Introduction: Engineering problems and computational methods

- 20 cm x 30 cm rectangular plate
- Initially at temperature f(x,y). Then, insulated at x=0, zero temperature at y=0, and convective heat transfer at x=20 and at y=30
- Find temperature variation with time at the center

Experimental: Advantages: No equations, Arbitrary Shape Issues: Size, Material, Time, f(x,y)

Analytical:
$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$
 $T(x, y, t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} c_{ij} e^{-\alpha \left(\beta_i^2 + \gamma_j^2 \right) t} \cos(\beta_i x) \sin(\gamma_j y)$

Adv: Fast, Adaptable, Accurate; Issues: Ideal conditions

Introduction: Engineering problems and computational methods Numerical Method: Reduce to algebraic equations

E.g.,

| | i,j+1 | | |
|-------|-------|-------|--|
| i-1,j | i,j | i+1,j | |
| | i,j-1 | | |

$$\frac{\partial T}{\partial t} = \frac{T_{i,j}^{t+\Delta t} - T_{i,j}^t}{\Delta t}$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1,j}^{t-\Delta t} - T_{i,j}^t}{\Delta x} - \frac{T_{i,j}^{t-\Delta t} - T_{i-1,j}^t}{\Delta x} = \frac{T_{i+1,j}^{t-\Delta t} - 2T_{i,j}^t + T_{i-1,j}^t}{\Delta x^2}$$

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Results in a set of linear (or nonlinear, if α is a function of temperature) equations

Adv: Arbitrary shape, initial and boundary conditions; Usually fast.

Issues: Convergence, Accuracy, Efficiency

Error Analysis: Round-off and Truncation errors Backward and Forward error analysis

All computational results have errors: Computers have finite storage length and computations cannot be carried out infinitely (We do not consider Model error and Data error)

Round-off Error: Due to finite storage length. E.g., with 8 significant digits: $\sqrt{2}$ is stored as 1.4142136 (actually as 0.14142136x10¹), an error of about $3x10^{-6}$ percent.

Truncation Error: Due to finite steps in computation. E.g., exp(2) is computed using the infinite series, truncated after a finite number of terms. True value is 7.389056098930650. 1 term – 1; 2 terms–3, 3–5, 4–6.333, 5-7, 6-7.356,...,15-7.3890561.

Error Analysis: Round-off and Truncation errors Backward and Forward error analysis

Round-off Error: Considering decimal storage, real numbers are stored as mantissa (m) x 10 $^{power(p)}$ with $0.1 \le m < 1$. If mantissa rounded-off at the tth digit, maximum error = 0.5×10^{-t} . Maximum relative error = 5×10^{-t} called the round-off unit, u.

Definitions:

True Error (e) = True Value – Approximate Value

Approximate Error (ε) = Current Approximation – Previous Approximation

(e.g., x=x/2+1/x, x=1,1.5, 1.4166667,1.4142157,1.4142136)

True Relative Error (e_r) = (True Value – Approximate Value) / True Value

Approximate Relative Error (ε_r) = (Current Approximation – Previous Approximation) / Current Approximation

Error Propagation

y is a function of n independent variables, $x_1, x_2, ..., x_n$, i.e. vector x y=f(x)

Due to error in the variables $(\Delta x_i = x_i - \widetilde{x}_i)$, there is error in y

$$\widetilde{y} = f(\widetilde{x})$$
 Error: $\Delta y = y - \widetilde{y} = f(x) - f(\widetilde{x}) = \sum_{i=1}^{n} \Delta x_i \frac{\partial f}{\partial x_i}\Big|_{\widetilde{x}_i}$

(Neglecting higher order terms in the Taylor's series)

Error Propagation

$$g = \frac{2h}{t^2}$$

Height measurement accurate to a mm, time to 100^{th} of sec. Error in g, if h=100.000 m and t=4.52 s?

$$\frac{\partial g}{\partial h} = \frac{2}{t^2}; \frac{\partial g}{\partial t} = -\frac{4h}{t^3}$$

$$\Delta g \cong \frac{2}{\widetilde{t}^2} \Delta h - \frac{4\widetilde{h}}{\widetilde{t}^3} \Delta t$$

$$= 0.0978933 \Delta h - 4.33156 \Delta t$$

Max value 0.0434 (Relative error is more meaningful, roughly 0.4%.)

Error Propagation and Condition Number of a problem

Condition number: Ratio of the relative change in the function, f(x), to the relative change in the variable for a small perturbation Δx in the variable x.

$$C_{P} = \frac{\left| \frac{f(x + \Delta x) - f(x)}{f(x)} \right|}{\left| \frac{\Delta x}{x} \right|} \text{ or, as } \Delta x \to 0, \frac{xf'(x)}{f(x)}$$

Well-Conditioned (<1) and *Ill-conditioned (>1)*

E.g.: Hyperbola xy-y+1=0. Measure x, compute y=f(x)=1/(1-x).

 $C_p = |x/(1-x)|$ Ill-conditioned for x>0.5 (x=0.8, y=5; x=0.808,y=5.2083)

Similarly, $y = \sqrt{1+x} - 1$ for small x;

$$C_p = \left| \frac{x}{2(1+x-\sqrt{1+x})} \right|$$
 close to but <1. (x=0.01, y=.004988; x=0.0101,y=.005037)

Error Analysis: Forward and Backward error analysis

Forward Error: requires the T.V.

 $(Recall\ that\ True\ Error\ (e) = True\ Value\ -Approximate\ Value)$

E.g.: $\sqrt{2} = 1.414213562373095$. With 4 digit accuracy (u=5x10⁻⁴), approx. value = 1.414. True error, $e = 2.134x10^{-4}$. True relative error = 0.015%.

Backward Error: determines the change necessary in the input variable (or data) to explain the final error in the output (or result) obtained through errors introduced at various stages of calculation.

E.g.: $1.414^2 = 1.999396$. Error= 6.04×10^{-4} , Relative error = 0.03%. $y = \sqrt{1+x}-1$ with x=0.001616 gives y = $\sqrt{1.002}-1$ = 0.0009995, which is exact for x=0.002 (error=0.000384, 24%)

Condition Number of an algorithm

• Condition number: Exact input data, x; Corresponding function value y; Algorithm A operating on x produces y_A on a machine with precision unit u. Input data, x_A , which would produce y, if exact computations are done. Condition number

of the algorithm $C_{A} = \frac{\left| \frac{x - x_{A}}{x} \right|}{u}$

Well-Conditioned (<1) and Ill-conditioned (>1)

$$y = \sqrt{1+x} - 1$$
 for $x = 0.001616$, we get $x_A = 0.002$.

$$C_A = \frac{\left| \frac{0.001616 - 0.002}{0.001616} \right|}{5 \times 10^{-4}} = 475$$

$$y = \sqrt{1+x} - 1 = \frac{x}{\sqrt{1+x} + 1}$$
 x=0.001616, y=0.0008076, x_A=0.00161585, C_A=0.18

Error Analysis: Vector Norms

What if the computed result is a vector?

$$[A]{x} = {b}$$

Error vector

$$\{\varepsilon\} = \{x\} - \{\widetilde{x}\}$$

Or, relative error vector

$$\left\{ \mathcal{E}_r \right\} = \left\{ \frac{x - \widetilde{x}}{x} \right\}$$

Magnitude: In terms of the "Norm" of the vector

Error Analysis: Vector Norms

Some properties of the vector norms are (α is a scalar):

- ||x|| = 0, only if x is a null vector, otherwise ||x|| > 0
- $\|\alpha x\| = |\alpha| \|x\|$
- $||x_1 + x_2|| \le ||x_1|| + ||x_2||$

Magnitude: The L_p norm of an *n*-dimensional vector, $\{x\}$, *i.e.*, $(x_1,x_2,...,x_n)^T$, is given by

$$||x||_p = (|x_1|^p + |x_2|^p + |x_3|^p + \dots + |x_n|^p)^{1/p} \quad p \ge 1$$

Common Vector Norms

- p=2, Euclidean norm: (length) $||x||_2 = \sqrt{x_1^2 + x_2^2 + ... + x_n^2}$
- p=1, (total distance) $||x||_1 = \sum_{i=1}^n |x_i|$
- p= ∞ , Maximum norm $||x||_{\infty} = \max_{i} |x_{i}|$