Numerical Integration and Differentiation

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Integration

- **Goal**: Solve $I(f) = \int_a^b f(x)\ dx$
- WLOG, let $a = 0, b = 1$
- **Numerical integration** or **quadrature**
- **Question**: How is integration related to interpolation?

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- WLOG, let $a = 0, b = 1$
- **Numerical integration** or **quadrature**
- **Question**: How is integration related to interpolation?
- Suppose $f \approx p_n$
- $E_n = I(f) - I(p_n) = \int_a^b f(x) - p_n(x)\ dx$
- $|E_n| \le (b-a)\|f - p_n\|_\infty$
- Usually write $I(p_n) = \sum_{j=1}^n w_j f(x_j)$
- Focus on single interval for simplicity
- **Def**: w_j are called integration/quadrature **weights**, x_j are called **nodes**
- **Question**: What are optimal weights and nodes and what are corresponding errors?

Simple quadratures

Gaussian quadratures

Numerical differentiation

Trapezoidal's rule

- **Endpoints rule**: $I(p_0) = (b-a)f(a)$ or $(b-a)f(b)$
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- Assume $f(x) = a_0 + a_1 x$,
- $p_1(a) = f(a)$ and $p_1(b) = f(b)$
- $p_1(x) = f(a) + (x-a)\frac{f(b)-f(a)}{b-a}$
- $I(p_1) = \left(\frac{b-a}{2}\right)(f(a) + f(b))$
- **Question**: How to evaluate the error?

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- **Question**: How to evaluate the error?
- $|f(x) - p_1(x)| = \left|(x-a)(x-b)\frac{f''(\xi)}{2}\right| \leq \frac{K}{2}|(x-a)(x-b)|$
- $|E| \leq \frac{K}{2}\left|\int_a^b (x-a)(x-b)\ dx\right| = \frac{K}{2}\left(\frac{1}{6}(b-a)^3\right)$
- **Question**: When is the approximation accurate?

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- **Question**: When is the approximation accurate?
- $b-a$ small
- $I(f) = \int_a^b f(x)\ dx = \sum_{j=1}^n \int_{x_{j-1}}^{x_j} f(x)\ dx \approx \frac{b-a}{2n}\sum_{j=1}^n f(x_{j-1}) + f(x_j)$

General methods

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- Use higher-degree polynomials p_n and more nodes $x_0, \ldots, x_n$
- **Def**: A numerical integration formula $\widetilde{I}(f)$ that approximates $I(f)$ have **degree** m if
  - $\widetilde{I}(f) = I(f), \forall f$ of degree $\leq m$.
  - $\widetilde{I}(f) \neq I(f)$ for some polynomial f of degree $m+1$.
- E.g. Endpoints rule, zero degree
- E.g. Trapezoidal's rule, first degree
- **Question**: Suppose $\{x_j\}$ are know, how to calculate $\widetilde{I}(f)$?

Integration vector

- One general approach: use the integration vector
- Recall $\mathbf{S} = \widetilde{\mathbf{A}}\mathbf{B}\mathbf{A}^{-1}$
- $\widetilde{\mathbf{A}} = \begin{bmatrix} x_0 & x_0^2 & \dots & x_0^{n+1} \\ x_1 & x_1^2 & \dots & x_1^{n+1} \\ \vdots & \ddots & \ddots & \vdots \\ x_n & x_n^2 & \dots & x_n^{n+1} \end{bmatrix}$
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- **Question**: Equispaced vs Chebyshev?
- Chebyshev has better approximation ability
- **Question**: Is it possible to do better?

Simple quadratures

Gaussian quadratures

Numerical differentiation

Case 1

- Suppose $[a, b] = [-1, 1]$
- $E(f) = \int_a^b f(x) - \widetilde{f}(x)\ dx$
- **Question**: Suppose $\widetilde{I}(f) = w_1 f(x_1)$, can we choose w_1, x_1 s.t. $\widetilde{I}(f)$ is the first degree method?

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- Conditions:

$$E(1) = 0,$$
$$E(x) = 0.$$

- Solve

$$\int_{-1}^{1} 1\ dx - w_1 = 0,$$
$$\int_{-1}^{1} x\ dx - w_1 x_1 = 0.$$

- **Midpoint rule**: $\widetilde{I}(f) = 2f(0)$

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- $E_n(x^i) = \int_{-1}^{1} x^i \, dx - (w_1 x_1^i + w_2 x_2^i) = 0$
- Nonlinear system

$$
\begin{aligned}
w_1 + w_2 &= 2, \\
w_1 x_1 + w_2 x_2 &= 0, \\
w_1 x_1^2 + w_2 x_2^2 &= \frac{2}{3}, \\
w_1 x_1^3 + w_2 x_2^3 &= 0.
\end{aligned}
$$

- $\widetilde{I}(f) = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$

General case

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- **Question**: How about this general case?
- $E(x^i) = 0, i = 0, 1, \dots, 2n-1$
- $\sum_{j=1}^{n} w_j x_j^i = \begin{cases} 0, & i = 1, 3, \dots, 2n-1, \\ \frac{2}{i+1}, & i = 0, 2, \dots, 2n-2. \end{cases}$
- **THM**: This can be solved by **Gaussian quadrature**, whereas nodes $\{x_j\}$ are zeros of Legendre polynomial $p_n(x)$ on $[-1, 1]$. The weights are

$$w_j = \frac{-2}{(n+1)p_n'(x_j)p_{n+1}(x_j)}.$$

- **Def**: **Legendre polynomials**: $p_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}(x^2-1)^n$

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- Fix h, say $h = 0.01$, calculate $f'(0) \approx \frac{f(h)-f(0)}{h}$
- $f(x) = f(0) + f'(0)x + \frac{f''(0)}{2}x^2 + \dots$
- $|R_1(x)| \approx \left|\frac{f''(0)}{2}x\right|$ for x near 0
- E.g. $f(x) = e^x$
- $h = 0.01 : f'(0) \approx \frac{e^h-1}{h} = 1.005$
- $h = 0.001 : f'(0) \approx 1.0005$
- $h = 0.0001 : f'(0) \approx 1.00005$
- Error decays linearly, i.e., $|R_1(x)| \le Ch$ if $\left|\frac{f''(0)}{2}\right| \le C$

Central difference

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- Central difference
- $f(x) = f(0) + f'(0)x + \frac{f''(0)}{2}x^2 + \frac{f'''(0)}{6}x^3 + \dots$
- $f(h) = f(0) + f'(0)h + \frac{f''(0)}{2}h^2 + \frac{f'''(0)}{6}h^3 + \dots$
- $f(-h) = f(0) - f'(0)h + \frac{f''(0)}{2}h^2 - \frac{f'''(0)}{6}h^3 + \dots$
- $f(h) - f(-h) = 2f'(0)h + \frac{f'''(0)}{3}h^3 + \dots$
- $\frac{f(h)-f(-h)}{2h} - f'(0) = \frac{f'''(0)}{6}h^2 + \dots$
- $\left|\frac{f(h)-f(-h)}{2h} - f'(0)\right| \approx \left|\frac{f'''(0)}{6}\right| h^2$
- E.g. $f(x) = e^x$ with $h = 0.01$
- $\frac{e^h-1}{h} = 1.005$
- $\frac{e^h-e^{-h}}{2h} = 1.00002$, much more accurate!

Second-order derivative

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- $f(h) = f(0) + f'(0)h + \frac{f''(0)}{2}h^2 + \frac{f'''(0)}{6}h^3 + \frac{f^{(4)}(0)}{24}h^4$
- $f(-h) = f(0) - f'(0)h + \frac{f''(0)}{2}h^2 - \frac{f'''(0)}{6}h^3 + \frac{f^{(4)}(0)}{24}h^4$
- $\left| f''(0) - \frac{f(-h)-2f(0)+f(h)}{h^2} \right| \approx \frac{h^2}{12} f^{(4)}(0).$
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- **Question**: Advantages of local approximation?

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- Sparse matrix

General approach

- **Question**: Use $f(-h), f(0), f(h)$ to approximate $f''(0)$
- $f''(0) \approx af(-h) + bf(0) + cf(h)$
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- Let $f''(0) = af(-h) + bf(0) + cf(h)$ when $f = 1, x, x^2$
- $\begin{bmatrix} 1 & 1 & 1 \\ -h & 0 & h \\ h^2 & 0 & h^2 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} \Rightarrow \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \frac{1}{h^2} \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$
- General problem: use $f(x_0), \ldots, f(x_n)$ to approximate $f''(0)$