

Mathematical Models for Engineering Problems and Differential Equations

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December 10, 2009

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Numerical Methods

- ▶ What do we really need in practical problems (differential equations with initial conditions)?
→ $y(0.1), y(0.2), y(0.3), \dots, y(100)$
- ▶ 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

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Polygonal Method

Used to start finding $y(x_0 + h), y(x_0 + 2h), \dots$ 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) . $\rightarrow f(x_0, y_0)$
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.
→ 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.
→ *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:

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

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

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

→ 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.

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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.:

$$\rightarrow y'(x_0 + h/2) = f\left[x_0 + \frac{h}{2}, y(x_0) + y'(x_0)\frac{h}{2}\right]$$

3. Compute the value of $y(x_0 + h)$ using the slope just computed:

$$\rightarrow y(x_0 + h) = y(x_0) + hf\left[x_0 + \frac{h}{2}, y(x_0) + y'(x_0)\frac{h}{2}\right].$$

4. The right-hand side is the first three terms of the Taylor series expansion. (See the proof on p.642.)

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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 :

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

→ “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.”

→ We need $y(x_0), y'(x_0), y''(x_0), \dots, y^{(n)}(x_0), \dots$.

- ▶ 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 $y'(x), y''(x), \dots, y^{(n)}(x), \dots$.
2. Starting from the initial condition $y(x_0) = y_0$, find $y'(x_0), y''(x_0), \dots, y^{(n)}(x_0), \dots$.
3. Now we have the Taylor series near $x = x_0$.

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

→ Ignoring the cumulative error, accuracy keeps the same (due to the fixed h in each step), but more labor required.

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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.

→ e.g., $A = B = 1/2$ and $C = D = 1$.

4. Runge-Kutta formula (second order form)

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

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Finite Difference

First difference

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

In general,

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

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,

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

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)

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

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

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

- ▶ When the “abscissa” points are evenly spaced
→ Newton’s interpolation formula.

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Newton's Forward Interpolation Formula

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

1. In general,

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

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 $f(x)$.

→ 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 forward 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,

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

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

The same argument applies to the backward interpolation formula,

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

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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

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

→ f is a function of x alone.

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

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

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

→ We need to find $f(x, y(x))$!

Approximation Formulas (cont'd)

2. Let $F(x)$ be a (forward) interpolating polynomial of $f(x, y(x))$.

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

$$\begin{aligned} \rightarrow \int_{x_0}^{x_0+nh} f(x, y(x)) dx &\approx \int_{x_0}^{x_0+nh} F(x) dx \\ &= \int_{x_0}^{x_0+nh} \sum_{k=0}^m \left(\frac{\prod_{j=0}^{k-1} (x - x_0 - jh)}{k!h^k} \Delta^k \right) y'(x_0) dx \\ &= \int_0^{nh} \sum_{k=0}^m \left(\frac{\prod_{j=0}^{k-1} (u - jh)}{k!h^k} \Delta^k \right) y'(x_0) du \quad (u = x - x_0) \end{aligned}$$

→ Can be computed. (See (50.22) and (50.23) on p.674)

→ 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,

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

therefore (trapezoidal rule)

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

NOTE: It is called “trapezoidal rule” because it approximates an definite interval with a trapezoid:

$$\int_a^b f(x)dx \approx (b - a)\frac{f(b) + f(a)}{2}.$$

2. Simpson's Rule

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

$$\begin{aligned}\int_{x_0}^{x_0+2h} F(x)dx &= 2h \left(1 + \Delta + \frac{1}{6}\Delta^2 \right) y'(x_0) \\ &= \frac{h}{3} (y'(x_0) + 4y'(x_0 + h) + y'(x_0 + 2h))\end{aligned}$$

therefore (Simpson's rule)

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

...And More

3. With $n = 4$ and the degree of $F(x) \leq 3$
→ “third degree polynomial” (50.35).
 4. With $n = 5$ and the degree of $F(x) \leq 5$
→ “fifth degree polynomial” (50.37).
 5. With $n = 6$ and the degree of $F(x) \leq 6$
→ modified to (50.4)
→ “Weddle’s rule” (50.41).
- 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 obtained from $y(x_0 + nh)$, to find $y(x_0 + nh)$
 - Not starting/continuing formulas.
 - 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 $f(x_0), f(x_0 + h), \dots, f(x_0 + (n - 1)h)$
 - Cannot be used as a starting formula.

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Milne's Method

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

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

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

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

- ▶ 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 from 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.

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Comment on Errors

Three suggestions:

1. Start with many more decimals than you need.
2. Calculate the estimate error by making all calculations over again with $h/2$.
3. Apply a corrector formula to get the accuracy 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,
→ decrease h .
- ▶ if the *estimate* error is very much less than the desired error,
→ increase h .
- ▶ if the *estimate* error is reasonably less than the desired error,
→ keep h .

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