Mathematical Models for Engineering Problems and Differential Equations

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Numerical Methods

- What do we really need in practical problems (differential equations with initial conditions)?
  $\rightarrow y(0.1), y(0.2), y(0.3), \cdots, y(100)$
- The solution of most practical differential equations are not composed of elementary functions.
- Even when we have solutions composed of elementary functions, getting values by numerical methods is easier at times.
- Implicit solutions are not useful.
- Three categories
  - Starting methods: to start the construction of a table
  - Continuing methods: requires more values of y to be used
  - Corrector methods to correct values of y obtained by starting and continuing methods

Outline

Polygonal Method

Used to start finding $y(x_0 + h), y(x_0 + 2h), \cdots$ where h is a (small) constant and $y(x)$ is the unique particular solution of

$$y' = f(x, y)$$

satisfying the initial condition

$$y(x_0) = y_0.$$

Procedure:

1. Find the value of y' at (x_0, y_0). $\to f(x_0, y_0)$
2. The equation of the tangent to the integral curve $y(x)$ at (x_0, y_0) is
$$y - y(x_0) = (x - x_0)y'(x_0).$$
3. Find the value of tangent line at $x = x_1 := x_0 + h$:
$$y_1 := y(x_1) = y(x_0) + y'(x_0)h.$$
4. Assuming (x_1, y_1) is actually on the integral curve $y(x)$, repeat the procedure.

Error of Polygonal Method

- A *formular error* is introduced in the first step.
  $|Y(x+h) - y_1|$ ($Y(x)$ is the actual solution.)
- At each step, a *starting error* and a *formula error* are introduced, so that the *cumulative error* may soon become large.
  $\rightarrow$ Useful only if too great accuracy is not required or if h is very small.

Computing the Error

1. We want to compute $|Y(x_0 + h) - y_1|$ where $Y(x)$ is the actual solution and y_1 is the value of the (approximate) solution at $x = x_0 + h$ we found by polygonal method.
2. The formular
$$y(x_0 + h) = y(x_0) + y'(x_0)h$$
is the first two terms of a Taylor series.
The remainder (or error) term is (Lagrange formula)
$$E(x_0 + h) := ch^2, \quad c := \frac{y''(X)}{2!}.$$
3. If we half the interval, assuming the variation of $y''(X)$ is negligible in each $h/2$, the same c can be used for each $h/2$ interval.
$\rightarrow$ *approximate error*

Computing the Error (cont'd)

4. $E\left(x_0 + \frac{h}{2}\right) = c\left(\frac{h}{2}\right)^2 = \frac{1}{4}E(x_0 + h).$
5. A starting error $E(x_0 + h/2)$ and a formular error $E(x_0 + h/2)$ are introduced when computing $y(x_0 + h)$ in the next step:

$$\rightarrow \quad E\left[\left(x_0 + \frac{h}{2}\right) + \frac{h}{2}\right] = \frac{1}{2}E(x_0 + h).$$

6. We get

$$E(x_0 + h) := Y(x_0 + h) - y(x_0 + h)$$
$$E\left[\left(x_0 + \frac{h}{2}\right) + \frac{h}{2}\right] := Y(x_0 + h) - y\left[\left(x_0 + \frac{h}{2}\right) + \frac{h}{2}\right]$$

- $E(x_0 + h)$: approximate error in the value of $y(x_0 + h)$ computed in one step.
- $E((x_0 + h/2) + h/2)$: approximate error in the value of $y(x_0 + h)$ computed in two steps.

Computing the Error (cont'd)

7. Therefore we get

$$E\left[\left(x_0 + \frac{h}{2}\right) + \frac{h}{2}\right] = y\left[\left(x_0 + \frac{h}{2}\right) + \frac{h}{2}\right] - y(x_0 + h)$$

$\rightarrow$ difference of the values computed in two steps and one step.

Error of Polygonal Method (cont'd)

- Practical error checking
  If $E[(x_0 + h/2) + h/2]$ and $E(x_0 + h)$ agree up to k decimal places, their common numerical value has k decimal place accuracy.
- Can be used as a continuing method, but is a poor method due to the low accuracy.

Outline

Improving the Polygonal Starting Method

"Can we obtain more terms of the Taylor series expansion of $y(x)$?"

1. Approximate the value $y(x_0 + h/2)$ by the mid point of $(x_0, y(x_0))$ and $(x_0 + h, y(x_0) + y'(x_0)h)$
   $\rightarrow P\left(x_0 + \frac{h}{2}, y(x_0) + y'(x_0)\frac{h}{2}\right)$
2. Approximate the value $y'(x_0 + h/2)$ by applying the value just computed into the D.E.:
   $$\rightarrow \quad y'(x_0 + h/2) = f\left[x_0 + \frac{h}{2}, y(x_0) + y'(x_0)\frac{h}{2}\right]$$
3. Compute the value of $y(x_0 + h)$ using the slope just computed:
   $$\rightarrow \quad y(x_0 + h) = y(x_0) + hf\left[x_0 + \frac{h}{2}, y(x_0) + y'(x_0)\frac{h}{2}\right].$$
4. The right-hand side is the first three terms of the Taylor series expansion. (See the proof on p.642.)

Outline

Chapter 10: Numerical Methods

Taylor Series Method

- "...greater accuracy may be achieved if, for a starting method, we use a Taylor series to terms of order greater than two...." (p.645)
- Taylor series expansion near x_0:

$$y(x_0 + h) = \sum_{j=0}^{\infty} \frac{y^{(j)}(x_0)}{j!} h^j$$

  $\rightarrow$ "If one knows the values of the function $y(x)$ and its derivatives at a point $x = x_0$, then one can find the values of the function for a neighboring point h units away."
  $\rightarrow$ We need $y(x_0), y'(x_0), y''(x_0), \cdots, y^{(n)}(x_0), \cdots$.
- Two methods
  1. Direct substitution
  2. "Creeping up" process
- Difficulties
  - $y' = f(x, y)$ may not have a Taylor series expansion in the interval.
  - It may be extremely difficult to obtain the derivatives.

1. Direct Substitution

1. Starting from the D.E., find the formula for $y'(x), y''(x), \cdots, y^{(n)}(x), \cdots$.
2. Starting from the initial condition $y(x_0) = y_0$, find $y'(x_0), y''(x_0), \cdots, y^{(n)}(x_0), \cdots$.
3. Now we have the Taylor series near $x = x_0$.

$\rightarrow$ "More and more terms of the series must be included, as h increases, in order to maintain a desired degree of accuracy."

2. “Creeping Up” Process

1. Find the approximate value of $y(x_0 + h)$ by Taylor series at $x = x_0$ up to order n.
2. Find the Taylor series at $x = x_0 + h$ by computing $y'(x_0 + h), y''(x_0 + h), \cdots, y^{(n)}(x_0 + h)$.
3. Find the approximate value of $y(x_0 + 2h)$ by Taylor series at $x = x_0 + h$ up to order n.
4. Repeat.

$\rightarrow$ Ignoring the cummulative error, accuracy kepts the same (due to the fixed h in each step), but more labor required.

Outline

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Runge-Kutta Formulas

- Derivatives not required.
- High degree of accuracy.
- Two methods: direct substitution and creeping up process.
- Large number of computation required when used as a continuing method.

Runge-Kutta Formulas (cont'd)

1. Differentiating the D.E. $y'(x) = f(x, y)$, we get

$$y''(x) = \frac{\partial}{\partial x} f(x, y) + \frac{\partial}{\partial y} f(x, y) y'(x).$$

2. Applying $y'(x)$ and $y''(x)$ in the Taylor series expansion, (up to order 2)

$$y(x_0+h) = y(x_0)+f(x_0, y_0)h+\left[\frac{\partial f(x_0, y_0)}{\partial x} f(x, y) + \frac{\partial f(x_0, y_0)}{\partial y} f(x_0, y_0)\right] \frac{h^2}{2}.$$

3. Find (non-unique) A, B, C, D such that

$$y(x_0 + h) = y(x_0) + Ahf(x_0, y_0) + Bhf[x_0 + Ch, y_0 + Dhf(x_0, y_0)]$$

   equals the right-hand side of the previous equation.
   $\rightarrow$ e.g., $A = B = 1/2$ and $C = D = 1$.

4. Runge-Kutta formula (second order form)

$$y(x_0 + h) = y(x_0) + \frac{1}{2} hf(x_0, y_0) + \frac{1}{2} hf[x_0 + h, y_0 + hf(x_0, y_0)]$$

Outline

Finite Difference

First difference

$$\Delta f(x) := f(x+h) - f(x)$$

In general,

$$\Delta^n f(x) := \Delta[\Delta^{n-1} f(x)], \quad n = 1, 2, \cdots$$

and

$$\Delta^n f(x_0) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} f[x_0 + (n-k)h],$$

where

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}.$$

Interpolating Polynomials

Given function values at $m+1$ different points,

$$f(x_0), f(x_1), \cdots, f(x_m),$$

what is the best approximate function value at an arbitrary point?

- There is a *unique* polynomial of degree m (or less), $p(x) = \sum_{j=0}^{m} a_j x^j$, which agrees with the $m+1$ function values: (Theorem 48.2)

$$p(x_0) = f(x_0), p(x_1) = f(x_1), \cdots, p(x_m) = f(x_m).$$

- This polynomials can be found by solving an $(m+1) \times (m+1)$ linear system.

$$\left[x_k^j\right][a_k] = \left[f(x_j)\right] \quad \rightarrow \quad [a_k] = \left[x_k^j\right]^{-1}\left[f(x_j)\right].$$

- When the "abscissa" points are evenly spaced $\rightarrow$ Newton's interpolation formula.

Outline

Chapter 10: Numerical Methods

Newton's Forward Interpolation Formula

To find the interpolating polynomial for the given function values at $m+1$ distinct abscissa points, $x = x_0, x_0 + h, x_0 + 2h, \cdots, x_0 + mh$.

1. In general,

$$f(x_0 + nh) = \sum_{k=0}^{n} \binom{n}{k} \Delta^k f(x_0) = \sum_{k=0}^{m} \binom{n}{k} \Delta^k f(x_0), \quad n = 0, \cdots, m,$$

   since $\binom{n}{k} = 0$ for $k > n$.

2. For $x = x_0 + nh$ and $n = (x - x_0)/h$ (n not necessarily an integer), we get the first formula

$$F(x) = \sum_{k=0}^{m} \binom{n}{k} \Delta^k f(x_0).$$

3. Applying $n = (x - x_0)/h$, we get the second formula

$$F(x) = \sum_{k=0}^{m} \frac{\Delta^k f(x_0)}{k! h^k} \prod_{j=0}^{k-1} (x - x_0 - jh).$$

Newton's Forward Interpolation Formula (cont'd)

4. Since
   - $F(x_0 + kh) = f(x_0 + kh)$, $\forall 0 \leq k \leq m$ and
   - $F(x)$ is a polynomial of degree $\leq m$,

   $F(x)$ is the *unique* interpolating polynomial of $f(x)$.
   $\rightarrow$ Newton's forward interpolation formula.

Newton's Backward Interpolation Formula

- Backward difference:

$$\nabla f(x) := f(x) - f(x-h).$$

- The first formula:

$$F(x) = \sum_{k=0}^{m} (-1)^k \binom{n}{k} \nabla^k f(x_0).$$

- The second formula:

$$F(x) = \sum_{k=0}^{m} \frac{\nabla^k f(x_0)}{k! h^k} \prod_{j=0}^{k-1} (x - x_0 + jh).$$

The Error in Polynomial Interpolation

The error formula (for forawrd interpolation formula):

$$E(x) := f(x) - F(x) = \frac{\prod_{j=0}^{m}(x - x_0 - jh)}{(m+1)!} f^{(m+1)}(X)$$

where $x_0 \leq X \leq x_0 + mh$. Therefore,

$$C_f \min |f^{(m+1)}(x)| \leq |E(x)| \leq C_f \max |f^{(m+1)}(x)|, \quad x_0 \leq x \leq x_0 + mh,$$

where $C_f := \left| \frac{\prod_{j=0}^{m}(x - x_0 - jh)}{(m+1)!} \right|$.

The same argument applies to the backward interpolation formual, with $C_b := \left| \frac{\prod_{j=0}^{m}(x - x_0 + jh)}{(m+1)!} \right|$.

Outline

Approximation Formulas

To solve the differential equation

$$y' = f(x, y), \quad y(x_0) = y_0.$$

1. Let $y(x)$ be a solution, which we do not know. Then

$$y'(x) = f(x, y(x)).$$

$\rightarrow f$ is a function of x alone.

$$\rightarrow \int_{\tilde{y}=y_0}^{y} d\tilde{y} = \int_{\tilde{x}=x_0}^{x} f(x, y(x))d\tilde{x}$$

$$\rightarrow y(x) = y_0 + \int_{\tilde{x}=x_0}^{x} f(x, y(x))dx$$

$$\rightarrow y(x_0 + nh) = y(x_0) + \int_{x_0}^{x_0+nh} f(x, y(x))dx$$

$\rightarrow$ We need to find $f(x, y(x))$!

Approximation Formulas (cont'd)

2. Let $F(x)$ be a (forward) interpolating polynomialof $f(x, y(x))$. Then,

$$F(x) = \sum_{k=0}^{m} \frac{\Delta^k f(x_0, y(x_0))}{k!h^k} \prod_{j=0}^{k-1} (x - x_0 - jh)$$
$$= \left(\frac{\prod_{j=0}^{k-1}(x - x_0 - jh)}{k!h^k} \Delta^k \right) y'(x_0).$$

$$\rightarrow \int_{x_0}^{x_0+nh} f(x, y(x))dx \approx \int_{x_0}^{x_0+nh} F(x)dx$$
$$= \int_{x_0}^{x_0+nh} \left(\frac{\prod_{j=0}^{k-1}(x - x_0 - jh)}{k!h^k} \Delta^k \right) y'(x_0)dx$$
$$= \int_{0}^{nh} \left(\frac{\prod_{j=0}^{k-1}(u - jh)}{k!h^k} \Delta^k \right) y'(x_0)du \quad (u = x - x_0)$$

$\rightarrow$ Can be computed. (See (50.22) and (50.23) on p.674)

$\rightarrow$ Different formulas depending on the degree of $F(x)$.

1. Trapezoidal Rule

With $n = 1$, if the degree of $F(x)$ is less than or equal to 1,

$$\int_{x_0}^{x_0+h} = h(1 + \frac{1}{2}\Delta)y'(x_0) = \frac{h}{2}\left(y'(x_0) + y'(x_0 + h)\right),$$

therefore (trapezoidal rule)

$$y(x_0 + h) \approx y(x_0) + \frac{h}{2}(y'(x_0) + y'(x_0 + h)).$$

2. Simpson's Rule

With $n = 2$, if the degree of $F(x)$ is less than or equal to 2,

$$\int_{x_0}^{x_0+2h} F(x)dx = 2h\left(1 + \Delta + \frac{1}{6}\Delta^2\right)y'(x_0)$$

$$= \frac{h}{3}\left(y'(x_0) + 4y'(x_0 + h) + y'(x_0 + 2h)\right)$$

therefore (Simpson's rule)

$$y(x_0 + 2h) = y(x_0) + \frac{h}{3}\left(y'(x_0) + 4y'(x_0 + h) + y'(x_0 + 2h)\right).$$

...And More

3. With $n = 4$ and the degree of $F(x) \leq 3$
   $\rightarrow$ "third degree polynomial" (50.35).
4. With $n = 5$ and the degree of $F(x) \leq 5$
   $\rightarrow$ "fifth degree polynomial" (50.37).
5. With $n = 6$ and the degree of $F(x) \leq 6$
   $\rightarrow$ modified to (50.4)
   $\rightarrow$ "Weddle's rule" (50.41).

$\rightarrow$ See the table on p.678.

How to use them?

- Except the “third degree polynomial,” all the formulas require $y'(x_0 + nh)$, which can be obtaind from $y(x_0 + nh)$, to find $y(x_0 + nh)$
  $\rightarrow$ Not starting/continuing formulas.
  $\rightarrow$ A corrector formula: repeated application of the formula will improve an estimated approximation of $y(x_0 + nh)$ computed by a less accurate formula than itself.
- “Third degree polynomial” is a continuing formula.
- To compute $f(x_0 + nh)$, we need $f(x_0), f(x_0 + h), \cdots, f(x_0 + (n - 1)h)$
  $\rightarrow$ Cannot be used as a staring formula.

Outline

Milne's Method

- Simple form and relatively high degree of accuracy
  $\rightarrow$ most widely used
- Composed of
  - "Third degree polynomial" (50.62) as a continuing formula to estimate/predict a value of $y(x_0 + 4h)$.

$$y_p(x_0 + 4h) = y(x_0) + \frac{4h}{3}\left(2y'(x_0 + h) - y'(x_0 + 2h) + 2y'(x_0 + 3h)\right)$$

  - Simpson's formula (50.61) as a corrector formula

$$y_c(x_0{+}4h) = y(x_0{+}2h){+}\frac{h}{3}\left(y'(x_0 + 2h) + 4y'(x_0 + 3h) + y_p'(x_0 + 4h)\right)$$

- Requires a starting formulas to know
  $y'(x_0 + h), y'(x_0 + 2h), y'(x_0 + 3h)$.
- Repeated process will converge as long as
  - the original estimate is not too far away fro the true value and
  - h is sufficiently small.

Milne's Method (cont'd)

Solving

$$y' = f(x, y), \quad y(x_0) = y_0.$$

1. Find $y(x_0 + h), y(x_0 + 2h), y(x_0 + 3h)$ using a starting formula, e.g., Taylor series method.
2. Find $y'(x_0 + h), y'(x_0 + 2h), y'(x_0 + 3h)$ by the differential equation.
3. Compute an estimate of $y(x_0 + 4h)$ using the "third degree polynomial" formula.
4. Correct it using the Simpson's formula.
5. Repeat until the value does not change.
6. Find $y'(x_0 + 4h)$.
7. Compute an estimate of $y(x_0 + 5h)$ and repeat the process.

Outline

Comment on Errors

Three suggestions:

1. Start with many more decimals than you need.
2. Calculate the estimate error by make all calculations over again with $h/2$.
3. Apply a corrector formula to get the accurary and adjust h accordingly.

Caution: Practical error estimate formulas do not give exact error bound. Use *upper bound* of the error if exact error bound is required.

Choosing the Size of h

After calculating the value $y(x_0 + h)$,

- if the *estimate* error is greater than the desired error,
  $\rightarrow$ decrease h.
- if the *estimate* error is very much less than the desired error,
  $\rightarrow$ increase h.
- if the *estimate* error is reasonably less than the desired error,
  $\rightarrow$ keep h.

Outline

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