THE UNIVERSITY OF TEXAS AT DALLAS

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EVALUATION OF FUNCTIONS

Notes prepared for EE 6481

by

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EVALUATION OF FUNCTIONS

- Sensitivity of the computed value of a function to changes in the values of the arguments

  Example: Roots of a polynomial

- Newton-Raphson method for finding roots
- Numerical integration
- Other methods for evaluating functions include:

  Evaluation of series (see slides on floating-point computation)

  Solution of ordinary di erential equations

  Solution of partial di erential equations

SENSITIVITY/CONDITION NUMBER (1)

- **Sensitivity** of the value $f(x, y)$ of a function f to changes in the input y:

$$S(f; x, y) := \left| \frac{y\left[f(x, y\ ) - f(x, y)\right]}{(y\ - y)\, f(x, y)} \right|$$

$$\approx \left| \frac{y}{f(x, y)} \frac{\partial f(x, y)}{\partial y} \right|$$

Also known as the **condition number**

S is the ratio of the relative errors in the output and the input:

$$S \approx \frac{\Delta f / f}{\Delta y / y}$$

Example: $f(x, y) = x - y$

$$S(f; x, y) = \frac{|y|}{|x - y|}$$

SENSITIVITY/CONDITION NUMBER (2)

- Sensitivity of the value of a repeated root of a polynomial to changes in the constant term:

$$p(z,\alpha) := \sum_{k=1}^{n} \binom{n}{k} z^k (-1)^{n-k} + \alpha$$

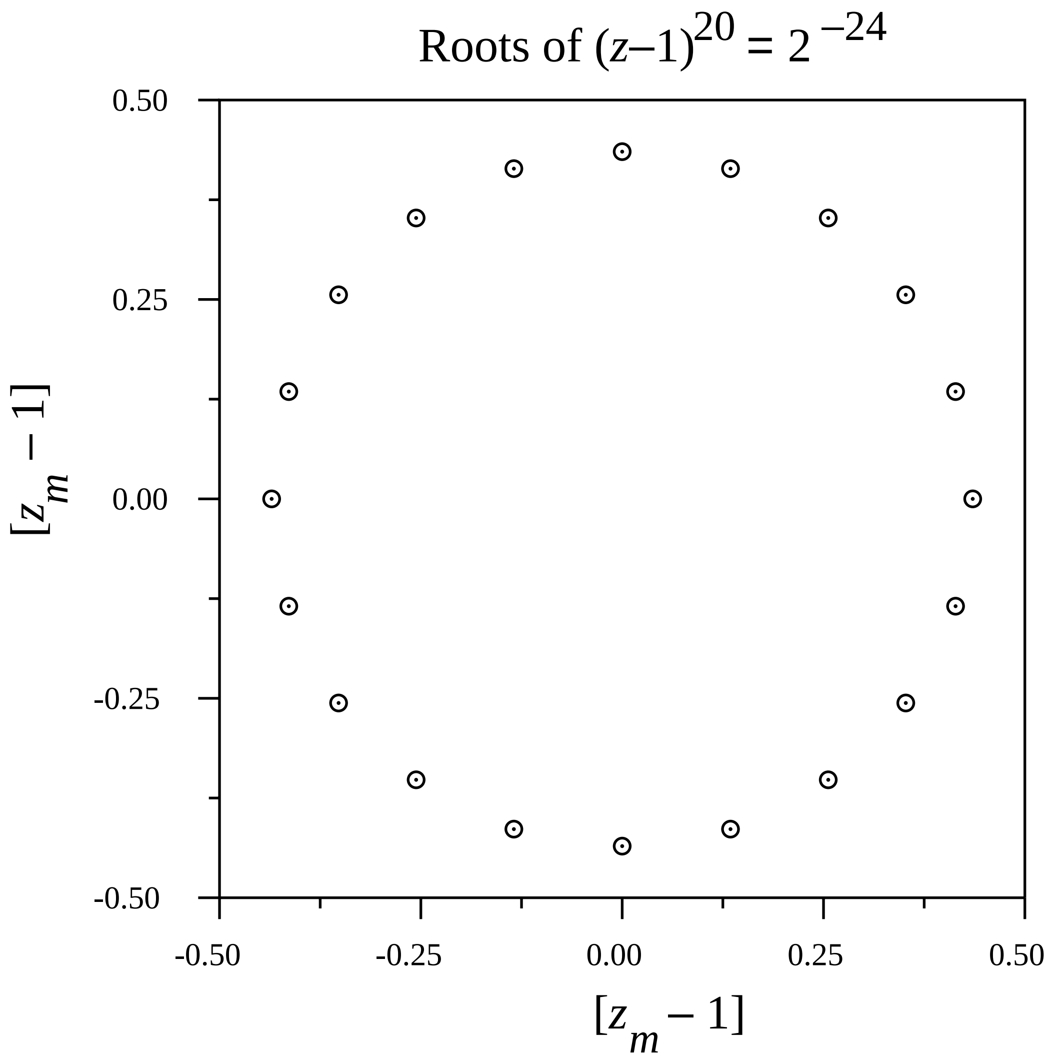
$p(z,(-1)^n) = (z-1)^n$ $\qquad$ n roots, each equal to 1

One ulp (unit in the last place) is $u = 2^{-24}$ in IEEE-754 single precision

Sensitivity of the roots of $p(z,\alpha)$ to a change of one ulp near $\alpha = 1$:

$$S(z_1;\,\alpha) = \left| \frac{\alpha\left[z_1(\alpha\ ) - z_1(\alpha)\right]}{(\alpha\ \ - \alpha)\, z_1(\alpha)} \right| \approx \left| \frac{u^{1/n}}{u} \right| = \frac{1}{u^{(n-1)/n}} \approx \frac{1}{u} \quad 1$$

SENSITIVITY/CONDITION NUMBER (3)



NEWTON-RAPHSON METHOD (1)

- The Newton-Raphson method is one of the better iterative methods for finding roots of a function f

Let a be a zero of f; if $x \approx a$, then

$$f(x) \approx f(a) + (x - a)f'(x)$$
$$\approx (x - a)f'(x)$$
$$a \approx x - \frac{f(x)}{f'(x)}$$

Newton-Raphson method: Iterate the difference equation

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

to convergence

NEWTON-RAPHSON METHOD (3)

- Rate of convergence for

$$f(x) = B(x - a) + C(x - a)^2$$

Di erence equation:

$$x_{k+1} = x_k - \frac{(x_k - a) + \frac{C}{B}(x_k - a)^2}{1 + 2\frac{C}{B}(x_k - a)} \approx a + \frac{C}{B}(x_k - a)^2$$

if x is su ciently close to a that

$$2\frac{C}{B}|x_k - a| \qquad 1$$

If this inequality holds already when $k = 0$, then

$$x_{k+1} - a \approx \left(\frac{C}{B}\right)^k (x_0 - a)^{2k}$$

The number of significant digits doubles with each iteration!

NEWTON-RAPHSON METHOD (4)

- Reciprocal approximation instead of floating-point division (used on Seymour Cray's machines)

  To find the number a such that

  $$a = \frac{1}{b}$$

  one can find the zeros of

  $$f(x) = \frac{1}{x} - b$$

  Newton-Raphson di erence equation:

  $$x_{k+1} = x_k - (-x_k + x_k^2 b) = 2x_k - x_k^2 b$$

NUMERICAL INTEGRATION (1)

- Problem: Evaluate the Riemann integral

$$I = \int_a^b f(x)\,dx$$

Sample f at $N+1$ points $x_0 = a$, $x_1 = a + h$, ..., $x_N = b$ and approximate I as a weighted sum of sampled values of f

$$I \approx \sum_{i=0}^{N} w_i\, f(x_i) = \sum_{i=1}^{N} I_i$$

where

$$I_i := \int_{x_{i-1}}^{x_i} f(x)\,dx$$

is the approximate integral of f over the panel (x_{i-1}, x_i)

Common rules for integration:

◦ Newton-Cotes methods (including rectangle rules)

◦ Gaussian quadrature

NUMERICAL INTEGRATION (2)

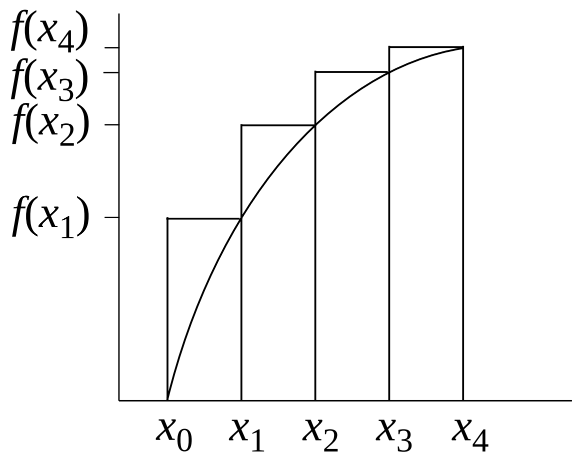
- Rectangle rules: Use a staircase approximation for f

  Right-hand rectangle rule:

$$\int_a^b f(x)\,dx \approx R_h[f] = \sum_{i=1}^{N} r_i[f]$$

  where

$$r_i[f] = h_i f(x_i), \quad h_i = x_i - x_{i-1}$$



NUMERICAL INTEGRATION (3)

- Centered rectangle rule:

$$\int_a^b f(x)\,dx \approx C_h[f] = \sum_{i=1}^{N} c_i[f]$$

where

$$c_i[f] = h_i f(x_{i-\frac{1}{2}}), \quad h_i = x_i - x_{i-1}, \quad x_{i-\frac{1}{2}} = \frac{x_i - x_{i-1}}{2}$$

- Trapezoidal rule:

$$\int_a^b f(x)\,dx \approx Th_h[f] = \frac{h}{2} f(x_0) + h \sum_{i=1}^{N-1} f(x_i) + \frac{h}{2} f(x_N)$$

NUMERICAL INTEGRATION (4)

- Numerical example: Evaluate $\int_0^1 x^2\,dx = \frac{1}{3}$ using 3 di erent rules and $h = \frac{1}{4}$

i	$f(x_i)$	$f\left(x_{i-\frac{1}{2}}\right)$
0	0	n/a
1	$\frac{1}{16}$	$\frac{1}{64}$
2	$\frac{1}{4}$	$\frac{9}{64}$
3	$\frac{9}{16}$	$\frac{25}{64}$
4	1	$\frac{49}{64}$

rule	computed integral	error
right-hand rectangle	0.4687	0.1354
midpoint	0.3281	−0.0052
trapezoidal	0.3438	0.0104

Note that the error of the trapezoidal method is −2 times the error of the midpoint method for this example

LOCAL vs. GLOBAL ERROR IN NUMERICAL INTEGRATION

- Local error in computed value of integral

  Error after 1 step of integration

  Equal to computed 1-panel integral − exact 1-panel integral

- Global error in computed value of integral

  Error after N steps of integration

  Equal to algebraic sum of local errors (classical approach)

  Can also be analyzed by global methods

  - Transfer function (comes from considering numerical integration rule as a digital filter)
  - Numerical dispersion function $\big(\omega(k)\big)$ vs. physical dispersion function

LOCAL ERROR ANALYSIS IN NUMERICAL INTEGRATION (1)

- Right-hand rectangle rule (algebraic derivation)

  Expand f about one of the sampling points:

$$f(x) = f(x_i) + \left.\frac{df}{dx}\right|_{x_i} (x - x_i) + \cdots$$

  Integrate over one panel:

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = h_i f(x_i) - \frac{1}{2} h_i^2 \left.\frac{df}{dx}\right|_{x_i} + \cdots$$

  Obtain global error by summing local errors:

$$\int_a^b f(x)\,dx \approx R_h[f] - \frac{h^2}{2} \sum_{i=1}^{N} \left.\frac{df}{dx}\right|_{x_i}$$

$$\approx R_h[f] - h\left(\frac{b-a}{2}\right)\left(\frac{1}{N}\sum_{i=1}^{N}\left.\frac{df}{dx}\right|_{x_i}\right)$$

LOCAL ERROR ANALYSIS IN NUMERICAL INTEGRATION (2)

- Right-hand rectangle rule (geometrical derivation)

  Local error ≈ area of triangle:

$$\text{local error}_i \approx \tfrac{1}{2}h\big(f(x_i) - f(x_{i-1})\big)$$

  Global error = sum of local errors:

$$\begin{aligned}\text{global error} &\approx \tfrac{1}{2}h\big(f(x_1) - f(x_0) + f(x_2) - f(x_1) + \cdots + f(x_N) - f(x_{N-1})\big)\\ &\approx \tfrac{1}{2}h\big(f(x_N) - f(x_0)\big)\end{aligned}$$

  - Global error   step size times change in f (in this case)
  - Note the cool telescoping sum

LOCAL ERROR ANALYSIS IN NUMERICAL INTEGRATION (3)

- Centered rectangle (midpoint) rule

Expand f about one of the sampling points:

$$f(x) = f(x_{i-\frac{1}{2}}) + \left.\frac{df}{dx}\right|_{x_{i-\frac{1}{2}}} \left(x - x_{i-\frac{1}{2}}\right) + \frac{1}{2} \left.\frac{d^2 f}{dx^2}\right|_{x_{i-\frac{1}{2}}} \left(x - x_{i-\frac{1}{2}}\right)^2 + \frac{1}{6} \left.\frac{d^3 f}{dx^3}\right|_{x_{i-\frac{1}{2}}} \left(x - x_{i-\frac{1}{2}}\right)^3 + \frac{1}{24} \left.\frac{d^4 f}{dx^4}\right|_{x_{i-\frac{1}{2}}} \left(x - x_{i-\frac{1}{2}}\right)^4 + \cdots$$

Integrate a typical term:

$$\int_{x_{i-1}}^{x_i} (x - x_{i-\frac{1}{2}})^p \, dx = \begin{cases} h_i & \text{if } p = 0; \\ 0 & \text{if } p = 1; \\ \frac{1}{12} h_i^3 & \text{if } p = 2; \\ 0 & \text{if } p = 3; \\ \frac{1}{80} h_i^5 & \text{if } p = 4. \end{cases}$$

LOCAL ERROR ANALYSIS IN NUMERICAL INTEGRATION (4)

- Centered rectangle (midpoint) rule

  Local error:

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = c_i[f] + p_i[f] + q_i[f] + \cdots = t_i[f] - 2p_i[f] - 4q_i[f] + \cdots$$

  where

$$p_i[f] := \frac{1}{24} h_i^3 \left.\frac{d^2 f}{dx^2}\right|_{x_{i-\frac{1}{2}}}, \qquad q_i[f] := \frac{1}{1920} h_i^5 \left.\frac{d^4 f}{dx^4}\right|_{x_{i-\frac{1}{2}}}$$

  Obtain global error by summing local errors:

$$\int_a^b f(x)\,dx \approx C_h[f] + \frac{h^3}{24} \sum_{i=1}^{N} \left.\frac{d^2 f}{dx^2}\right|_{x_{i-\frac{1}{2}}}$$

$$\approx C_h[f] + h^2 \left(\frac{b-a}{24}\right) \left(\frac{1}{N} \sum_{i=1}^{N} \left.\frac{d^2 f}{dx^2}\right|_{x_{i-\frac{1}{2}}} \right)$$

LOCAL ERROR ANALYSIS IN NUMERICAL INTEGRATION (5)

- Trapezoidal rule

  Local error:

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = c_i[f] + p_i[f] + q_i[f] + \cdots = t_i[f] - 2p_i[f] - 4q_i[f] + \cdots$$

  Note that (3rd order trapezoidal error) = $-2\times$ (3rd order midpoint error)

  Obtain global error by summing local errors:

$$\int_a^b f(x)\,dx \approx T_h[f] - \frac{h^3}{12}\sum_{i=1}^{N} \left.\frac{d^2 f}{dx^2}\right|_{x_{i-\frac{1}{2}}}$$

$$\approx T_h[f] - h^2\left(\frac{b-a}{12}\right)\left(\frac{1}{N}\sum_{i=1}^{N} \left.\frac{d^2 f}{dx^2}\right|_{x_{i-\frac{1}{2}}}\right)$$

LOCAL ERROR ANALYSIS IN NUMERICAL INTEGRATION (6)

- Simpson's rule

Combine the one-panel formulas for the trapezoidal and midpoint rules so that the 3rd order error vanishes

Let

$$s_i[f] := \tfrac{2}{3}c_i[f] + \tfrac{1}{3}t_i[f] = \tfrac{1}{6}h_i\left[f(x_{i-1}) + 4f(x_{i-\frac{1}{2}}) + f(x_i)\right]$$

Local error:

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = s_i[f] + \tfrac{2}{3}q_i[f] + \cdots$$

Obtain global error by summing local errors:

$$\int_a^b f(x)\,dx \approx S_h[f] - \frac{b-a}{180}\left(\frac{h}{2}\right)^4 \left(\frac{1}{N}\sum_{i=1}^{N} \left.\frac{d^4 f}{dx^4}\right|_{x_{i-\frac{1}{2}}}\right)$$

LOCAL ERROR ANALYSIS IN NUMERICAL INTEGRATION (7)

- Simpson's rule

  Multi-panel rule using a redefined step size $h' = h/2$ and redefined sampling points $x_{2i} = x_i$, $x_{2i-1} = x_{i-\frac{1}{2}}$:

$$\int_a^b f(x)\,dx \approx \frac{h'}{3}\Big(f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 4f(x_{2N-3}) + 2f(x_{2N-2}) + 4f(x_{2N-1}) + f(x_{2N})\Big) - \frac{b-a}{180}(h')^4 \left(\frac{1}{N}\sum_{i=1}^{N} \left.\frac{d^4 f}{dx^4}\right|_{x_{i-\frac{1}{2}}}\right)$$

  Note that the weights oscillate at the Nyquist frequency