Day 13: Higher Order Methods

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1 Problem 4 with Euler Method

We have the problem

$$y'' = ty \qquad y(0) = 1 \qquad y'(0) = 1$$

We turn this into two equations

$$y' = w \qquad y(0) = 1 \qquad w' = ty \qquad w(0) = 1$$

To solve this, we wish to use the Trapezoid method. But before we do that, let's solve the problem using Euler's Method and get our bearings.

We create a table, and stuff it with what we know.

time	y	w	slope y	slope w	Euler y	Euler w
0	1	1				

We compute the slopes of y and w

time	y	w	slope y	slope w	Euler y	Euler w
0	1	1	1	0		

We use these slopes to estimate the new values of y and w using Euler's Method.

time	y	w	slope y	slope w	Euler y	Euler w
0	1	1	1	0	1.25	1

Plug these back into the table, and start again

time	y	w	slope y	slope w	Euler y	Euler w
0	1	1	1	0	1.25	1
0.25	1.25	1				

Compute the slopes at these points:

time	y	w	slope y	slope w	Euler y	Euler w
0	1	1	1	0	1.25	1
0.25	1.25	1	1	0.3125		

We can plug these slopes into the Euler Method to get the next step.

2 Problem 4 with Trapezoid Method

To compute the Trapezoid method, we would extend our table. We have already filled in the first steps above.

Our equations were

$$y' = w \qquad y(0) = 1 \qquad w' = ty \qquad w(0) = 1$$

time	y	w	slope y	slope w	Euler y	Euler w	Trap y	Trap w
0	1	1	1	0	1.25	1		

We take use these values to compute the Trapezoid method

$$y_1 = y_0 + \frac{h}{2}[w_0 + w_1] = 1 + \frac{1}{8}[1 + 1]$$

$$w_1 = w_0 + \frac{h}{2}[t_0 y_0 + t_1 y_1] = w_0 + \frac{h}{2}[0 + \frac{1}{4} \times \frac{5}{4}] = 1 + \frac{5}{128}$$

time	y	w	slope y	slope w	Euler y	Euler w	Trap y	Trap w
0	1	1	1	0	1.25	1	1.25	1.04
0	1.25	1.04						

3 Extended Example

Before we dive into Taylor Methods, let's look at an example to see how we can find the derivative of y'.

We look at the following example. It is instructive to look at the vector field.

$$y' = -\frac{t}{y} \qquad y(0) = 1$$

Can we derive y'' without knowing $y(t)$? Well, we could differentiate y' with respect to t by using the chain rule.

$$f'(t, y) = \frac{\partial f(t, y)}{\partial t} + \frac{\partial f(t, y)}{\partial y} f(t, y)$$

We have an expression for y' in two variables: t and y. The independent variable is t, and we assume that y is a function of t. To show this, we sometimes write $y(t)$.

Since $\frac{dy}{dt} = f(t, y(t)) = -\frac{t}{y}$

$$y'' = -\frac{1}{y} + \frac{t}{y^2}\frac{dy}{dt} = -\frac{1}{y} - \frac{t^2}{y^3} = -\frac{y^2 + t^2}{y^3}$$

But $y^2 = 1 - t^2$, so we know $y^2 + t^2 = 1$, and we can replace the numerator and get

$$y'' = -\frac{1}{y^3}$$

We can solve the original problem by separating variables:

$$\int y dy = -\int t dt$$

$$y^2 = C - t^2$$

Evaluate at y(0) = 1.

$$1 = C - 0$$

$$y^2 = 1 - t^2$$

$$y = \sqrt{1 - t^2} = (1 - t^2)^{\frac{1}{2}}$$

So we have an explicit analytic solution. We could then check our notes by differentiating twice, and explicitly derive y' and y'' from our formula for $y(t)$.

$$\frac{dy}{dt} = \frac{1}{2}(1 - t^2)^{-\frac{1}{2}}(-2t) = -\frac{t}{(1 - t^2)^{\frac{3}{2}}}$$

As a check, note that we plug in y and get our original definition of $f(t, y(t))$.

$$-\frac{t}{(1 - t^2)^{\frac{1}{2}}} = -\frac{t}{y}$$

4 Runge Kutta Methods through Taylor Series

We derived the Euler method from the Taylor series. To derive a second order method, we could add another term to our estimate.

$$y(t+h) = y(t) + hy'(t) + \frac{1}{2}h^2y''(t) + \frac{1}{6}h^3y'''(c)$$

This would give us

$$w_{i+1} = w_i + hf(t_i, w_i) + \frac{h^2}{2}f'(t_i, w_i)$$

However, we don't know $y(t)$ - all we know is that $y' = f(t, y(t))$.
What do we know about $f'(t, y)$?

$$f'(t,y) = \frac{\partial f(t,y)}{\partial t} + \frac{\partial f(t,y)}{\partial y}\frac{dy}{dt} = \frac{\partial f(t,y)}{\partial t} + \frac{\partial f(t,y)}{\partial y}f(t,y)$$

We are trying to design an equation of the form

$$\frac{w_{i+1} - w_i}{h} = c_1f(t_i, w_i) + c_2f(t_i + b_2, w_i + af(t_i, w_i))$$

We expand the last function call using the two dimensional Taylor Series

$$\frac{w_{i+1} - w_i}{h} = c_1f(t_i, w_i) + c_2\left(f(t_i, w_i) + b_2\frac{\partial f}{\partial t}(t_i, y_i) + af(t_i, y_i)\frac{\partial f}{\partial y}(t_i, y_i) + O(h^2)\right)$$

$$\frac{w_{i+1} - w_i}{h} = (c_1 + c_2)f(t_i, w_i) + c_2b_2\frac{\partial f}{\partial t}(t_i, y_i) + c_2af(t_i, y_i)\frac{\partial f}{\partial y}(t_i, y_i) + c_2O(h^2)$$

Compare to a Taylor Series Expansion

$$\frac{y_{i+1} - y_i}{h} = y'(t_i, y_i) + \frac{h}{2}y''(t_i, y_i) + \frac{h^2}{6}y'''(c)$$

We set this to equal to the Taylor Series Expansion above, and find

$$c_1 + c_2 = 1$$

$$c_2b_2 = \frac{h}{2}$$

$$c_2a = \frac{h}{2}$$

We can solve this with

$$a = b_2 = \frac{h}{2c_2}$$

This gives us a number of equations of similar form

$$\frac{w_{i+1} - w_i}{h} = (1 - c_2)f(t_i, w_i) + c_2 f(t_i + \frac{h}{2c_2}, w_i + \frac{h}{2c_2} f(t_i, w_i))$$

Some notable examples

Euler's method with a step size of $\frac{h}{2}$: $c_1 = 0$, $c_2 = 1$, $a = b_2 = \frac{h}{2}$

$$w_{i+1} = w_i + hf(t_i + \frac{h}{2}, w_i + \frac{h}{2} f(t_i, w_i))$$

Trapezoid method: $c_1 = c_2 = \frac{1}{2}$, $a = b_2 = \frac{h}{2\times\frac{1}{2}} = h$

$$w_{i+1} = w_i + \frac{h}{2}\left(f(t_i, w_i)) + f(t_i + h, w_i + hf(t_i, w_i))\right)$$

Optimal RK2, with smallest error term:: $c_1 = \frac{1}{4}, c_2 = \frac{3}{4}$, $b_1 = a = \frac{h}{2\times\frac{3}{4}} = \frac{2h}{3}$

$$w_{i+1} = w_i + \frac{h}{4} f(t_i, w_i) + \frac{3h}{4} f(t_i + \frac{2h}{3}, w_i + \frac{2h}{3} f(t_i, w_i))$$

The are often represented in a tabular form as follows:

$$\begin{array}{c|cc} c_0 & & \\ c_1 & a & \\ \hline & b_1 & b_2 \end{array}$$

$k_1 = hf(t_i, w_i)$

$k_2 = hf(t_i + c_1 h, w_i + ak_1)$

$w_{i+1} = w_i + (b_1 k_1 + b_2 k_2)$

$$\begin{array}{c|cc} 0 & & \\ \frac{1}{2} & \frac{1}{2} & \\ \hline & 0 & 1 \end{array}$$

$$w_{i+1} = w_i + hf(t_i + \frac{h}{2}, w_i + \frac{h}{2} f(t_i, w_i))$$

Trapezoid method: $b_1 = b_2 = \frac{1}{2}$, $a = c_2 = \frac{h}{2b2} = h$

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

$$w_{i+1} = w_i + \frac{h}{2}\left(f(t_i, w_i)) + f(t_i + h, w_i + hf(t_i, w_i))\right)$$

Optimal RK2 (smallest error term): $b_1 = \frac{1}{4}, b_2 = \frac{3}{4}$, $c_1 = a = \frac{2h}{3}$

$$\begin{array}{c|cc}
0 & & \\
\frac{2}{3} & \frac{2}{3} & \\
\hline
 & \frac{1}{4} & \frac{3}{4}
\end{array}$$

$$w_{i+1} = w_i + \frac{h}{4}f(t_i, w_i) + \frac{3h}{4}f(t_i + \frac{2h}{3}, w_i + \frac{2h}{3}f(t_i, w_i))$$

It is possible to derive systems of equations for higher order Runge-Kutta methods. Here are two fourth order equations, We start with the Classical Fourth Order Runge-Kutta:

$$\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
1 & 0 & 0 & 1 & \\
\hline
 & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6}
\end{array}$$

Each of the first 4 rows of this table describes a term in the final sum.

$$k_1 = f(t_i, w_i)$$

$$k_2 = f\left(t_i + \frac{h}{2}, w_i + \frac{h}{2}k_1\right)$$

$$k_3 = f\left(t_i + \frac{h}{2}, w_i + \frac{h}{2}k_2\right)$$

$$k_4 = f(t_i + h, w_i + hk_3)$$

$$w_{i+1} = w_i + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

Kutta's Original extension was the following. Again, each of the first 4 rows of this table describes a term in the final sum. Since the rows are not equal to the columns in this case, it is easier to figure out what is going on.

$$\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{3} & \frac{1}{3} & & & \\
\frac{2}{3} & -\frac{1}{3} & 1 & & \\
1 & 1 & -1 & 1 & \\
\hline
 & \frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8}
\end{array}$$

$$k_1 = f(t_i, w_i)$$

$$k_2 = f\left(t_i + \frac{h}{3}, w_i + \frac{h}{3}k_1\right)$$

$$k_3 = f\left(t_i + \frac{2h}{3}, w_i + h(-\frac{1}{3}k_1 + k_2)\right)$$

$$k_4 = f(t_i + h, w_i + h(k_1 - k_2 + k_3))$$

$$w_{i+1} = w_i + \frac{h}{8}(k_1 + 3k_2 + 3k_3 + k_4)$$

5 Adaptive methods

As with Adaptive Quadrature, we attempt to move forward in time, estimating the next step two different ways.

If the ways are close enough, we declare the step done, and select the most accurate of the two.

If they are not close enough, we decrease h and try again.

The trick is to find two ways of estimating the next step that can share some work.

To this end, there are nested RK pairs.

6 Stiff Equations

Some equations are stiff: Attracting Solutions surrounded by fast changing solutions. Solvers tend to overshoot the solution to stiff equations.

$$y' = 10(1 - y), y(0) = \frac{1}{2}, t \in [0, 100]$$

There is an attracting solution $y(t) = 1$.

Apply Euler's Method

$$w_{i+1} = w_i + hf(t_i, w_i)$$

$$= w_i + 10h(1 - w_i)$$

$$= w_i(1 - 10h) + 10h$$

We are looking for a fixed point of $g(x) = x(1 - 10h) + 10h$

This converges if $|g'(x)| < 1$

Since $g'(x) = (1 - 10h)$, this says $|1 - 10h| < 1$ or $h < 0.2$

Now consider an Implicit method, such as **Backwards Euler**

$$\begin{aligned} w_0 &= y_0 \\ w_{i+1} &= w_i + hf(t_{i+1}, w_{i+1}) \end{aligned}$$

In our example, that is

$$\begin{aligned} w_{i+1} &= w_i + h10(1 - w_{i+1}) \\ w_{i+1}(1 + 10h) &= w_i + 10h \\ w_{i+1} &= \frac{w_i + 10h}{1 + 10h} \end{aligned}$$

We can look at $g'(x)$ to see that this converges for any h. If $h = 0.2$ this gives

$$w_{i+1} = \frac{w_i + 2}{3}$$

In general, we can solve for w_{i+1} analytically, or through root finding or iteration.

7 Adams-Bashforth

Adams-Bashforth is a multistep method.

Rather than start fresh, each new point w_{i+1} is computed on the p previous estimates.

The new value is the weighted sum of prior parts. For example, the order two-step method is

$$w_{i+1} = w_i + h\left(\frac{3}{2}f(t_i, w_i) - \frac{1}{2}f(t_{i-1}, w_{i-1})\right)$$

Two questions present themselves

We need w_0 and w_1 to get going: How do we start the series?

Once again, we see weights that sum to 1. But where do the weights come from?

The book has an interesting discussion, and includes an important observation about stability.

But we will derive the system above, as well as the three-step Adams-Bashforth method, from first principles.

Our starting point, as always, is the equation

$$y'(t) = f(t, y(t))$$

We wish to integrate this from $t = t_i$ to $t = t_{i+1}$. If f was simply a function of t, that would be

$$y(t_{i+1}) - y(t_i) = \int_{t_i}^{t_{i+1}} f(t, y(t))dt$$

The next insight is to approximate $f(t, y(t))$ with a polynomial $P(x)$ using the last n points.

Given this, we extrapolate to find $y(t_{i+1})$.

The polynomial $P(x)$ for the two stage method is, using the Lagrange form

$$f(t, y(t)) \approx \frac{t - t_{i-1}}{t_i - t_{i-1}} f(t_i, w_i) + \frac{t - t_1}{t_{i-1} - t_1} f(t_{i-1}, w_{i-1})$$

Integrate both sides

$$\int_{t_i}^{t_{i+1}} f(t, y(t))dt \approx \int_{t_i}^{t_{i+1}} \frac{t - t_{i-1}}{t_i - t_{i-1}} f(t_i, w_i)dt + \int_{t_i}^{t_{i+1}} \frac{t - t_1}{t_{i-1} - t_1} f(t_{i-1}, w_{i-1})dt$$

This is the integral of two linear functions, as the terms like $f(t_i, w_i)$ are constant.

$$\int_{t_i}^{t_{i+1}} f(t, y(t))dt \approx f(t_i, w_i) \int_{t_i}^{t_{i+1}} \frac{t - t_{i-1}}{t_i - t_{i-1}} dt + f(t_{i-1}, w_{i-1}) \int_{t_i}^{t_{i+1}} \frac{t - t_1}{t_{i-1} - t_1} dt$$

To integrate the first term on the right side, make a change of variables $t = t_i + sh$

This means that $dt = h\ ds$

$$\int_{t_i}^{t_{i+1}} \frac{t - t_{i-1}}{t_i - t_{i-1}} dt = h \int_0^1 (s + 1)ds = \frac{3h}{2}$$

LIkewise, we can make the same substitution

$$\int_{t_i}^{t_{i+1}} \frac{t - t_1}{t_{i-1} - t_1} dt = -h \int_0^1 s ds = \frac{h}{2}$$

Putting this together, we get

$$w_{i+1} = w_i + \int_{t_i}^{t_{i+1}} f(t, y(t))dt \approx w_i + \frac{h}{2}(3f(t_i, w_i) - f(t_{i-1}, w_{i-1}))$$

For higher order methods, the argument is the same

The difference lies in the integrals

$$\frac{1}{2}\int_2^3 (t-1)(t-2)dt = \frac{1}{2}\int_1^2 s(s-1)ds$$

$$= \frac{1}{2}\left(\frac{s^3}{3} - \frac{s^2}{2}\right)|_1^2 = \frac{1}{2}\left(\frac{8}{3} - \frac{1}{3} - \frac{4}{2} + \frac{1}{2}\right) = \frac{5}{12}$$

Next one

$$-\int_2^3 t(t-2)dt = \left(t^2 - \frac{t^3}{3}\right)|_2^3 = \left(9 - 4 - \frac{27}{3} + \frac{8}{3}\right)$$

$$= \left(5 - \frac{19}{3}\right) = \left(\frac{15}{6} - \frac{19}{3}\right) = -\frac{4}{3}$$

One more

$$\frac{1}{2}\int_2^3 t(t-1)dt = \frac{1}{2}\left(\frac{t^3}{3} - \frac{t^2}{2}\right)|_2^3 = \left(\frac{27}{3} - \frac{8}{3} - \frac{9}{2} + \frac{4}{2}\right)$$

$$= \left(\frac{19}{3} - \frac{5}{2}\right) = \left(\frac{38}{6} - \frac{15}{6}\right) = \frac{23}{6}$$

$$w_{i+1} = w_i + \int_{t_i}^{t_{i+1}} f(t, y(t))dt \approx w_i + \frac{h}{2}(3f(t_i, w_i) - f(t_{i-1}, w_{i-1}))$$

Put it all together

$$w_{i+1} = w_i + \frac{h}{12}\left(23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1})\right) + 5f(t_{i-2}, w_{i-2}))$$

Fourth order Adams-Bashforth:

$$w_{i+1} = w_i + \frac{h}{24}\left(55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1})\right) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3}))$$

8 Derivation of Adams

We are looking for a two-step Adams method. It will have the general form

$$
\begin{aligned}
w_{i+1} &= a_1 w_i + a_2 w_{i-1} + h[b_0 f_{i+1} + b_1 f_i + b_2 f_{i-1}] \\
&= a_1[y_i] \\
&+ a_2[y_i - hy_i' + \frac{h^2}{2} y_i'' - \frac{h^3}{6} y_i''' + \frac{h^4}{24} y_i'''' + \ldots] \\
&+ b_0[\qquad hy_i' + h^2 y_i'' + \frac{h^3}{2} y_i''' + \frac{h^4}{6} y_i'''' + \ldots] \\
&+ b_1[\qquad hy_i'] \\
&+ b_0[\qquad hy_i' - h^2 y_i'' + \frac{h^3}{2} y_i''' - \frac{h^4}{6} y_i'''' + \ldots]
\end{aligned}
$$

Gather terms to see that

$$
\begin{aligned}
w_i = (a_1 + a_2) y_i + (b_0 + b_1 + b_2 - a_2) hy' + (a_2 - 2b_2 + 2b_0) \frac{h^2}{2} y_i'' \\
+ (a_2 + 3b_0 + 3b_2) \frac{h^3}{6} y_i''' + (a_2 + 4b_0 - 4b_2) \frac{h^4}{24} y_i'''' + \ldots
\end{aligned}
$$

Compare with the Taylor Series Expansion

$$
y(t+h) = y_{i+1} = y_i + hy_i' + \frac{h^2}{2} y_i'' + \frac{h^3}{6} y_i''' + \ldots
$$

Set up the equations

$$
\begin{aligned}
a_1 + a_2 &= 1 \\
b_0 + b_1 + b_2 - a_2 &= 1 \\
a_2 - 2b_2 + 2b_0 &= 1
\end{aligned}
$$

For an explicit method, $b_0 = 0$

$$
\begin{aligned}
a_1 + a_2 &= 1 \\
b_1 + b_2 - a_2 &= 1 \\
a_2 - 2b_2 &= 1
\end{aligned}
$$

We can solve in terms of a_1

$$a_2 = 1 - a_1$$
$$b_2 = -\frac{1}{2}a_1$$
$$b_1 = 2 - \frac{1}{2}a_1$$

We are free to set a_1 arbitrarily - Any choice leads to an explicit second-order method.

The error is

$$\begin{aligned} y_{i+1} - w_{i+1} &= \frac{1}{6}h^3 y_i''' - \frac{3b_2 - a_2}{6}h^3 y_i''' + O(h^4) \\ &= \frac{1 - 3b_2 + a_2}{6}h^3 y_i''' + O(h^4) \\ &= \frac{4 + a_1}{12}h^3 y_i''' + O(h^4) \end{aligned}$$

9 Stability of Multistep methods

The general form of a 2-step method is

$$w_{i+1} = a_1 w_i + a_2 w_{i-1} + h[b_0 f_{i+1} + b_i f_1 + b_2 f_{i-1}]$$

The presence of f_{i+1} seems a bit troubling: if present, the system is implicit. For now, let's assume that $b_0 = 0$.

In Adams-Bashforth methods, all of the a_i but the first are zero.

Section 6.7.2 looks at what happens if they are not. In particular, the book considers

$$w_{i+1} = -w_i + 2w_{i-1} + h[\frac{5}{2}f_i + \frac{1}{2}f_{i-1}]$$

This method is unstable, as seen in the figure.

To explore this, Sauer proposes a thought experiment. Considers the system

$$y' = 0 \qquad y(0) = 0 \qquad t \in [0, 1]$$

Clearly $y(t) = 0$ is a stable solution, and the system reduces to

$$w_{i+1} = -w_i + 2w_{i-1} + h[0] = -w_i + 2w_{i-1}$$

This recurrence has the following "characteristic polynomial" -

$$\lambda^2 = -\lambda + 2$$

That is, if r is a root of this equation, solutions of the form cr^i will solve the system.

If $|r| > 1$, his allows small rounding errors to add up to observable size, and to swamp the computation. If the root is less than 1 in absolute value, the error is damped.

In the example above, we have

$$0 = \lambda^2 + \lambda - 2 = (\lambda + 2)(\lambda - 1)$$

This means that any error c will be magnified, quickly becoming $(-2)^i c$.

$$w_{i+1} = -w_i + 2w_{i-1}$$

For example, let $w_{i-1} = 0.001$, $w_i = -0.002$ and you will see that $w_{i+1} = 0.004$.

The Adams-Bashforth two step method has the form

$$w_{i+1} = w_i + h[b_i f_1 + b_2 f_{i-1}]$$

which gives the characteristic equation $\lambda - 1 = 0$ and a single root, $r = 1$. Errors are not magnified.