

Quadratic approximation for derivatives at end points

Three points x_0, x_0+h, x_0+2h with values of function $u(x)$ $u_1=u(x_0)$, $u_2=u(x_0+h)$, $u_3=u(x_0+2h)$. Consider the polynomial $p(x) = ax^2 + bx + c$ such that $p(x_0)=u_1$, $p(x_0+h)=u_2$, $p(x_0+2h)=u_3$. Then a, b, c are the solutions of:

```
In[8]:= sols = Solve[{u1 == a x0^2 + b x0 + c, u2 == a (x0 + h)^2 + b (x0 + h) + c,
                    u3 == a (x0 + 2 h)^2 + b (x0 + 2 h) + c}, {a, b, c}] // Simplify
```

```
Out[8]= {{a -> (u1 - 2 u2 + u3)/(2 h^2), b -> -1/(2 h^2) (h (3 u1 - 4 u2 + u3) + 2 (u1 - 2 u2 + u3) x0),
          c -> 1/(2 h^2) (2 h^2 u1 + h (3 u1 - 4 u2 + u3) x0 + (u1 - 2 u2 + u3) x0^2)}}}
```

The constant $2a$ is the value of $p''(x)$ for all values of x . The first derivative $p'(x)=2ax+b$ can be calculated at each point.

First Derivative at middle point:

```
In[9]:= 2 a (x0 + h) + b /. sols // Simplify
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Out[9]= {-u1 + u3/(2 h)}
```

First derivative at right most point x_0+2h

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In[10]:= 2 a (x0 + 2 h) + b /. sols // Simplify
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Out[10]= {(u1 - 4 u2 + 3 u3)/(2 h)}
```

First derivative at leftmost point x_0

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In[11]:= 2 a (x0) + b /. sols // Simplify
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Out[11]= {-3 u1 + 4 u2 + u3/(2 h)}
```

The approximation is $O(h^2)$ for both end points:

```
In[15]:= Series[-(3 u[x0] - 4 u[x0 + h] + u[x0 + 2 h])/(2 h), {h, 0, 3}]
```

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Out[15]= u'[x0] - 1/3 u^{(3)}[x0] h^2 - 1/4 u^{(4)}[x0] h^3 + O[h]^4
```

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In[16]:= Series[(u[x0 - 2 h] - 4 u[x0 - h] + 3 u[x0])/(2 h), {h, 0, 3}]
```

```
Out[16]= u'[x0] - 1/3 u^{(3)}[x0] h^2 + 1/4 u^{(4)}[x0] h^3 + O[h]^4
```

For the second derivative, the approximation is $O(h^2)$ only for the middle point. For the left/right points are only $O(h)$.

$$\text{In[17]:= Series}\left[\frac{u[x0 - 2 h] - 2 u[x0 - h] + u[x0]}{h^2}, \{h, 0, 3\}\right]$$

$$\text{Out[17]= } u''[x0] - u^{(3)}[x0] h + \frac{7}{12} u^{(4)}[x0] h^2 - \frac{1}{4} u^{(5)}[x0] h^3 + O[h]^4$$

$$\text{In[18]:= Series}\left[\frac{u[x0 - h] - 2 u[x0] + u[x0 + h]}{h^2}, \{h, 0, 3\}\right]$$

$$\text{Out[18]= } u''[x0] + \frac{1}{12} u^{(4)}[x0] h^2 + O[h]^4$$

$$\text{In[19]:= Series}\left[\frac{u[x0] - 2 u[x0 + h] + u[x0 + 2 h]}{h^2}, \{h, 0, 3\}\right]$$

$$\text{Out[19]= } u''[x0] + u^{(3)}[x0] h + \frac{7}{12} u^{(4)}[x0] h^2 + \frac{1}{4} u^{(5)}[x0] h^3 + O[h]^4$$

Look for $O(h^2)$ solutions for the left point:

$$\text{In[24]:= Series}\left[\frac{1}{h^2} \alpha u[x0] + \beta u[x0 + h] + \gamma u[x0 + 2 h] + \delta u[x0 + 3 h], \{h, 0, 3\}\right]$$

$$\begin{aligned} \text{Out[24]= } & \frac{\alpha u[x0] + \beta u[x0] + \gamma u[x0] + \delta u[x0]}{h^2} + \frac{\beta u'[x0] + 2 \gamma u'[x0] + 3 \delta u'[x0]}{h} + \\ & \frac{1}{2} (\beta u''[x0] + 4 \gamma u''[x0] + 9 \delta u''[x0]) + \frac{1}{6} (\beta u^{(3)}[x0] + 8 \gamma u^{(3)}[x0] + 27 \delta u^{(3)}[x0]) h + \\ & \frac{1}{24} (\beta u^{(4)}[x0] + 16 \gamma u^{(4)}[x0] + 81 \delta u^{(4)}[x0]) h^2 + \\ & \frac{1}{120} (\beta u^{(5)}[x0] + 32 \gamma u^{(5)}[x0] + 243 \delta u^{(5)}[x0]) h^3 + O[h]^4 \end{aligned}$$

$$\text{In[29]:= sols2 = Solve}\left[\{\alpha + \beta + \gamma + \delta == 0, \beta + 2 \gamma + 3 \delta == 0, \beta / 6 + 8 \gamma / 6 + 27 \delta / 6 == 0\}, \{\alpha, \beta, \gamma, \delta\}\right]$$

Solve::svars : Equations may not give solutions for all "solve" variables. >>

$$\text{Out[29]= } \left\{\left\{\beta \rightarrow -\frac{5 \alpha}{2}, \gamma \rightarrow 2 \alpha, \delta \rightarrow -\frac{\alpha}{2}\right\}\right\}$$

$$\text{In[32]:= Series}\left[\frac{1}{h^2} \alpha u[x0] + \beta u[x0 + h] + \gamma u[x0 + 2 h] + \delta u[x0 + 3 h] /. \text{sols2} /. \alpha \rightarrow 2, \{h, 0, 3\}\right]$$

$$\text{Out[32]= } \left\{u''[x0] - \frac{11}{12} u^{(4)}[x0] h^2 - u^{(5)}[x0] h^3 + O[h]^4\right\}$$

$$\text{In[33]:= sols2 /. } \alpha \rightarrow 2$$

$$\text{Out[33]= } \{\{\beta \rightarrow -5, \gamma \rightarrow 4, \delta \rightarrow -1\}\}$$

In[37]:= **second1** =
$$\frac{\alpha u[x0] + \beta u[x0 + h] + \gamma u[x0 + 2 h] + \delta u[x0 + 3 h]}{h^2}$$
 /. **sols2** /. $\alpha \rightarrow 2$

Out[37]=
$$\left\{ \frac{2 u[x0] - 5 u[h + x0] + 4 u[2 h + x0] - u[3 h + x0]}{h^2} \right\}$$

Verify:

In[38]:= **Series**[**second1**, {**h**, 0, 3}]

Out[38]=
$$\left\{ u''[x0] - \frac{11}{12} u^{(4)}[x0] h^2 - u^{(5)}[x0] h^3 + O[h]^4 \right\}$$

Look for $O(h^2)$ solutions for the right point: We see that the solution is completely symmetric by taking $h \rightarrow -h$

In[36]:= **Series**
$$\left[\frac{\alpha u[x0] + \beta u[x0 - h] + \gamma u[x0 - 2 h] + \delta u[x0 - 3 h]}{h^2}, \{h, 0, 3\} \right]$$

Out[36]=
$$\begin{aligned} & \frac{\alpha u[x0] + \beta u[x0] + \gamma u[x0] + \delta u[x0]}{h^2} + \frac{-\beta u'[x0] - 2 \gamma u'[x0] - 3 \delta u'[x0]}{h} + \\ & \frac{1}{2} (\beta u''[x0] + 4 \gamma u''[x0] + 9 \delta u''[x0]) + \frac{1}{6} (-\beta u^{(3)}[x0] - 8 \gamma u^{(3)}[x0] - 27 \delta u^{(3)}[x0]) h + \\ & \frac{1}{24} (\beta u^{(4)}[x0] + 16 \gamma u^{(4)}[x0] + 81 \delta u^{(4)}[x0]) h^2 + \\ & \frac{1}{120} (-\beta u^{(5)}[x0] - 32 \gamma u^{(5)}[x0] - 243 \delta u^{(5)}[x0]) h^3 + O[h]^4 \end{aligned}$$

sols3 = **Solve**[$\{\alpha + \beta + \gamma + \delta = 0, \beta - 2 \gamma - 3 \delta = 0, \beta / 6 + 8 \gamma / 6 + 27 \delta / 6 = 0\}, \{\alpha, \beta, \gamma, \delta\}$]