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Heun's method

Introduction

- In this topic, we will
  - Derive Heun's method by estimating and averaging slopes
  - Look at the technique visually
  - See the error is O(h^3) for a single step
  - Look at two examples of a single step
  - See how to apply Heun's method under multiple steps
    - We will implement this in C++
  - Look at two examples of multiple steps
  - Derive the formula based on integration

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Trapezoidal rule

- A simple Reimann sum approximates an integral with one value:

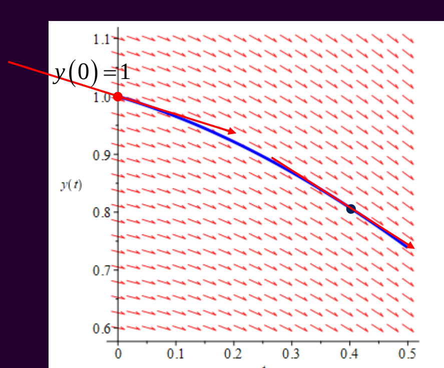
$$\int_a^b f(x)\,\mathrm{d}x \approx f(a)(b-a)$$

- The value of the function, however, changes across $[a, b]$, so the trapezoidal rule averages the two end-points:

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{f(a)+f(b)}{2}(b-a)$$

Heun's method

- Euler's method uses one slope $y_1 \leftarrow y_0 + hf\left(t_0, y(t_0)\right)$
  - However, the slope changes across the interval
  - It would be better to average the slopes $\dfrac{f\left(t_0, y(t_0)\right) + f\left(t_1, y(t_1)\right)}{2}$?



$$y^{(1)}(t) = -0.2y(t) - \sin(t) - 0.1$$
$$y(0) = 1$$

Heun’s method

- The issue here is we don’t know the value $y(t_1)$

$$y_1 \leftarrow y_0 + h\frac{f\left(t_0, y(t_0)\right) + f\left(t_1, y(t_1)\right)}{2}$$

- Can we approximate $y(t_1)$?
  - How about using Euler’s approximation of $y(t_1)$?

- Start with:

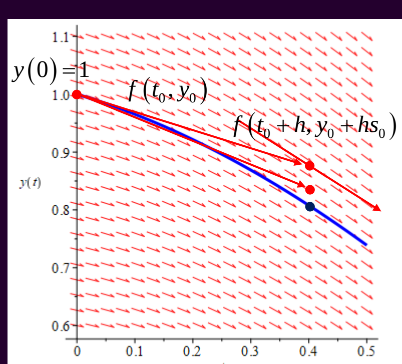
$$s_0 \leftarrow f\left(t_k, y_k\right)$$

$$s_1 \leftarrow f\left(t_k + h, y_k + hs_0\right)$$

$$y_{k+1} \leftarrow y_k + h\frac{s_0 + s_1}{2}$$

Heun’s method

- Visually, we proceed as follows



$$y^{(1)}(t) = -0.2y(t) - \sin(t) - 0.1$$

$$y(0) = 1$$

One step of Heun's method

- What is the error? $O(h^2)$ or $O(h^3)$ or better?
  - We will look at two initial-value problems and approximate $y(t_0 + h)$ for successively smaller values of h
  - For example, approximate $y(0.4)$ with:

$$y^{(1)}(t) = -y(t)$$
$$y(0) = 1$$

$$s_0 \leftarrow f(0, 1) = -1$$
$$s_1 \leftarrow f(0.4, 1 + 0.4s_0) = -0.6$$
$$y_1 \leftarrow y_0 + h\frac{s_0 + s_1}{2}$$
$$= 1 + 0.4\frac{(-1) + (-0.6)}{2} = 0.68$$

$$e^{-0.4} = 0.67032004603563\,93$$

Heun's method

One step of Heun's method

- Let's approximate the solution at $y(0 + h)$ to

$$y^{(1)}(t) = -y(t)$$
$$y(0) = 1$$

n	$h = 2^{-n}$	Exact	Approximation	Error	Ratio
1	0.5	0.606530659712633	0.625	–0.0185	
2	0.25	0.7788007830714049	0.78125	–0.002449	0.1326
3	0.125	0.8824969025845955	0.8828125	–0.0003156	0.1289
4	0.0625	0.9394130628134758	0.939453125	–0.00004006	0.1269
5	0.03125	0.9692332344763441	0.96923828125	–0.000005047	0.1260
6	0.015625	0.9844964370054085	0.9844970703125	–0.0000006333	0.1255
7	0.0078125	0.9922179382602435	0.992218017578125	–0.00000007932	0.1252
8	0.00390625	0.9961013694701175	0.9961013793945312	–0.000000009924	0.1251
9	0.001953125	0.9980487811074755	0.9980487823486328	–0.000000001241	0.1251
10	0.0009765625	0.9990239141819757	0.9990239143371582	–0.0000000001552	0.1250

Heun's method

One step of Heun's method

- Let's approximate the solution at $y(0 + h)$ to

$$y^{(1)}(t) = -0.2y(t) - \sin(t) - 0.1$$
$$y(0) = 1$$

$$y(t) = \frac{-13 + 25\cos(t) - 5\sin(t) + 14e^{-\frac{t}{5}}}{26}$$

n	$h = 2^{-n}$	Exact	Approximation	Error	Ratio
1	0.5	0.738852315643913	0.737643615348949	0.001209	
2	0.25	0.8962693342116731	0.8959495050931846	0.0003198	0.2646
3	0.125	0.9552271839309132	0.9551765791634232	0.00006048	0.1582
4	0.0625	0.9794223225078814	0.9794153338174256	0.000006989	0.1381
5	0.03125	0.9901670100357426	0.9901660950939792	0.0000009149	0.1309
6	0.015625	0.9951978758220640	0.9951977588732431	0.0000001169	0.1278
7	0.0078125	0.9976275785667972	0.9976275637870025	0.00000001478	0.1264
8	0.00390625	0.9988209552460877	0.9988209533885432	0.000000001858	0.1257
9	0.001953125	0.9994122698263201	0.9994122695934978	0.0000000002328	0.1253
10	0.0009765625	0.9997065830522891	0.9997065830231471	0.00000000002914	0.1252

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Heun's method

Multiple steps of Heun's method

- Can we see that the error is indeed $O(h^3)$?

$$y(t_0 + h) = y(t_0) + y^{(1)}(t_0)h + \frac{1}{2}y^{(2)}(t_0)h^2 + \frac{1}{6}y^{(3)}(\tau_0)h^3$$
$$= y_0 + f(t_0, y_0)h + \frac{1}{2}y^{(2)}(t_0)h^2 + \frac{1}{6}y^{(3)}(\tau_0)h^3$$

- Let us label $s_0 = f(t_0, y_0)$, so we have

$$y(t_0 + h) = y_0 + s_0 h + \frac{1}{2}y^{(2)}(t_0)h^2 + \frac{1}{6}y^{(3)}(\tau_0)h^3$$

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Multiple steps of Heun's method

- Next, let us use the forward divided-difference approximation of the second derivative:

$$y^{(2)}(t_0) = \frac{y^{(1)}(t_0+h) - y^{(1)}(t_0)}{h} - \frac{1}{2}y^{(3)}(\tau_1)h$$
$$= \frac{y^{(1)}(t_0+h) - s_0}{h} - \frac{1}{2}y^{(3)}(\tau_1)h$$

- Substituting this into the previous equation, we have

$$y(t_0+h) = y_0 + s_0 h + \frac{1}{2}\left(\frac{y^{(1)}(t_0+h) - s_0}{h} - \frac{1}{2}y^{(3)}(\tau_1)h\right)h^2 + \frac{1}{6}y^{(3)}(\tau_0)h^3$$

- Expand and collect on powers of h to get:

$$y(t_0+h) = y_0 + s_0 h - \frac{1}{2}s_0 h + \frac{1}{2}y^{(1)}(t_0+h)h + \left(\frac{1}{6}y^{(3)}(\tau_0) - \frac{1}{4}y^{(3)}(\tau_1)\right)h^3$$

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Heun's method

Multiple steps of Heun's method

- We can now simplify this to the following:

$$y(t_0+h) = y_0 + \frac{1}{2}s_0 h + \frac{1}{2}y^{(1)}(t_0+h)h - \frac{1}{12}y^{(3)}(t_0)h^3 + o(h^3)$$

- Next, we must observe the next term of interest:

$$y^{(1)}(t_0+h) = f(t_0+h, y(t_0+h))$$

- From calculus, you will recall that

$$g(a, b+c) = g(a,b) + \frac{\partial}{\partial b}g(a,\beta)c$$

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Multiple steps of Heun's method

- Thus, we now have that:

$$y(t_0+h) = y_0 + s_0 h + \frac{1}{2} y^{(2)}(\tau_2) h^2$$

$$\begin{aligned} y^{(1)}(t_0+h) &= f(t_0+h, y(t_0+h)) \\ &= f\left(t_0+h, y_0+s_0 h+\frac{1}{2}y^{(2)}(\tau_2)h^2\right) \\ &= f\left(t_0+h, (y_0+s_0 h)+\left(\frac{1}{2}y^{(2)}(\tau_2)h^2\right)\right) \\ &= f(t_0+h, y_0+s_0 h)+\frac{\partial}{\partial y}f(t_0+h, y(\tau_3))\left(\frac{1}{2}y^{(2)}(\tau_2)h^2\right) \\ &= f(t_0+h, y_0+s_0 h)+\frac{1}{2}\left(\frac{\partial}{\partial y}f(t_0+h, y(\tau_3))y^{(2)}(\tau_2)\right)h^2 \end{aligned}$$

Multiple steps of Heun's method

- We will substitute

$$y^{(1)}(t_0+h) = f(t_0+h, y_0+s_0 h)+\frac{1}{2}\left(\frac{\partial}{\partial y}f(t_0+h, y(\tau_3))y^{(2)}(\tau_2)\right)h^2$$

into the equation

$$y(t_0+h) = y_0 + \frac{1}{2}s_0 h + \frac{1}{2}y^{(1)}(t_0+h)h - \frac{1}{12}y^{(3)}(t_0)h^3 + o(h^3)$$

- This yields:

$$y(t_0+h) = y_0 + \frac{1}{2}s_0 h + \frac{1}{2}\left(f(t_0+h, y_0+s_0 h)+\frac{1}{2}\left(\frac{\partial}{\partial y}f(t_0+h, y(\tau_3))y^{(2)}(\tau_2)\right)h^2\right)h$$
$$-\frac{1}{12}y^{(3)}(t_0)h^3 + o(h^3)$$

Multiple steps of Heun's method

- Can we simplify this?

$$y(t_0+h) = y_0 + \frac{1}{2}s_0 h + \frac{1}{2}\left(f(t_0+h, y_0+s_0h) + \frac{1}{2}\left(\frac{\partial}{\partial y} f(t_0+h, y(\tau_3)) y^{(2)}(\tau_2) \right) h^2 \right) h$$

$$-\frac{1}{12} y^{(3)}(t_0) h^3 + o(h^3)$$

$$s_1 = f(t_0+h, y_0+s_0h)$$

$$y(t_0+h) = y_0 + \frac{1}{2}s_0 h + \frac{1}{2} f(t_0+h, y_0+s_0h) h$$

$$+\left(\frac{1}{4}\frac{\partial}{\partial y} f(t_0+h, y(\tau_3)) y^{(2)}(\tau_2) - \frac{1}{12} y^{(3)}(t_0) \right) h^3 + o(h^3)$$

$$y(t_0+h) = y_0 + \frac{s_0+s_1}{2} h + \left(\frac{1}{4}\frac{\partial}{\partial y} f(t_0+h, y(\tau_3)) y^{(2)}(\tau_2) - \frac{1}{12} y^{(3)}(t_0) \right) h^3 + o(h^3)$$

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Multiple steps of Heun's method

- As with Euler's method:
  - First, we will implement a function to find the *n* approximations by dividing a range $[t_0, t_f]$ into *n* sub-intervals
  - For two IVPs with the initial condition $y(0) = 1$, we will approximate $y(5)$ by using 2^n intervals

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Implementation

```
std::tuple<double *, double *, double *> heun(
    double f( double t, double y ), std::pair<double, double> t_rng, double y0,
    unsigned int n
) {
    double h{ (t_rng.second - t_rng.first)/n };

    double  *ts{ new double[n + 1] };
    double  *ys{ new double[n + 1] };
    double *dys{ new double[n + 1] };

    ts[0] = t_rng.first;
    ys[0] = y0;
    dys[0] = f( ts[0], ys[0] );

    for ( unsigned int k{0}; k < n; ++k ) {
         ts[k + 1] = t_rng.first + h*(k + 1);     // ts[k + 1] = ts[k] + h;
         double s0{ dys[k] };
         double s1{ f( ts[k + 1], ys[k] + h*s0 ) };
         ys[k + 1] = ys[k] + h*(s0 + s1)/2.0;
        dys[k + 1] = f( ts[k + 1], ys[k + 1] );
    }

    return std::make_tuple( ts, ys, dys );
}
```


Multiple steps of Heun's method

- Let's approximate the solution at $y(5)$ to

$$y^{(1)}(t) = -y(t)$$
$$y(0) = 1$$

n	Approximation	Error	Ratio
2	2.640625	–2.634	
4	0.07965183258056641	–0.0729	0.02768
8	0.0111918820307766	–0.004454	0.06108
16	0.007466932539429057	–0.0007290	0.1637
32	0.006893866059610459	–0.0001559	0.2139
64	0.006774386822159493	–0.00003644	0.2337
128	0.006746775448351634	–0.000008828	0.2423
256	0.006740120906468897	–0.000002174	0.2462
512	0.006738486441915978	–0.0000005394	0.2481
1024	0.006738081362611961	–0.0000001344	0.2491
	0.006737946999085467		

Multiple steps of Heun's method

- Let's approximate the solution at $y(5)$ to

$$y^{(1)}(t) = -0.2y(t) - \sin(t) - 0.1$$
$$y(0) = 1$$

$$y(t) = \frac{-13 + 25\cos(t) - 5\sin(t) + 14e^{-\frac{t}{5}}}{26}$$

n	Approximation	Error	Ratio
2	0.442991390682734	–0.2877	
4	0.2033310765216377	–0.04808	0.1671
8	0.1652850891391681	–0.01004	0.2087
16	0.1575662171471889	–0.002317	0.2308
32	0.1558079696338854	–0.0005584	0.2410
64	0.1553867579336197	–0.0001372	0.2457
128	0.155283561779206	–0.00003402	0.2479
256	0.1552580145623753	–0.000008469	0.2490
512	0.1552516585204115	–0.000002113	0.2495
1024	0.1552500733106273	–0.0000005277	0.2497

0.1552495456267901

Error analysis

- As with integration and Euler's method,
  the error accumulates and thus the $O(h^3)$ error of one step
  is reduced to an $O(h^2)$ error over multiple steps

Integration?

- Recall I mentioned that finding a solution to an initial-value problem is equivalent to performing an integration

$$y^{(1)}(t) = f(t, y(t))$$
$$y(t_0) = y_0$$
$$y(t_0 + h) = y(t_0) + \int_{t_0}^{t_0+h} f(\tau, y(\tau))\,d\tau$$
$$\approx y(t_0) + h\frac{f(t_0, y(t_0)) + f(t_0 + h, y(t_0 + h))}{2}$$
$$\approx y_0 + h\frac{f(t_0, y_0) + f(t_0 + h, y_0 + hf(t_0, y_0))}{2}$$

Summary

- Following this topic, you now
  - Understand Heun's method for approximating a solution to a 1st-order initial-value problem
  - Are aware of a visual interpretation with respect to slopes
  - Understand the error is O(h^3) for a single step
  - Are aware that we must apply this technique multiple times to estimate the solution on a larger interval
  - Know that the error drops in this case to O(h^2)
  - Have seen a number of examples and an implementation
  - Understand the derivation and the parallel to the trapezoidal rule

References

[1] https://en.wikipedia.org/wiki/Heun%27s_method

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Acknowledgments

None so far.

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Colophon

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Mathematical equations are prepared in MathType by Design Science, Inc.
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