-k-p)!} = 0, \qquad \sum_{p=0}^{l-1} \frac{p!\, b_p}{(b-a)^p} \binom{l}{p} = 0, \qquad l \geq 2$$

Based on the following identity of the Bernoulli numbers

$$\sum_{p=0}^{l-1} B_p \binom{l}{p} = 0, \qquad l \geq 2$$

The coefficients b_p are solved as

$$b_p = \frac{(b-a)^p}{p!} B_p$$

Therefore, we choose $g(x)$ as

$$g_m(x) = \sum_{p=0}^{m} \frac{(b-a)^p}{p!} B_p \frac{(x-a)^{m-p}}{(m-p)!}$$

$$= \frac{(b-a)^m}{m!} \sum_{p=0}^{m} B_P \binom{m}{p} \left(\frac{x-a}{b-a}\right)^{m-p} = \frac{(b-a)^m}{m!} B_m \left(\frac{x-a}{b-a}\right)$$

Its derivative becomes

$$g_m^{(k)}(x) = \sum_{p=0}^{m-k} \frac{(b-a)^p}{p!} B_p \frac{(x-a)^{m-k-p}}{(m-k-p)!} = g_{m-k}(x)$$

Substitute into $(*)$, we have

$$\int_a^b f(x)\,\mathrm{d}x = \frac{b-a}{2}[f(a)+f(b)] - \sum_{k=2}^{m} \frac{B_k}{k!}(b-a)^k \left[f^{(k-1)}(b) - f^{(k-1)}(a)\right] + R_{m1}$$

For the remainder term, note that

$$B_m(1-x) = (-1)^m B_m(x)$$

This can be demonstrated from the generating function of $B_m(x)$, which is

$$\frac{ze^{xz}}{e^z-1}=\sum_{m=0}^{\infty}B_m(x)\frac{z^m}{m!}$$

Substitute $x\to 1-x$, and we have

$$\sum_{m=0}^{\infty}B_m(1-x)\frac{z^m}{m!}=\frac{ze^{(1-x)z}}{e^z-1}=\frac{-ze^{-xz}}{e^{-z}-1}=\sum_{m=0}^{\infty}B_m(x)\frac{(-z)^m}{m!}$$

With this, we can show that

$$R_{m1}=\frac{(b-a)^m}{m!}\int_a^b f^{(m)}(x)B_m\left(\frac{b-x}{b-a}\right)\,\mathrm{d}x$$

$$=\frac{(-1)^m}{m!}(b-a)^m\int_a^b B_m\left(\frac{x-a}{b-a}\right)f^{(m)}(x)\,\mathrm{d}x$$

For all other cases with $n>1$, within each interval $I_i=[x_{i-1},x_i]$ with $i=1,2,\cdots,n$, we can apply the E-M formula as

$$\int_{x_{i-1}}^{x_i}f(x)\,\mathrm{d}x=\frac{h}{2}[f(x_{i-1})+f(x_i)]-\sum_{k=2}^{m}\frac{B_k}{k!}h^k\left[f^{(k-1)}(x_i)-f^{(k-1)}(x_{i-1})\right]$$

$$+\frac{(-1)^m}{m!}h^m\int_{x_{i-1}}^{x_i}B_m\left(\frac{x-x_{i-1}}{h}\right)f^{(m)}(x)\,\mathrm{d}x$$

Before adding up the results from each I_i, we need to manipulate the remainder term. Note that

$$x_{i-1}=a+(i-1)h\le x<x_i=a+ih,\qquad i-1\le\frac{x-a}{b-a}n<i,\qquad i-1=\left[\frac{x-a}{b-a}n\right]$$

Then we have

$$B_m\left(\frac{x-x_{i-1}}{h}\right)=B_m\left(\frac{x-a}{b-a}n-\left[\frac{x-a}{b-a}n\right]\right)=B_m\left(\left\{\frac{x-a}{b-a}n\right\}\right)$$

The sum over all intervals gives the final E-M formula. ■

Corollary

Let $f\in C^m(\mathbb{R}_{>0})$, with $a,b\in\mathbb{N}$ and $a<b$. We have

$$\sum_{a\le k<b}f(k)=\int_a^b f(x)\,\mathrm{d}x+\sum_{l=1}^{m}\frac{B_l}{l!}\left[f^{(l-1)}(b)-f^{(l-1)}(a)\right]$$

$$+\frac{(-1)^{m+1}}{m!}\int_a^b B_m(\{x\})\,f^{(m)}(x)\,\mathrm{d}x$$

To prove this, consider $n=b-a$ and $h=1$. ■

Properties of Bernoulli polynomial / function

$$B_0(x) = 1, \qquad B_1(\{x\}) = \{x\} - \frac{1}{2}$$
$$B_m'(x) = mB_{m-1}(x)$$
$$\int_0^1 B_m(x)\,\mathrm{d}x = 0, \qquad \text{for } m \geq 1$$
$$B_m(0) = B_m(1), \qquad \text{for } m \geq 2$$

Fourier series of Bernoulli function

$B_m(\{x\})$ is continuous, piecewise smooth with period 1. This implies that its Fourier series is pointwise convergent. Denote

$$a_{mk} = \int_0^1 B_m(x)\, e^{-i2\pi kx}\,\mathrm{d}x\,, \qquad k \in \mathbb{Z}$$

Specifically, we have

$$a_{00} = 1, \qquad a_{0k} = 0, \qquad \text{for } k \neq 0, \qquad a_{m0} = 0, \qquad \text{for } m \geq 1$$

We can first calculate

$$a_{1k} = \int_0^1 \left(x - \frac{1}{2}\right) e^{-i2\pi kx}\,\mathrm{d}x = \frac{i}{2\pi k}$$

For $m \geq 2$, using the recursive relation and integration by parts gives

$$a_{mk} = \frac{m}{2\pi ik} a_{(m-1)k}, \qquad a_{mk} = -\frac{m!}{(2\pi ik)^m}, \qquad \text{for } m \geq 1 \text{ and } k \neq 0$$

The Fourier series becomes

$$B_m(\{x\}) = -\frac{m!}{(2\pi i)^m} \sum_{k \neq 0} \frac{e^{i2\pi kx}}{k^m}$$

The series is absolutely convergent for $m \geq 2$.

Bernoulli number

In the Fourier series, taking $x = 0$ gives

$$B_m = -(-i)^m \frac{m!}{(2\pi)^m} \sum_{k \neq 0} \frac{1}{k^m}$$

When m is odd, we have $B_m = 0$ due to cancellation for positive and negative k. When m is even with $m = 2l$, we have

$$B_{2l} = (-1)^{l+1} \frac{(2l)!}{(2\pi)^{2l}} \cdot 2\zeta(2l), \qquad \zeta(2l) = (-1)^{l+1} B_{2l} \frac{2^{2l-1}\pi^{2l}}{(2l)!}$$

This is the relation between the Riemann zeta function and Bernoulli number.

As $l \to \infty$, the Bernoulli number behaves as

$$|B_{2l}| \sim \frac{2 \cdot (2l)!}{(2\pi)^{2l}} \sim \sqrt{2\pi \cdot 2l}\left(\frac{2l}{e}\right)^{2l} \frac{1}{2^{2l-1}\pi^{2l}}\,, \qquad \text{as } l \to \infty$$

Bound of the Bernoulli function

$$|B_m(\{x\})| \le \frac{m!}{(2\pi)^m} \sum_{k \neq 0} \frac{1}{k^m} = |B_m|$$

Example 1

$$f(x) = x^s, \qquad s \in \mathbb{N}$$

Note that when we choose $m > s$, we have

$$f^{(m)}(x) = 0, \qquad \text{for } m > s$$

From E-M formula, with $[a, b] = [0, n]$, we have

$$\sum_{1 \le k < n} k^s = \frac{n^{s+1}}{s+1} - \frac{n^s}{2} + \sum_{l=2}^{s} \frac{B_l}{l!} \frac{s!}{(s-l+1)!} n^{s-l+1}$$

The sum of powers is thus obtained as

$$\sum_{1 \le k \le n} k^s = \frac{1}{s+1}\left[n^{s+1} + \frac{s+1}{2} n^s + \sum_{l=2}^{s} B_l \binom{s+1}{l} n^{s-l+1}\right]$$

As an example, for $s = 4$ we have

$$B_2 = \frac{1}{6}, \qquad B_4 = -\frac{1}{30}, \qquad \sum_{1 \le k \le n} k^4 = \frac{1}{5}\left(n^5 + \frac{5}{2} n^4 + \frac{5}{3} n^3 - \frac{1}{6} n\right)$$

Example 2

$$f(x) = \frac{1}{x}, \qquad [a, b] = [1, n]$$

The partial sum of the harmonic series can be written as

$$\sum_{1 \le k < n} \frac{1}{k} = \ln n + \sum_{l=1}^{2m} \frac{B_l}{l!}\left[(-1)^{l-1}(l-1)!\left(\frac{1}{n^l} - 1\right)\right]$$

$$+ \frac{(-1)^{2m+1}}{(2m)!} \int_1^n B_{2m}(\{x\})\,(-1)^{2m} \frac{(2m)!}{x^{2m+1}}\,\mathrm{d}x$$

$$= \ln n + \left(-\frac{1}{2}\right)\left(\frac{1}{n} - 1\right) + \sum_{l=1}^{m} \frac{B_{2l}}{2l}\left(1 - \frac{1}{n^{2l}}\right) - \int_1^n B_{2m}(\{x\}) \frac{1}{x^{2m+1}}\,\mathrm{d}x$$

We thus obtain

$$H_n = \sum_{1\le k\le n} \frac{1}{k} = \ln n + \frac{1}{2} + \frac{1}{2n} + \sum_{l=1}^{m} \frac{B_{2l}}{2l}\left(1 - \frac{1}{n^{2l}}\right) - \int_1^n \frac{B_{2m}(\{x\})}{x^{2m+1}}\,\mathrm{d}x$$

Consider the limit $n \to \infty$, we can express the Euler's constant γ as

$$H_n - \ln n \to \gamma, \qquad \gamma = \frac{1}{2} + \sum_{l=1}^{m} \frac{B_{2l}}{2l} - \int_1^\infty \frac{B_{2m}(\{x\})}{x^{2m+1}}\,\mathrm{d}x$$

Therefore, we have

$$H_n = \ln n + \gamma + \frac{1}{2n} - \sum_{l=1}^{m} \frac{B_{2l}}{2l}\frac{1}{n^{2l}} + \int_n^\infty \frac{B_{2m}(\{x\})}{x^{2m+1}}\,\mathrm{d}x$$

The remainder term is now bounded as

$$\left|\int_n^\infty \frac{B_{2m}(\{x\})}{x^{2m+1}}\,\mathrm{d}x\right| \le |B_{2m}| \cdot \int_n^\infty \frac{1}{x^{2m+1}}\,\mathrm{d}x = \frac{|B_{2m}|}{2m}\frac{1}{n^{2m}}$$

The partial sum H_n is usually expressed as

$$H_n = \ln n + \gamma + \frac{1}{2n} - \sum_{l=1}^{m-1} \frac{B_{2l}}{2l}\frac{1}{n^{2l}} - \theta_{mn}\frac{B_{2m}}{2m}\frac{1}{n^{2m}}, \qquad 0 < \theta_{mn} < 1$$

For $n = m = 5$, we can achieve an accuracy of

$$\left|\theta_{mn}\frac{B_{2m}}{2m}\frac{1}{n^{2m}}\right| < 10^{-10}$$

This is the general procedure of using E-M formula to obtain a well-constrained remainder.

Example 3

$$f(x) = \frac{1}{x^s}, \qquad s > 1, \qquad [a, b] = [1, n]$$

Note that

$$f^{(k)}(x) = (-1)^k \frac{\Gamma(s+k)}{\Gamma(s)}\frac{1}{x^{s+k}}$$

Following the same procedure, we can obtain a way to compute Riemann ζ function

$$\zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^s} = \sum_{1\le k\le n} \frac{1}{k^s} + \frac{1}{s-1}\frac{1}{n^{s-1}} - \frac{1}{2n^s} + \sum_{l=1}^{m-1} \frac{B_{2l}}{(2l)!}\frac{\Gamma(s+2l-1)}{\Gamma(s)}\frac{1}{n^{s+2l-1}}$$
$$+\theta_{mn}\frac{B_{2m}}{(2m)!}\frac{\Gamma(s+2m-1)}{\Gamma(s)}\frac{1}{n^{s+2m-1}}$$

For $s = 2$, we have

$$\zeta(2) = \frac{\pi^2}{6} \approx \sum_{1\le k\le n} \frac{1}{k^2} + \frac{1}{n} - \frac{1}{2n^2} + \sum_{l=1}^{m-1} \frac{B_{2l}}{n^{2l+1}}$$

Example 4

$$f(x) = \ln x\,, \qquad [a,b] = [1,n]$$

Note that

$$f^{(k)}(x) = (-1)^{k-1}\frac{(k-1)!}{x^k}$$

Following the same procedure, we obtain the Stirling formula

$$\ln n! = \left(n+\frac{1}{2}\right)\ln n - n + C + \sum_{l=1}^{m}\frac{B_{2l}}{2l(2l-1)}\frac{1}{n^{2l-1}} + \theta_{mn}\frac{B_{2m+2}}{(2m+2)(2m+1)}\frac{1}{n^{2m+1}}$$

The constant C is given as

$$C = \frac{1}{2}\ln(2\pi)\,, \qquad e^C = \lim_{n\to\infty}\frac{n!}{\sqrt{n}\left(\frac{n}{e}\right)^n} = \lim_{n\to\infty}\frac{(2n)!}{\sqrt{2n}\left(\frac{2n}{e}\right)^{2n}} = \sqrt{2\pi}$$

This result uses the Wallis formula

$$\lim_{n\to\infty}\frac{2^{2n}(n!)^2}{\sqrt{n}\,(2n)!} = \sqrt{\pi}$$

In the previous examples, we all have

$$\int_a^b f(x)\,\mathrm{d}x \ \text{ integrable}, \qquad \int_1^\infty \left|f^{(m)}(x)\right|\mathrm{d}x \ \text{ convergent}$$

Example 5

$$f(x) = x^x$$

Note that

$$S_n = \sum_{k=1}^{n} k^k\,, \qquad \lim_{n\to\infty}\frac{S_n}{n^n} = \lim_{n\to\infty}\frac{S_n - S_{n-1}}{n^n - (n-1)^{n-1}} = 1$$

Therefore, we can consider

$$S_n = n^n\left(1 + \frac{C}{n} + o\left(\frac{1}{n}\right)\right)$$

The coefficient C is

$$C = \lim_{n\to\infty} n\left(\frac{S_n}{n^n} - 1\right) = \lim_{n\to\infty}\frac{S_{n-1}}{(n+1)^n} = \frac{1}{e}$$

We can iteratively solve all coefficients, but it is not efficient.

Now consider

$$S_n = n^n\left(C_0 + \frac{C_1}{n} + \frac{C_2}{n^2} + \cdots \frac{C_m}{n^m} + o\left(\frac{1}{n^m}\right)\right)$$

We have

$$n^n = S_n - S_{n-1} = n^n \sum_{k=0}^{m} \frac{C_k}{n^k} - (n-1)^{n-1} \sum_{k=0}^{m} \frac{C_k}{(n-1)^k}$$

$$1 = \sum_{k=0}^{m} \frac{C_k}{n^k} - \left(1 - \frac{1}{n}\right)^n \sum_{k=0}^{m} \frac{C_k}{(n-1)^{k+1}}$$

Substitute $x = 1/n$ and we obtain

$$1 = \sum_{k=0}^{m} C_k x^k - \frac{1}{e}\left(\sum_{n\geq 0} b_n x^n\right)\left[\sum_{k=0}^{m} C_k x^{k+1}\left(\sum_{l\geq 0} d_{kl} x^l\right)\right] + o(x^m)$$

The two series with coefficients $\{b_n\}$ and $\{d_n\}$ are obtained as

$$(1-x)^{\frac{1}{x}} = \frac{1}{e}\sum_{n\geq 0} b_n x^n = \frac{1}{e}\left(1 - \frac{x}{2} - \frac{5}{24}x^2 - \frac{5}{48}x^3 - \frac{337}{5760}x^4 + o(x^4)\right)$$

$$\frac{1}{(1-x)^{k+1}} = \sum_{l\geq 0} d_{kl} x^l = \sum_{l\geq 0} \binom{k+l}{l} x^l$$

Comparing the coefficients, we can solve for C_k as

$$C_0 = 1, \qquad C_1 = \frac{1}{e}, \qquad C_2 = \frac{1}{e^2} + \frac{1}{2e}, \qquad C_3 = \frac{1}{e^3} + \frac{2}{e^2} + \frac{7}{24e}$$

$$C_4 = \frac{1}{e^4} + \frac{9}{2e^3} + \frac{10}{3e^2} + \frac{3}{16e}, \qquad C_5 = \frac{1}{e^5} + \frac{8}{e^4} + \frac{117}{8e^3} + \frac{16}{3e^2} + \frac{743}{5760e}$$

- Exercise

Barnes G-function

We directly start from the following representation of $G(1+z)$

$$\ln G(1+z) = \frac{z(1-z)}{2} + \frac{z}{2}\ln(2\pi) + z\ln\Gamma(z) - \int_0^z \ln\Gamma(x)\,\mathrm{d}x$$

From the Stirling formula, we have the asymptotic expansion

$$\ln\Gamma(z) = \left(z - \frac{1}{2}\right)\ln z - z + \frac{1}{2}\ln(2\pi) + \frac{1}{12z} + \sum_{l=2}^{N} \frac{B_{2l}}{2l(2l-1)}\frac{1}{z^{2l-1}} + o\left(\frac{1}{z^{2N+1}}\right)$$

$$= \left(z - \frac{1}{2}\right)\ln z - z + \frac{1}{2}\ln(2\pi) + \frac{1}{12z} + \sum_{l=1}^{N} \frac{B_{2l+2}}{(2l+1)(2l+2)}\frac{1}{z^{2l+1}} + o\left(\frac{1}{z^{2N+3}}\right)$$

The integral of $\ln\Gamma(x)$ can be decomposed into two parts. The integral from 0 to 1 is a constant, while from 1 to z we have

$$-\int_1^z \ln\Gamma(x)\,\mathrm{d}x = -\frac{z^2}{2}\ln z + \frac{3}{4}z^2 + \frac{z}{2}\ln z - \frac{z}{2} - \frac{z}{2}\ln(2\pi) - \frac{1}{12}\ln z - \frac{1}{4} + \frac{1}{2}\ln(2\pi)$$

$$+\sum_{l=1}^{N}\frac{B_{2l+2}}{2l(2l+1)(2l+2)}\left(\frac{1}{z^{2l}}-1\right)+o\left(\frac{1}{z^{2N+2}}\right)$$

Also note that

$$\sum_{l=1}^{N}\frac{B_{2l+2}}{(2l+1)(2l+2)}\frac{1}{z^{2l}}\cdot\left(\frac{1}{2l}+1\right)=\sum_{l=1}^{N}\frac{B_{2l+2}}{4l(l+1)}\frac{1}{z^{2l}}$$

Therefore, we have

$$\ln G(1+z)=z^2\ln z-\frac{3}{4}z^2+\frac{z}{2}\ln(2\pi)-\frac{1}{12}\ln z+\frac{1}{12}-\ln A$$
$$+\sum_{l=1}^{N}\frac{B_{2l+2}}{4l(l+1)}\frac{1}{z^{2l}}+o\left(\frac{1}{z^{2N+2}}\right)$$

Smoothed sum of arithmetic functions (link)

The asymptotic behavior of a divergent partial sum can be analyzed by introducing a smoothing function $\eta(x)$ and consider the infinite sum

$$\sum_{n=1}^{\infty}a(n)\,\eta\left(\frac{n}{N}\right)$$

We study the case $a(x)=x^s$ for $s\in\mathbb{N}$ using the cutoff function $\eta(x)$, a compactly supported bounded function in C^∞ with $\eta(x)=1$ for $x\leq 1/2$ and $\eta(x)=0$ for $x\geq 1$. Note that

$$f(x)=x^s\eta\left(\frac{x}{N}\right),\qquad f^{(k)}(x)=\begin{cases}0, & x\geq N\\ \dfrac{s!}{(s-k)!}x^{s-k}, & x\leq\dfrac{N}{2}\ \text{ and }\ k\leq s\end{cases}$$

The Euler-Maclaurin formula gives (as $N\to\infty$)

$$\sum_{n=0}^{N-1}f(n)=\int_0^N f(x)\,\mathrm{d}x-\frac{1}{2}[f(N)-f(0)]$$
$$+\sum_{l=1}^{m}\frac{B_{2l}}{(2l)!}\left[f^{(2l-1)}(N)-f^{(2l-1)}(0)\right]-\frac{1}{(2m)!}\int_0^N B_{2m}(\{x\})f^{(2m)}(x)\,\mathrm{d}x$$

The integral term is evaluated as

$$\int_0^N x^s\eta\left(\frac{x}{N}\right)\,\mathrm{d}x=N^{s+1}\int_0^1 x^s\eta(x)\,\mathrm{d}x=C_{\eta,s}N^{s+1}$$

The remainder term is bounded as

$$|R|\leq\frac{B_{2m}}{(2m)!}\int_0^N f^{(2m)}(x)\,\mathrm{d}x=O(N\cdot\|f\|_{C^{2m}}),\qquad\|f\|_{C^{2m}}=\sup_{x\in\mathbb{R}}\left|f^{(2m)}(x)\right|$$

For $s \geq 1$, we can choose $2m \geq s + 2$ and obtain

$$\sum_{n=1}^{\infty} f(n) = \sum_{n=0}^{N-1} x^s \eta\left(\frac{x}{N}\right) = C_{\eta,s} N^{s+1} - \frac{B_{s+1}}{(s+1)!} f^{(s)}(0) + O(N \cdot \|f\|_{C^{s+2}})$$

$$= -\frac{B_{s+1}}{s+1} + C_{\eta,s} N^{s+1} + O\left(\frac{1}{N}\right), \qquad N \to \infty$$

For $s = 0$, we can choose $m = 1$ and obtain

$$\sum_{n=1}^{\infty} f(n) = \sum_{n=0}^{N-1} \eta\left(\frac{x}{N}\right) - 1 = C_{\eta,0} N + \frac{1}{2}\eta(0) + O(N \cdot \|f\|_{C^2}) - 1$$

$$= -\frac{1}{2} + C_{\eta,0} N + O\left(\frac{1}{N}\right), \qquad N \to \infty$$

We recognize that the leading term is the specific values of the Riemann zeta function

$$\zeta(-s) = -\frac{B_{s+1}^{+}}{s+1}, \qquad \text{with } B_1^{+} = \frac{1}{2}$$

Now we extend to complex s with function

$$g(x) = \frac{1}{x^s}\left[\eta\left(\frac{x}{N}\right) - \eta\left(\frac{2x}{N}\right)\right], \qquad s \in \mathbb{C}, \qquad \mathrm{Re(s)} < 1$$

The reason is that now x^{-s} is singular at the origin, which prevents us from taking the value at $x = 0$. With this telescoped sum, we immediately obtain

$$G_N(n) = \sum_{n=1}^{\infty} g(n) = C_{\eta,-s}\left[N^{1-s} - \left(\frac{N}{2}\right)^{1-s}\right] + O\left(\frac{1}{N}\right), \qquad N \to \infty$$

By summing the telescoping series, we have

$$\sum_{k=1}^{\log_2 N} G_{2^k}(n) = \left[\sum_{n=1}^{\infty} \frac{1}{n^s}\eta\left(\frac{n}{2}\right) - \sum_{n=1}^{\infty} \frac{1}{n^s}\eta(n)\right] + \left[\sum_{n=1}^{\infty} \frac{1}{n^s}\eta\left(\frac{n}{4}\right) - \sum_{n=1}^{\infty} \frac{1}{n^s}\eta\left(\frac{n}{2}\right)\right] + \cdots$$

$$= C_{\eta,-s}[2^{1-s} - 1^{1-s}] + C_{\eta,-s}[4^{1-s} - 2^{1-s}] + \cdots + O\left(\frac{1}{N}\right)$$

This shows that

$$\sum_{n=1}^{\infty} \frac{1}{n^s}\eta\left(\frac{n}{N}\right) = \zeta(s) + C_{\eta,-s} N^{1-s} + O\left(\frac{1}{N}\right)$$

The following limit thus exists

$$\zeta(s) = \lim_{N \to \infty}\left[\sum_{n=1}^{\infty} \frac{1}{n^s}\eta\left(\frac{n}{N}\right) - C_{\eta,-s} N^{1-s}\right]$$

Formal Power Series & Lagrange Inversion Theorem

➢ Formal power series

Definitions

For a domain K with char $K = 0$ (e.g., $\mathbb{Q}, \mathbb{R}, \mathbb{C}$)

- Series: $\{a_n\},\ \mathbb{Z} \to K$
- Laurent series: There exists $n_0 \in \mathbb{Z}$ such that $a_n = 0$ for $n < n_0$
- Formal power series

$$f(z) = \sum_{n\in\mathbb{Z}} a_n z^n$$

- Addition, multiplication

$$(f+g)(z) = \sum_{n\in\mathbb{Z}} (a_n + b_n) z^n, \qquad (\lambda f)(z) = \sum_{n\in\mathbb{Z}} (\lambda a_n) z^n$$

$$(f\cdot g)(z) = \sum_{n\in\mathbb{Z}} c_n z^n, \qquad c_n = \sum_{p\in\mathbb{Z}} a_p b_{n-p}$$

- Division: Given two formal power series

$$f(z) = \sum_{n\geq n_0} a_n z^n, \qquad g(z) = \sum_{m\geq m_0} b_m z^m, \qquad b_{m_0} \neq 0$$

  Consider $h(z) = (f/g)(z)$ has the form

$$h(z) = \sum_{k\geq n_0 - m_0} d_k z^k$$

  From multiplication, we obtain the linear system and can solve for all coefficients d_k

$$a_n = \sum_{p\in\mathbb{Z}} b_p d_{n-p}$$

- The set $\mathcal{A}(K) = \{f(z) \mid \{a_n\} \text{ is a Laurent series}\}$ is also a domain.
- For $f \in \mathcal{A}$, define the order of f as the minimal n such that $a_n \neq 0$, denoted as $\operatorname{ord}(f)$. We specify $\operatorname{ord}(0) = +\infty$.
- For $f, g \in \mathcal{A}$, define distance as

$$d(f,g) = e^{-\operatorname{ord}(f-g)}$$

- **Corollary.** Distance $d(f,g)$ is a complete metric, and $(\mathcal{A}, d)$ is complete. Consider a Cauchy series $\{f_n\} \subset \mathcal{A}$, we have

$$\forall \varepsilon > 0,\ \exists N \in \mathbb{N},\ \forall m,n > N,\ d(f_m, f_m) < \varepsilon,\ \operatorname{ord}(f_m - f_n) > -\ln \varepsilon$$

  Let $M = [-\ln \varepsilon]$, then for any $k < M$, the z^k coefficients of f_m and f_n are the same.

- If $\mathrm{ord}(f) = 1$, then f is invertible. Denote the set $\mathcal{A}^* = \{f \in \mathcal{A} \mid f \text{ invertible}\}$
- For $n \in \mathbb{Z}$, denote $[z^n]: f \to K$ as the operation

$$[z^n]\left(\sum_{n\in\mathbb{Z}} a_n z^n\right) = a_n$$

- **Corollary.** For $f, g \in \mathcal{A}$ with $\mathrm{ord}(g) \geq 1$, we have

$$f\big(g(z)\big) = \sum_{n\geq n_0} a_n \big(g(z)\big)^n \in \mathcal{A}$$

Proof. Denote $\mathrm{ord}(g) = m_0 \geq 1$, and

$$\big(g(z)\big)^n = \sum_{m\geq nm_0} b_m^{(n)} z^m, \qquad f\big(g(z)\big) = \sum_{n\geq n_0} a_n \sum_{m\geq nm_0} b_m^{(n)} z^m$$

Since $m_0 \geq 1$, we have

$$f\big(g(z)\big) = \sum_{m\geq n_0 m_0} \sum_{n=n_0}^{[m/m_0]} a_n b_m^{(n)} z^m \in \mathcal{A}$$

■

- **Corollary.** For $g \in \mathcal{A}^*$, there exists a unique $h = g^{-1} \in \mathcal{A}^*$ such that

$$g\big(h(z)\big) = h\big(g(z)\big) = z$$

Proof. Since $g \in \mathcal{A}^*$, we have $b_1 \neq 0$ and $b_n^{(n)} = b_1^n \neq 0$. We have

$$h(z) = \sum_{n\geq 1} a_n z^n, \qquad h\big(g(z)\big) = z$$

This leads to a linear system, and we can solve for coefficients as

$$a_1 = \frac{1}{b_1}, \qquad a_2 = -\frac{a_1 b_2^{(1)}}{b_1^2}, \cdots$$

We then need to show that $g\big(h(z)\big) = z$ also holds. For $h \in \mathcal{A}^*$, we can also find $\tilde{h} \in \mathcal{A}^*$ such that $\tilde{h}\big(h(z)\big) = z$. Now with $z \to h(z)$, we have

$$h\big(g(z)\big) = z, \qquad h\Big(g\big(h(z)\big)\Big) = h(z), \qquad \tilde{h}\Big(h\Big(g\big(h(z)\big)\Big)\Big) = \tilde{h}\big(h(z)\big)$$

From the property of $\tilde{h}(z)$, we prove

$$g\big(h(z)\big) = z$$

■

- $(\mathcal{A}^*, \cdot)$ is a group, where $\cdot$ denotes composition.

- Multinomial theorem

For a commutative ring R

$$(y_1 + \cdots + y_m)^n = \sum_{\substack{d_1,\cdots,d_m \geq 0 \\ d_1+\cdots+d_m=n}} \frac{n!}{d_1! \cdots d_m!} y_1^{d_1} \cdots y_m^{d_m}, \qquad y_i \in R$$

This can be proved by induction over m. The binomial theorem corresponds to $m = 2$.

Inverse of a formal power series

To calculate f/g, we only need $1/g$, which is

$$g = b_{m_0} z^{m_0} + b_{m_0+1} z^{m_0+1} + \cdots, \qquad \frac{1}{g} = \frac{1}{b_{m_0} z^{m_0}} \cdot \frac{1}{1 + \frac{b_{m_0+1}}{b_{m_0}} z + \frac{b_{m_0+2}}{b_{m_0}} z^2 + \cdots}$$

Now we focus on a specific type of $g \in \mathcal{A}$ with

$$g = \sum_{n \geq 0} b_n z^n, \qquad b_0 \neq 0$$

Then for $m \in \mathbb{N}$, the coefficients of $1/g$ are given as

$$[z^m]\left(\frac{1}{g(z)}\right) = \frac{1}{b_0} \sum_{\substack{d_1,\cdots,d_m \geq 0 \\ d_1+2d_2+\cdots+md_m=m}} \frac{(d_1 + \cdots + d_m)!}{d_1! \cdots d_m!} \left(-\frac{b_1}{b_0}\right)^{d_1} \cdots \left(-\frac{b_m}{b_0}\right)^{d_m}$$

Proof. Define a new series $y(z)$ and we have

$$y(z) = \sum_{k \geq 1} c_k z^k = \sum_{k \geq 1} \left(-\frac{b_k}{b_0}\right) z^k, \qquad \frac{1}{g(z)} = \frac{1}{b_0} \cdot \frac{1}{1 - y(z)} = \sum_{n \geq 0} \big(y(z)\big)^n$$

The coefficients become

$$[z^m]\left(\frac{1}{g(z)}\right) = \frac{1}{b_0} \sum_{n=0}^{m} [z^m]\big(y(z)\big)^n$$

Note the truncation to $n = m$ as we focus on $[z^m]$. We only need to prove

$$[z^m]\big(y(z)\big)^n = \sum_{\substack{d_1,\cdots,d_m \geq 0 \\ d_1+d_2+\cdots+d_m=n \\ d_1+2d_2+\cdots+md_m=m}} \frac{n!}{d_1! \cdots d_m!} c_1^{d_1} \cdots c_m^{d_m}$$

Using the multinomial theorem, we have

$$[z^m]\big(y(z)\big)^n = [z^m](c_1 z + c_2 z^2 + \cdots + c_m z^m)^n$$

$$= [z^m] \sum_{\substack{d_1,\cdots,d_m \geq 0 \\ d_1+\cdots+d_m=n}} \frac{n!}{d_1! \cdots d_m!} (c_1 z)^{d_1} \cdots (c_m z^m)^{d_m}$$

$$= \sum_{\substack{d_1,\cdots,d_m \geq 0 \\ d_1+d_2+\cdots+d_m=n \\ d_1+2d_2+\cdots+md_m=m}} \frac{n!}{d_1! \cdots d_m!} c_1^{d_1} \cdots c_m^{d_m} \qquad \blacksquare$$

Example

Roll the dice 10 times. We want to find the probability of the total sum being equal to 30. This problem is equivalent to

$$P = [x^{30}] \left(\frac{1}{6} x + \frac{1}{6} x^2 + \cdots + \frac{1}{6} x^6 \right)^{10} = \frac{1}{6^{10}} [x^{20}] \left(\frac{1-x^6}{1-x} \right)^{10}$$

$$= \frac{1}{6^{10}} [x^{20}] \frac{1}{(1-x)^{10}} \left(1 - 10x^6 + \binom{10}{2} x^{12} - \binom{10}{3} x^{18} \right)$$

$$= \frac{1}{6^{10}} \left([x^{20}] - 10 \cdot [x^{14}] + \binom{10}{2} [x^8] - \binom{10}{3} [x^2] \right) \frac{1}{(1-x)^{10}}$$

Note that

$$[x^m] \frac{1}{(1-x)^{10}} = (-1)^m \binom{-10}{m}$$

Then this probability can be computed.

- Bell polynomials

For $m, n \in \mathbb{N}$ with $m \geq n$, we have a formal power series $y(z)$ with coefficients $C = \{c_i\}_{i \geq 1}$. The Bell polynomial is defined as

$$B_{mn}(C) = [z^m] \big(y(z)\big)^n = \sum_{\substack{d_1,\cdots,d_m \geq 0 \\ d_1+d_2+\cdots+d_m=n \\ d_1+2d_2+\cdots+md_m=m}} \frac{n!}{d_1! \cdots d_m!} c_1^{d_1} \cdots c_m^{d_m}$$

Theorem. Consider $g(z) \in \mathcal{A}^*$ with

$$g(z) = \sum_{n \geq 1} b_n z^n$$

Then for any $m, n \in \mathbb{Z}$ with $m \geq n$, we have

$$[z^m] \big(g(z)\big)^n = \sum_{k=0}^{m-n} \binom{n}{k} b_1^{n-k} B_{(m-n)k}(b'), \qquad b' = (b_2, b_3, \cdots)$$

Theorem. For $f, g \in \mathcal{A}$ with $\operatorname{ord}(f) \geq 0$ and $\operatorname{ord}(g) \geq 1$, we have

$$[z^m]f\big(g(z)\big) = \sum_{n=0}^{m} a_n B_{mn}(b)$$

The above result implies the formula of the higher derivatives. Consider $f, g \in C^\infty$ with

$$a_n = [z^n]f(z) = \frac{1}{n!}f^{(n)}(y_0), \qquad b_m = [z^m]g(z) = \frac{1}{m!}g^{(m)}(x_0)$$

Note that

$$[z^m]f(g(z)) = \frac{1}{m!}(f \circ g)^{(m)}(x_0)$$

From this, we can obtain the Faà di Bruno's formula

$$(f \circ g)^{(m)}(x_0) = m! \sum_{n=0}^{m} a_n B_{mn}(b)$$
$$= m! \sum_{n=0}^{m} \frac{f^{(n)}\big(g(x_0)\big)}{n!} B_{mn}\left(\frac{g^{(1)}(x_0)}{1!}, \frac{g^{(2)}(x_0)}{2!}, \cdots, \frac{g^{(m)}(x_0)}{m!}\right)$$

➢ Derivatives and residues of formal power series

$$f'(z) = \sum n a_n z^{n-1}, \qquad \operatorname{Res} f = a_{-1} = [z^{-1}]\, f$$

Properties of derivatives

- Derivative operator $\mathcal{A} \to \mathcal{A}$ is linear
- If $f' = g'$ and $[z^0]f = [z^0]g$, then $f = g$
- $(fg)' = f'g + fg'$
- If $\operatorname{ord}(g) \geq 1$, then

$$\big[f\big(g(z)\big)\big]' = f'\big(g(z)\big)g'(z)$$

- If $g \in \mathcal{A}^*$, then

$$[g^{-1}(z)]' = \frac{1}{g'\big(g^{-1}(z)\big)}$$

Proof. From 4 to 5, the result is obvious since

$$\big[g\big(g^{-1}(z)\big)\big]' = g'\big(g^{-1}(z)\big) \cdot [g^{-1}(z)]' = 1, \qquad [g^{-1}(z)]' = \frac{1}{g'\big(g^{-1}(z)\big)}$$

To prove property 4, first consider $f(z) = z^n$. By induction, we have

$$\left[\big(g(z)\big)^n\right]' = \left[g(z)\big(g(z)\big)^{n-1}\right]' = g'(z)\big(g(z)\big)^{n-1} + g(z) \cdot (n-1)\big(g(z)\big)^{n-2} g'(z)$$

This directly gives

$$\left[\left(g(z)\right)^n\right]' = n\left(g(z)\right)^{n-1} g'(z)$$

When $n < 0$, consider

$$\left(g(z)\right)^n \cdot \left(g(z)\right)^{-n} = 1, \qquad \left[\left(g(z)\right)^n\right]' \cdot \left(g(z)\right)^{-n} + \left(g(z)\right)^n \cdot \left[\left(g(z)\right)^{-n}\right]' = 0$$

Using the previous result for positive exponents, we also have

$$\left[\left(g(z)\right)^n\right]' = -\left(g(z)\right)^{2n} \cdot (-n)\left(g(z)\right)^{-n-1} g'(z) = n\left(g(z)\right)^{n-1} g'(z)$$

Now we return to a general $f(z)$, which can be expressed as

$$f(z) = \lim_{N\to\infty} \sum_{n=n_0}^{N} a_n z^n$$

We only need to prove

$$[z^m]\left[f\left(g(z)\right)\right]' = [z^m]\left[f'\left(g(z)\right) g'(z)\right]$$

For LHS, the truncated summation implies that we can switch the operators

$$[z^m]\left[f\left(g(z)\right)\right]' = [z^m]\left[\lim_{N\to\infty} \sum_{n=n_0}^{N} a_n\left(g(z)\right)^n\right]' = \sum_{n=n_0}^{m+1} [z^m]\left[a_n\left(g(z)\right)^n\right]'$$

For RHS we can similarly truncate the summation. The two sides are equal. ■

Properties of residue

- Taking the residue is a linear operation
- $\mathrm{Res}\, f' = 0,\ \mathrm{Res}(f'g) = -\mathrm{Res}(fg')$
- If $\mathrm{ord}(g) \geq 1$, then

  $$Res\left\{f\left(g(z)\right) g'(z)\right\} = \mathrm{ord}\left(g(z)\right) \cdot \mathrm{Res}\, f(z)$$

  When $f(z) = z^{-1}$, we have

  $$Res\left\{\frac{g'(z)}{g(z)}\right\} = \mathrm{Res}\left\{\frac{n_0 b_0 z^{n_0-1} + \cdots}{b_0 z^{n_0} + \cdots}\right\} = n_0 = \mathrm{ord}\left(g(z)\right)$$

  When $f(z) = z^n$ with $n \neq -1$, we have

  $$Res\{g^n(z)\, g'(z)\} = Res\left\{\left(\frac{g^{n+1}(z)}{n+1}\right)'\right\} = 0$$

➢ Lagrange inversion theorem

Theorem. For $f \in \mathcal{A}^*$, its inverse is denoted as $g = f^{-1}$. For $\forall m, n \in \mathbb{Z}^*$, we have

$$m[z^m]\left[\left(g(z)\right)^n\right] = n[z^{-n}]\left[\left(f(z)\right)^{-m}\right]$$

Proof. We can directly calculate both sides from the perspective of residue

$$m[z^m]\left[\left(g(z)\right)^n\right] = m \operatorname{Res}\{g^n(z) \cdot z^{-m-1}\}$$

Substitute $z \to f(z)$, and then use integration by parts

$$m[z^m]\left[\left(g(z)\right)^n\right] = m \operatorname{Res}\{z^n \cdot f^{-m-1}(z) \cdot f'(z)\} = -\operatorname{Res}\{z^n \cdot [f^{-m}(z)]'\}$$

$$= n \operatorname{Res}\{z^{n-1} \cdot f^{-m}(z)\} = n[z^{-n}]\left[\left(f(z)\right)^{-m}\right] \qquad \blacksquare$$

Corollary. For $f \in \mathcal{A}^*$, $g = f^{-1}$. For $\forall m, n \in \mathbb{Z}$, $n \neq 0$, $m \geq n$, we have

$$[z^m]\left[\left(g(z)\right)^n\right] = n \sum_{k=0}^{m-n} (-1)^k \frac{(m+1)\cdots(m+k-1)}{k!} a_1^{-m-k} B_{(m-n)k}(a')$$

Note that

$$a_n = [z^n]\, f(z), \qquad a' = (a_2, a_3, \cdots)$$

For $n = 1$, we have the higher derivatives of the inverse function.

Proof. When $m \neq 0$, we directly have

$$[z^m]\left[\left(g(z)\right)^n\right] = \frac{n}{m}[z^{-n}]\left[\left(f(z)\right)^{-m}\right] = \frac{n}{m}\sum_{k=0}^{m-n}\binom{-m}{k} a_1^{-m-k} B_{(m-n)k}(a')$$

When $m = 0$, we can consider $-n$ with $n \geq 1$. Substitute $z \to f(z)$, and we obtain

$$[z^0]\left[\left(g(z)\right)^{-n}\right] = \operatorname{Res}\left\{\frac{g^{-n}(z)}{z}\right\} = \operatorname{Res}\left\{z^{-n}\frac{f'(z)}{f(z)}\right\}$$

Define a new function $h(z)$ as

$$h(z) = \frac{f(z)}{a_1 z} - 1 = \frac{a_2}{a_1} z + \frac{a_3}{a_1} z^2 + \cdots, \qquad f(z) = a_1 z\left(1 + h(z)\right)$$

The residue becomes

$$\operatorname{Res}\left\{z^{-n}\frac{a_1(1+h) + h' a_1 z}{a_1 z(1+h)}\right\} = \operatorname{Res}\left\{z^{-n} \cdot \left(\frac{1}{z} + \frac{h'(z)}{1+h(z)}\right)\right\} = \operatorname{Res}\left\{z^{-n}\frac{h'(z)}{1+h(z)}\right\}$$

Define the logarithmic function $L(z)$ as

$$L(z) = \sum_{k\geq 1}\frac{(-1)^{k-1}}{k} z^k, \qquad L'(z) = \frac{1}{1+z}$$

We thus obtain

$$\operatorname{Res}\left\{z^{-n}\frac{h'(z)}{1+h(z)}\right\} = \operatorname{Res}\left\{z^{-n}\big[L\big(h(z)\big)\big]'\right\} = -\operatorname{Res}\left\{-nz^{-n-1}L\big(h(z)\big)\right\}$$

This shows that

$$[z^0]\left[\big(g(z)\big)^{-n}\right] = n\,[z^n]\,L\big(h(z)\big) = n\sum_{k=1}^{n}\frac{(-1)^{k-1}}{k}B_{nk}\left(\frac{a_2}{a_1},\frac{a_3}{a_1},\cdots\right) \qquad \blacksquare$$

Lagrange-Bürmann formula

For $h \in \mathcal{A}$ with $\operatorname{ord}(h) = 0$, define $f(z) = z/h(z) \in \mathcal{A}^*$ and $g = f^{-1}$. We have

$$[z^m]\,g(z) = \frac{1}{m}[z^{m-1}]\,\big(h(z)\big)^m, \qquad m \geq 1$$

$$[z^m]\,\phi\big(g(z)\big) = \frac{1}{m}[z^{m-1}]\,\phi'(z)\big(h(z)\big)^m, \qquad m \geq 1$$

Proof. Directly using the Lagrange inversion theorem with $n = 1$, we obtain

$$[z^m]\,g(z) = \frac{1}{m}[z^{-1}]\left[\frac{z}{h(z)}\right]^{-m} = \frac{1}{m}[z^{m-1}]\big(h(z)\big)^m \qquad \blacksquare$$

Example 1. Lambert W-function

$$z = xe^x \qquad \Longrightarrow \qquad x = W(z) = \sum_{n\geq 1} a_n z^n$$

Based on the Lagrange-Bürmann formula, denote $h(z) = e^{-z}$ and we have

$$x = ze^z = \frac{z}{h(z)}, \qquad [z^m]\,W(z) = \frac{1}{m}[z^{m-1}]\,e^{-mz} = (-1)^{m-1}\frac{m^{m-1}}{m!}$$

The Lambert W-function is defined as

$$W(z) = \sum_{m\geq 1}(-1)^{m-1}\frac{m^{m-1}}{m!}z^m$$

It is applied to solve equations with the form

$$ax + b = e^x, \qquad -\left(x+\frac{b}{a}\right)e^{-\left(x+\frac{b}{a}\right)} = -\frac{1}{a}e^{-\frac{b}{a}}, \qquad x + \frac{b}{a} = -W\left(-\frac{1}{a}e^{-\frac{b}{a}}\right)$$

Corollary. For $f \in \mathcal{A}$ with $\operatorname{ord}(f) \geq 2$, define $F(z) = z - f(z) \in \mathcal{A}^*$ and $W = F^{-1}$. For any $g \in \mathcal{A}$, we have

$$g\big(W(z)\big) = g(z) + \sum_{k\geq 1}\frac{1}{k!}[f^k(z)g'(z)]^{(k-1)}$$

Proof. We only need to consider $g(z) = z^n$, which gives

$$W^n(z) = z^n + \sum_{k\geq 1} \frac{1}{k!} [f^k(z)\, n z^{n-1}]^{(k-1)}$$

For $m \geq n$, we need to prove $[z^m]$ is the same for both sides. The case $m = n$ is trivial, and now we can set $m \geq n + 1$. Note that

$$[z^1]\, F(z) = 1, \qquad [z^n]\, F(z) = -a_n = -[z^n]\, f(z), \qquad n \geq 2$$

From the previous corollary, we have

$$[z^m]\big[\big(W(z)\big)^n\big] = n \sum_{k=0}^{m-n} \frac{(m+1)\cdots(m+k-1)}{k!} B_{(m-n)k}(a_2, a_3, \cdots)$$

For the RHS, using the following result

$$\begin{aligned}
[z^m] \left(\sum_{l\in\mathbb{Z}} c_l z^l\right)^{(k-1)} &= [z^m]\left(\sum_{l\in\mathbb{Z}} c_l \cdot l(l-1)\cdots(l-k+2)\, z^{l-k+1}\right) \\
&= (m+1)\cdots(m+k-1)\cdot [z^{m+k-1}] \sum_{l\in\mathbb{Z}} c_l z^l
\end{aligned}$$

We can switch the order between derivative and $[z^m]$ as

$$\begin{aligned}
[z^m]\ \text{RHS} = n[z^m] &\sum_{k\geq 1} \frac{1}{k!} [f^k(z)\, z^{n-1}]^{(k-1)} \\
&= n \sum_{k\geq 1} \frac{(m+1)\cdots(m+k-1)}{k!} \cdot [z^{m+k-1}]\, [f^k(z)\, z^{n-1}] \\
&= n \sum_{k=1}^{m-n} \frac{(m+1)\cdots(m+k-1)}{k!} \cdot [z^{m-n}] \left(\frac{f(z)}{z}\right)^k
\end{aligned}$$

We can show that both sides are equal to each other. ■

Lagrange reversion theorem

$$W(z) = z + \sum_{k\geq 1} \frac{1}{k!} [f^k(z)]^{(k-1)}, \qquad \text{ord}(f) \geq 2$$

Example 2

$$f(z) = z^d, \qquad F(z) = z - z^d, \qquad d \geq 2$$

The inverse $W = F^{-1}$ is given as

$$W(z) = z + \sum_{k\geq 1} \frac{1}{k!} [f^k(z)]^{(k-1)} = z + \sum_{k\geq 1} \binom{kd}{k} \frac{z^{kd-k+1}}{kd-k+1}$$

➢ Inversion formula for C^∞

For $f \in C^\infty(\mathbb{R})$ with a bounded derivative $|f'| \leq M$, consider the equation

$$v(x,y) = x + yf\big(v(x,y)\big)$$

We want to know when this defines a function $v(x,y)$. Denote the implicit equation as follows

$$u(x,y,v) = x + yf(v) - v = 0, \qquad \frac{\partial u}{\partial v} = yf'(v) - 1$$

When $|y| < M^{-1}$, the bound $|f'(v)| \leq M$ implies $\partial u/\partial v \neq 0$ and $v(x,y)$ exists. We can see that $v(x,y)$ satisfies the PDE with $v(x,0) = x$

$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial x}\left(\frac{\partial u}{\partial v}\right)^{-1} = \frac{1}{1 - yf'(v)}, \qquad \frac{\partial v}{\partial y} = \frac{f(v)}{1 - yf'(v)} = f(v)\frac{\partial v}{\partial x}$$

For $g \in C^\infty(\mathbb{R})$, if $g(v)$ converges then we have

$$g\big(v(x,y)\big) = g(x) + \sum_{k=1}^{\infty} \frac{y^k}{k!} \partial_x^{k-1}\Big(f^k(x)g'(x)\Big)$$

If $g(v)$ does not converge, we can truncate the series to $k = N$ and then add $o(y^N)$.

Corollary.

$$\partial_y^k g\big(v(x,y)\big) = \partial_x^{k-1}\big[g'\big(v(x,y)\big)f^k\big(v(x,y)\big)v_x\big]$$

Proof. When $k = 1$, the expression holds. By induction, for $k+1$ we have

$$\begin{aligned}
\partial_y^{k+1} g\big(v(x,y)\big) &= \partial_y\{\partial_x^{k-1}[g'(v)f^k(v)v_x]\} \\
&= \partial_x^{k-1}\left\{\frac{\partial g'(v)f^k(v)}{\partial v} v_y v_x + g'(v)f^k(v)v_{xy}\right\} \\
&= \partial_x^{k-1}\left\{\frac{\partial g'(v)f^k(v)}{\partial v} f(v)v_x^2 + g'(v)f^k(v)\frac{\partial f(v)v_x}{\partial x}\right\} \\
&= \partial_x^{k-1}\left\{\frac{\partial g'(v)f^k(v)}{\partial x} f(v)v_x + g'(v)f^k(v)\frac{\partial f(v)v_x}{\partial x}\right\} \\
&= \partial_x^k\big[g'\big(v(x,y)\big)f^k\big(v(x,y)\big)v_x\big]
\end{aligned}$$

■

Now we can prove the inversion formula for C^∞. We only need to show that

$$\partial_y^k g(v) = \partial_x^{k-1}\Big(g'(x)f^k(x)\Big), \qquad \text{at } y = 0$$

The result from the corollary can directly be applied with $v(x,0) = x$. Furthermore, we have

$$v_x(x,0) = \left.\frac{1}{1 - yf'(v)}\right|_{y=0} = 1$$

Therefore, we demonstrate the coefficients of the Taylor series. For $g(v) = v$, we have

$$v(x,y) = x + \sum_{k=1}^{\infty} \frac{y^k}{k!} \partial_x^{k-1} f^k(x), \qquad \text{for } v = x + f(v)y \qquad \blacksquare$$

Example 1. Kepler equation

For $f(v) = \sin v$ and $y = \varepsilon$ with $|\varepsilon| \ll 1$, we have

$$v - \varepsilon \sin v = x$$

We can obtain the solution as an expansion of ε as

$$v(x;\varepsilon) = x + \sum_{k=1}^{\infty} \frac{\varepsilon^k}{k!} \partial_x^{k-1} (\sin^k x)$$

As a comparison, the Fourier expansion of v is

$$v(x;\varepsilon) = x + \sum_{m=1}^{\infty} \frac{2}{m} J_m(m\varepsilon) \sin(mx)$$

Example 2

$$v(x,\boldsymbol{t}) = x + t_0 + t_1 v + \frac{1}{2!} t_2 v^2 + \frac{1}{3!} t_3 v^3 + \cdots$$

This is equivalent to the following PDE

$$\frac{\partial v}{\partial t_k} = \frac{v^k}{k!} v_x, \qquad k = 0,1,2,\cdots, \qquad v(x,\boldsymbol{0}) = x$$

We can consider $y = 1$ with $f(v) = t_0 + t_1 v + \cdots$. This leads to

$$v = x + \sum_{k=1}^{\infty} \frac{1}{k!} \partial_x^{k-1} \left[\left(\sum_{l \geq 0} \frac{t_l}{l!} x^l \right)^k \right]$$

Note that $v(x,\boldsymbol{t}) = v(0, x + t_0, t_1, \cdots)$, we can just solve for

$$v(0,\boldsymbol{t}) = \sum_{k=1}^{\infty} \frac{1}{k!} \partial_x^{k-1} \left.\left[\left(\sum_{l \geq 0} \frac{t_l}{l!} x^l \right)^k \right]\right|_{x=0} = \sum_{k \geq 1} \frac{1}{k!} \partial_x^{k-1} \left.\left[\left(\sum_{l=0}^{k-1} \frac{t_l}{l!} x^l \right)^k \right]\right|_{x=0}$$

$$= \sum_{k \geq 1} \sum_{\substack{d_0,\cdots,d_{k-1} \geq 0 \\ d_0 + \cdots + d_{k-1} = k \\ d_1 + 2d_2 + \cdots (k-1)d_{k-1} = k-1}} \frac{(k-1)!}{d_0! \cdots d_{k-1}!} \prod_{l=0}^{k-1} \left(\frac{t_l}{l!} \right)^{d_l}$$

- Exercise

Todd power series

We want to find a formal power series $f(z)$ such that

$$f(z) = \sum_{n\geq 0} a_n z^n, \qquad [z^m]\left(f(z)\right)^{m+1} = 1, \qquad \forall m \in \mathbb{N}$$

Define $h(z) = z/f(z)$ and its inverse $g = h^{-1}$. The Lagrange-Bürmann formula gives

$$[z^{m+1}]\, g(z) = \frac{1}{m+1}[z^m]\left(f(z)\right)^{m+1} = \frac{1}{m+1}, \qquad m \in \mathbb{N}$$

The invertibility implies $\operatorname{ord}(g) = 1$. Now we directly obtain

$$g(z) = \sum_{n\geq 1} \frac{z^n}{n} = -\ln(1-z)$$

Since $h = g^{-1}$, we have

$$h(z) = 1 - e^{-z}, \qquad f(z) = \frac{z}{h(z)} = \frac{z}{1-e^{-z}}$$

Faà di Bruno's formula

For two functions f and g, the chain rule for higher derivatives is

$$\frac{\mathrm{d}^m}{\mathrm{d}x^m} f\big(g(x_0)\big) = m! \sum_{n=0}^{m} \frac{f^{(n)}\big(g(x_0)\big)}{n!} B_{mn}\left(\frac{g^{(1)}(x_0)}{1!}, \frac{g^{(2)}(x_0)}{2!}, \cdots, \frac{g^{(m)}(x_0)}{m!}\right)$$

$$= \sum_{n=0}^{m} f^{(n)}\big(g(x_0)\big) \sum_{\substack{d_1,\cdots,d_m\geq 0 \\ d_1+d_2+\cdots+d_m=n \\ d_1+2d_2+\cdots+md_m=m}} \frac{m!}{d_1!\cdots d_m!}\left(\frac{g^{(1)}(x_0)}{1!}\right)^{d_1}\cdots\left(\frac{g^{(m)}(x_0)}{m!}\right)^{d_m}$$

Formula for higher derivatives of inverse function

Denote $g = f^{-1}$ as the inverse function of f. The higher derivatives for g are given as

$$\frac{\mathrm{d}^m}{\mathrm{d}x^m} g\big(f(x_0)\big) = m! \sum_{n=0}^{m-1} (-1)^n \frac{(m+1)\cdots(m+n-1)}{n!\,[f^{(1)}(x_0)]^{m+n}} B_{(m-1)n}\left(\frac{f^{(2)}(x_0)}{2!}, \cdots, \frac{f^{(m)}(x_0)}{m!}\right)$$

$$= \sum_{n=0}^{m-1} \frac{(-1)^n \cdot (m+n-1)!}{[f^{(1)}(x_0)]^{m+n}} \sum_{\substack{d_2,\cdots,d_m\geq 0 \\ d_2+d_3+\cdots+d_m=n \\ d_2+2d_3+\cdots+(m-1)d_m=m-1}} \frac{1}{d_2!\cdots d_m!}\left(\frac{f^{(2)}(x_0)}{2!}\right)^{d_2}\cdots\left(\frac{f^{(m)}(x_0)}{m!}\right)^{d_m}$$

Roll the dice

The probability of the total sum being equal to m after rolling n times can be expressed as

$$P(S_n = m) = [x^m]\left(\frac{1}{6}x + \frac{1}{6}x^2 + \cdots + \frac{1}{6}x^6\right)^n = \frac{1}{6^n}B_{mn}(1,1,1,1,1,1)$$

On the other hand, we have

$$\begin{aligned} x^n\left(\frac{1-x^6}{1-x}\right)^n &= x^n\sum_{k=0}^{n}(-1)^k\binom{n}{k}x^{6k}\sum_{l=0}^{+\infty}(-1)^l\binom{-n}{l}x^l \\ &= x^n\sum_{k=0}^{n}(-1)^k\binom{n}{k}x^{6k}\sum_{l=0}^{+\infty}\binom{n+l-1}{l}x^l \end{aligned}$$

This gives

$$P(S_n = m) = \frac{1}{6^n}[x^m]\,x^n\left(\frac{1-x^6}{1-x}\right)^n = \frac{1}{6^n}\sum_{k=0}^{n}(-1)^k\binom{n}{k}\binom{m-6k-1}{m-6k-n}$$

The summation only contributes when $m - 6k - n \geq 0$, which leads to

$$P(S_n = m) = \frac{1}{6^n}\sum_{k=0}^{\left\lfloor\frac{m-n}{6}\right\rfloor}(-1)^k\binom{n}{k}\binom{m-6k-1}{n-1}$$

Fuss-Catalan number

When we solve for the power series of the inverse $W = F^{-1}$ with $F(z) = z - z^d$, we obtain

$$W(z) = z + \sum_{k\geq 1}\binom{kd}{k}\frac{z^{kd-k+1}}{kd-k+1}$$

The coefficients are positive integers, and in fact they are the Fuss-Catalan numbers

$$_d c_k = \frac{1}{kd-k+1}\binom{kd}{k}$$