Lecture #6: Orthogonal Polynomials, Bernoulli Numbers, & Euler-MacLaurin Formula

I. Orthogonal Polynomials

A. Rodriguez Formulas

1. Consider a 2nd-order Sturm-Liouville ODE of the form

$$p(x)\, y'' + q(x)\, y' + \lambda y = 0, \quad p(x) = \alpha x^2 + \beta x + \gamma$$

$q(x) = \mu x + \nu$

$\lambda \Rightarrow$ eigenvalue

2. Recall:

a. For a polynomial solution $y_n(x) = \sum_{j=0}^{n} a_j x^j$, we can substitute into ODE to obtain an eigenvalue condition

$$\boxed{\lambda_n = -n(n-1)\alpha - n\mu}$$

by equating coefficients of like powers of x^n

b. If $p'(x) = q(x)$, ODE is self-adjoint

c. If not, ODE can be converted to self-adjoint form with weighting

$$\boxed{w(x) = \frac{1}{p(x)} \exp\left[\int^x \frac{q(x')}{p(x')} dx'\right]}$$

d. This yields the form,

$$\boxed{\frac{d}{dx}\left[w(x)\, p(x)\, y'\right] + \lambda w(x) y = 0}$$

3. Rodrigues Formula

$$\boxed{y_n(x) = \frac{1}{w(x)} \left(\frac{d}{dx}\right)^n \left\{w(x)[p(x)]^n\right\}}$$

Compact form for solutions to ODE

a. Formula yields a polynomial of degree n.

4. Ex: Hermite ODE

a. $$y'' - 2xy' + \lambda y = 0 \quad \begin{cases} p = 1 \\ q = -2x \end{cases}$$

b. $p' \neq q$, so not self-adjoint!

c. Compute $$W(x) = \frac{1}{p(x)} e^{\int^x \frac{q(x')}{p(x')}dx'} = \frac{1}{(1)} e^{\int^x \frac{-2x}{1}dx'} = e^{-x^2}$$

d. Thus, the Rodrigues Formula for the Hermite polynomials is
$$y_n(x) = \frac{(-1)^n}{e^{-x^2}} \frac{d^n}{dx^n}\left[e^{-x^2}(1)^n\right] = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right)$$
$(-1)^n$ to obtain conventional signs

e. Thus
$$H_0(x) = (-1)^0 e^{x^2} e^{-x^2} = 1 \quad ✓$$
$$H_1(x) = (-1)^1 e^{x^2}\left[-2x e^{-x^2}\right] = 2x \quad ✓$$
$$H_2(x) = (-1)^2 e^{x^2}\left[-2e^{-x^2} + 4x^2 e^{-x^2}\right] = 4x^2 - 2 \quad ✓$$

B. Schlaefli Integral

1. Consider Cauchy's Integral Formula for the nth derivative at $z_0 = x$:
$$f^{(n)}(x) = \frac{n!}{2\pi i}\oint_C \frac{f(z)\,dz}{(z-x)^{n+1}}$$

2. Here, let $f(z) = W(z)\left[p(z)\right]^n$
a. must be analytic within and on contour C
b. Contour must enclose $z = x$

3. Thus, the Rodrigues Formula may be written
$$\boxed{y_n(x) = \frac{1}{W(x)}\left\{\frac{n!}{2\pi i}\oint_C \frac{W(z)\left[p(z)\right]^n}{(z-x)^{n+1}}dz\right.}$$
Schlaefli Integral

4. Schlaefli Integral is useful in finding Generating Functions (see I.D. below), as well as working with Gamma, Bessel, and other special functions.

I. (Continued)

C. Generating Functions

1. A set of functions $f_n(x)$ can be described as coefficients of the expansion of a generating function $g(x,t)$ in variable t,

2. Generating Function: $\boxed{g(x,t) = \sum_n c_n f_n(x) t^n}$

3. Relation using Contour Integration between $c_n f_n(x)$ and $g(x,t)$:

a. Consider the function $\frac{g(x,t)}{t^{m+1}} = \sum_n c_n f_n(x) t^{n-m-1}$

b. If I integrate along a closed contour enclosing only the pole at $t=0$ [not enclosing singularities in t of $g(x,t)$],

$$\oint_C \frac{g(x,t)}{t^{m+1}} dt = 2\pi i \operatorname*{Res}_{t=0} \left[\frac{g(x,t)}{t^{m+1}}\right] \longleftarrow \text{Residue Theorem.}$$

c. The residue is just the coefficient of the t^{-1} term. Thus $n=m$ and the coefficient is $c_m f_m(x)$

d. Therefore $\boxed{c_n f_n(x) = \frac{1}{2\pi i} \oint_C \frac{g(x,t)}{t^{n+1}} dt}$

3. Uses of the generating function, $g(x,t)$

a. Taking $\frac{\partial}{\partial t} g(x,t)$ derives relation between $f_n(x)$ and $f_{n+1}(x)$

b. Taking $\frac{\partial}{\partial x} g(x,t)$ derives relation between $f_n(x)$ and $f_n'(x)$.

4. Ex: Hermite Polynomials

a. $g(x,t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!}$

I. C.4. (Continued)

b. Recurrence Formula: i. Take $\frac{\partial}{\partial t}\left(e^{-t^2+2tx}\right) = (2x-2t)\underbrace{e^{-t^2+2tx}}_{\text{Substitute}} = \sum_{n=0}^{\infty} n H_n(x)\frac{t^{n-1}}{n!}$

ii. $\sum_{n=0}^{\infty} 2x\, H_n(x)\frac{t^n}{n!} - \sum_{n=0}^{\infty} 2\, H_n(x)\frac{t^{n+1}}{n!} = \sum_{n=0}^{\infty} n\, H_n \frac{t^{n-1}}{n!}$

iii. Equating coefficients of t^n yields $\boxed{2x\, H_n(x) - 2n\, H_{n-1}(x) = H_{n+1}(x)}$

Recurrence Formula

iv. May easily compute H_n starting from H_0 and H_1!

c. Derivative Formula: i. Take $\frac{\partial}{\partial x}\left(e^{-t^2+2tx}\right) = 2te^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n'(x)\frac{t^n}{n!}$

ii. A similar procedure yields $\boxed{2n\, H_{n-1}(x) = H_n'(x)}$

D. Finding Generating Functions

1. Substituting Schlaefli Integral for $y_n(x)$ into $g(x,t) = \sum_n c_n y_n(x) t^n$,

$$\boxed{g(x,t) = \frac{1}{w(x)} \sum_n c_n t^n \frac{n!}{2\pi i} \oint_C \frac{w(z)[p(z)]^n}{(z-x)^{n+1}}\, dz}$$

a. Here Contour C encloses $z=x$ and $w(z)[p(z)]^n$ is analytic on & within C.

2. This formula can be used to compute $g(x,t)$ for specified c_n

a. Typically exchange sum and integral (requires uniform convergence of sum)

b. Evaluate the infinite sum

c. Evaluate Contour integral via Residue Theorem

3. The process is somewhat lengthy. Text provides worked example for Legendre Polynomials.

4. Table 12.1 in text provide Rodrigues Formula & Generating Function for common orthogonal polynomials.

II. Bernoulli Numbers and Polynomials

A. Bernoulli Numbers

1. Generating function: $\boxed{\dfrac{t}{e^t-1} = \sum_{n=0}^{\infty} \dfrac{B_n t^n}{n!}}$

Taylor series

Definitions differ in various works, so be careful.

2. Since this is a Taylor series, we may identify

$$\boxed{B_n = \frac{d^n}{dt^n}\left(\frac{t}{e^t-1}\right)\Bigg|_{t=0}}$$

3. Compute B_0: $B_0 = \lim_{t\to 0} \dfrac{t}{e^t-1} = \lim_{t\to 0} \dfrac{t}{(\cancel{1}+t+\frac{t^2}{2!}+\frac{t^3}{3!}+\dots) - \cancel{1}} = \lim_{t\to 0} \dfrac{1}{1+\frac{t}{2!}+\frac{t^2}{3!}+\dots}$

$$\boxed{B_0 = 1}$$

4. Compute B_1: $B_1 = \dfrac{d}{dt}\left(\dfrac{t}{e^t-1}\right) = \lim_{t\to 0}\left[\dfrac{1}{e^t-1} - \dfrac{te^t}{(e^t-1)^2}\right]$

$$= \lim_{t\to 0}\left[\frac{e^t-1-te^t}{(e^t-1)^2}\right] = \lim_{t\to 0}\left[\frac{(\cancel{t}+\frac{t^2}{2!}+\frac{t^3}{3!}) - (\cancel{t}+t^2+\frac{t^3}{2!}+\dots)}{(t+\frac{t^2}{2!}+\dots)^2}\right] = \lim_{t\to 0} \frac{-\frac{1}{2}t^2+O(t^3)}{t^2+O(t^3)}$$

$$\boxed{B_1 = -\frac{1}{2}}$$

5. One may derive Recursion Relations

a. $N - \frac{1}{2} = \sum_{n=1}^{N} \binom{2N+1}{2n} B_{2n}$

b. $N - 1 = \sum_{n=1}^{N-1} \binom{2N}{2n} B_{2n}$

Either can be used to determine B_{2n} sequentially, starting from B_2.

c. NOTE: $\boxed{B_n = 0 \text{ for odd } n > 1.}$

6. Connection to Zeta functions, $\zeta(n)$

a. Starting with the integral representation using $g(x,t)$ (See I C,3d.)

$$B_n = \frac{n!}{2\pi i}\oint \frac{t}{e^t-1}\frac{dt}{t^{n+1}}$$

b. A contour integration, excluding $t=0$, can be used to obtain

$$B_n = -\frac{n!}{(2\pi i)^n}\sum_{m=1}^{\infty}\left[\frac{1}{m^n}+\frac{1}{(-m)^n}\right]$$

c. This may be expressed as

Riemann Zeta Function.

$$\boxed{B_{2n} = (-1)^{n+1}\frac{(2n)!}{(2\pi)^{2n}}\sum_{m=1}^{\infty}\frac{2}{m^{2n}} = (-1)^{n+1}\frac{2(2n)!}{(2\pi)^{2n}}\zeta(2n)} \qquad 2n \geq 2$$

$$B_{2n+1} = 0$$

d. <u>Define</u>: Riemann Zeta Function $\boxed{\zeta(z) = \sum_{m=1}^{\infty}\frac{1}{m^z}}$

7. Importance of this result:

a. Recurrence Relations (II.A.5a&b) enable easy calculation of B_{2n}

b. Result above yields a <u>closed form</u> expression for $\zeta(2n)$ (does not require infinite sum to be performed)

B. <u>Bernoulli Polynomials</u>

1. <u>Def: Generating function</u> $\boxed{\frac{te^{ts}}{e^t-1} = \sum_{n=0}^{\infty} B_n(s)\frac{t^n}{n!}}$

a. Note: $B_n(0) = B_n$ ← evaluation at $s=0$ yields <u>Bernoulli Numbers</u>

b. $B_0(s) = 1$

$B_1(s) = x - \frac{1}{2}$

$B_2(s) = x^2 - x + \frac{1}{6}$, etc.

2. <u>Derivative Formula</u>: Taking $\frac{\partial}{\partial s}$ and equating coefficients yields

$$\boxed{\frac{d}{ds}B_n(s) = n\,B_{n-1}(s)} \qquad n=1,2,3,\ldots$$

3. <u>Symmetry Relation</u>: $\boxed{B_n(1) = (-1)^n B_n(0)}$

III. Euler-MacLaurin Integration Formula

A. 1. Used to develop asymptotic expansions and approximate values of summations.

a. Ex: Used to derive Stirling's Formula, asymptotic form of $\Gamma(z)$

2. Euler-MacLaurin Integration Formula

$$\boxed{\int_0^1 f(x)\,dx = \frac{1}{2}\left[f(1)+f(0)\right] - \sum_{p=1}^{q} \frac{1}{(2p)!} B_{2p}\left[f^{(2p-1)}(1) - f^{(2p-1)}(0)\right] + \frac{1}{(2q)!}\int_0^1 f^{(2q)}(x)\, B_{2q}(x)\,dx}$$

a. Derive by repeated integration by parts, starting with $\int_0^1 f(x)\,dx = \int_0^1 f(x) B_0(x)\,dx$, and using derivative formula & symmetry relation for $B_n(x)$ (see text)

b. Final term can be considered a remainder!

$\Rightarrow$ Use formula to sum series as integrals plus correction term.

3. For intervals other than $[0,1]$, add $[1,2]$, $[2,3]$, etc, to obtain

$$\boxed{\begin{aligned}\int_0^n f(x)\,dx &= \frac{1}{2}f(0) + f(1) + f(2) + \dots + f(n-1) + \frac{1}{2}f(n) \\ &- \sum_{p=1}^{q} \frac{1}{(2p)!} B_{2p}\left[f^{(2p-1)}(n) - f^{(2p-1)}(0)\right] + \frac{1}{(2q)!}\int_0^1 B_{2q}(x) \sum_{\nu=0}^{n-1} f^{(2q)}(x+\nu)\,dx\end{aligned}}$$

4. Ex: Estimating $\zeta(3) = \sum_{n=1}^{\infty} \frac{1}{n^3}$ $\rightarrow$ here use $f = \frac{1}{x^3}$

a. NOTE: $\sum_{n=1}^{\infty} f(n) = \frac{1}{2}f(1) + \underbrace{\left[\frac{1}{2}f(1) + f(2) + \dots + \frac{1}{2}\cancel{f(\infty)}^{\,0}\right]}_{\text{Sum in Euler-MacLaurin Integration Formula}} + \frac{1}{2}\cancel{f(\infty)}^{\,0}$

b. So $\zeta(3) - \frac{1}{2}f(1) = [\text{---Sum---}]$

III. A4 (Continued)

c. Note that $\lim_{x\to\infty} \frac{d^n}{dx}[f(x)] = 0$ for all derivatives of $f(x) = \frac{1}{x^3}$.

d. Thus, we may substitute into the formula

$$\int_1^\infty \frac{dx}{x^3} = \frac{-1}{2} f(1) + \zeta(3) - \sum_{p=1}^{q} \frac{B_{2p}}{(2p)!}\left[\cancel{f^{(2p-1)}(\infty)}^{\,0} - f^{(2p-1)}(1)\right] + \text{remainder}$$

e. Solving for $\zeta(3)$ (and using $f(1) = 1$ and $\int_1^\infty \frac{dx}{x^3} = \left[\frac{-1}{2x^2}\right]_1^\infty = \frac{-1}{2}$),

$$\zeta(3) = \frac{1}{2} + \frac{1}{2} - \sum_{p=1}^{q} \frac{B_{2p}}{(2p)!} f^{(2p-1)}(1) + \text{remainder}$$

f. NOTE: Evaluating $f^{(2n-1)}(x) = -\frac{(2n+1)!}{2x^{2n+2}} \Rightarrow f^{(2n-1)}(1) = -\frac{(2n+1)!}{2}$

g. Finally

$$\boxed{\zeta(3) = 1 + \sum_{p=1}^{q} \frac{(2p+1)\, B_{2p}}{2} + \text{remainder}}$$

h. Thus, the more terms we take (higher q), the more accurate.

i. But, Bernoulli numbers diverge. $\Rightarrow$ remainder becomes non-negligible.

ii. We can do better by explicitly evaluating more terms

$$\zeta(3) = 1 + \frac{1}{2^3} + \frac{1}{3^3} + \sum_{n=4}^{\infty} \frac{1}{n^3}$$

and apply Euler-MacLaurin Integration Formula to $\sum_{n=4}^{\infty} \frac{1}{n^3}$.

$\Rightarrow$ This yields a rapidly converging result!