The Derivation of Second and Fourth Order Differentiation Matrices

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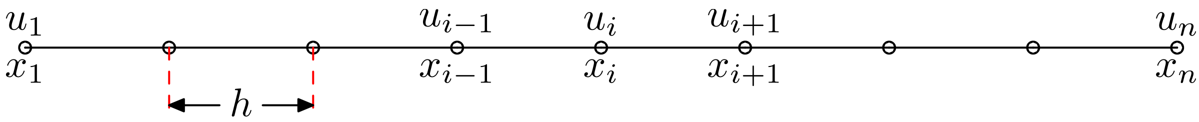
Introduction

Differentiation matrices are a class of band matrices that use methods of linear algebra to approximate derivatives. These matrices can be derived a number of different ways. We will derive a second order differentiation matrix from the Taylor polynomial and a fourth order differentiation matrix from the Lagrange interpolating polynomial.

The Problem

In many real life situations we don't have a simple function to differentiate. We may have a set of discrete points and we need to plot their derivative. Differentiation matrices are the perfect tool for this job. They take that set of discrete points and approximate the derivative as another set of discrete points.



Taylor's Theorem

The standard Taylor series has the following form.

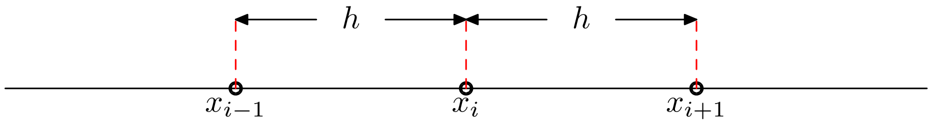
$$u(x) = u(a) + u'(a)(x - a) + \frac{u''(a)}{2!}(x - a)^2 + \cdots$$

For convenience we will substitute $a + h$ for x and then substitute x for a.

$$u(x + h) = u(x) + u'(x)(h) + \frac{u''(x)}{2!}h^2 + \cdots$$

The Second Order Difference Equation from Taylor's Theorem

The standard second-order finite difference approximation can be derived by considering the Taylor expansions of $u(x_{i+1})$ and $u(x_{i-1})$.



Note: $x_{i+1} = x_i + h$ and $x_{i-1} = x_i - h$

Using the Taylor series:

$$u(x_i + h) = u(x_i) + u'(x_i)h + \frac{u''(x_i)}{2i}h^2 + \cdots$$

$$u(x_i - h) = u(x_i) - u'(x_i)h + \frac{u''(x_i)}{2i}h^2 + \cdots$$

Difference Equation

Subtracting one equation from the other, and eliminating higher order terms, we get:

$$u(x_i + h) - u(x_i - h) = 2u^{'}(x_i)h$$
$$u'(x_i) = \frac{u(x_i + h) - u(x_i - h)}{2h}$$

.

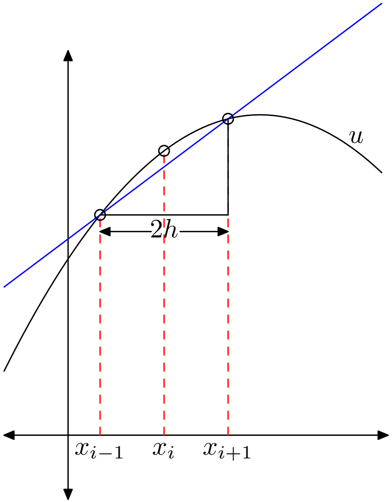
However, $x_{i+1} = x_i + h$ and $x_{i-1} = x_i - h$.

$$u'(x_i) = \frac{u(x_{i+1}) - u(x_{i-1})}{2h}$$

How the Difference Equation Works

The difference equation approximates the derivative at a point $(x_i, u(x_i))$ using the slope of the line that passes through the point before it $(x_{i-1}, u(x_{i-1}))$ and the point after it $(x_{i+1}, u(x_{i+1}))$.

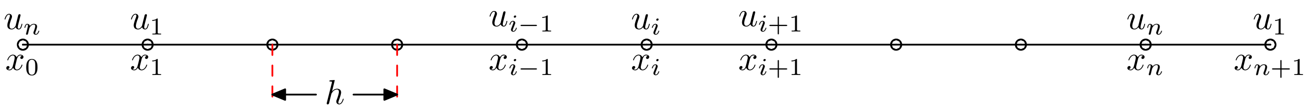
$$u'(x_i) = \frac{u(x_{i+1}) - u(x_{i-1})}{2h}$$



Assuming Periodicity

Before we can go any further we must assume that the function we are evaluating is periodic. We know that in most cassis it is not but it is going to be necessary so that we can set up our system of equations.

$$u_0 = u_n$$
$$u_1 = u_{n+1}$$



System of Equations

Our previous result:

$$u'(x_i) = \frac{u(x_{i+1}) - u(x_{i-1})}{2h}$$

Replacing $u'(x_i)$ with w_i, $u(x_{i+1})$ with u_{i+1}, and $u(x_{i-1})$ with u_{i-1} gives us the standard second order difference equation.

$$w_i = \frac{u_{i+1} - u_{i-1}}{2h}$$

We will now use this difference equation to set up a system of equations that represent the derivative of the function.

To set up the system of equations we will set $i = 1, 2, 3, \ldots, n$

System of Equations

$$
\begin{aligned}
w_1 &= \frac{u_2 - u_n}{2h} \\
w_2 &= \frac{u_3 - u_1}{2h} \\
w_3 &= \frac{u_4 - u_2}{2h} \\
&\vdots \\
w_{N-1} &= \frac{u_N - u_{N-2}}{2h} \\
w_N &= \frac{u_1 - u_{N-1}}{2h}
\end{aligned}
$$

Matrix Form

The system takes the form

$$\mathbf{w} = D\mathbf{u},$$

where

$$D = \begin{bmatrix} 0 & 1/2 & 0 & 0 & \dots & 0 & 0 & -1/2 \\ -1/2 & 0 & 1/2 & 0 & \dots & 0 & 0 & 0 \\ 0 & -1/2 & 0 & 1/2 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \ddots & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & \dots & -1/2 & 0 & 1/2 \\ 1/2 & 0 & 0 & 0 & \dots & 0 & -1/2 & 0 \end{bmatrix}.$$

Example

Lets look at an example using the following set of 8 discrete points (2,5),(4,15),(6,35),(8,65),(10,100),(12,145),(14,195), and (16,255).

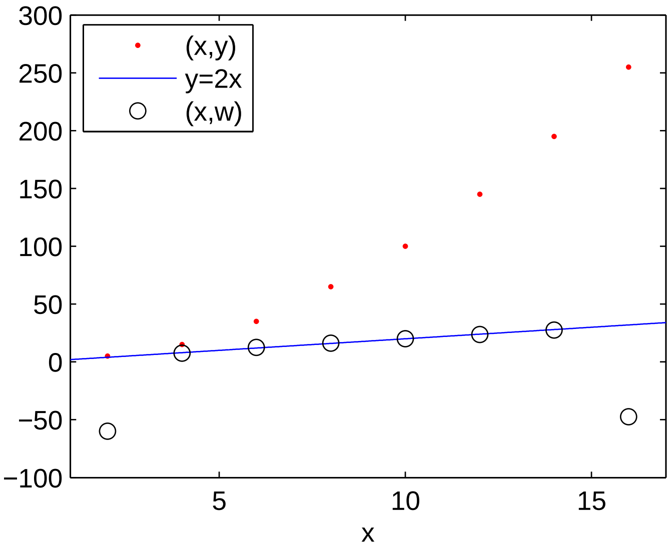
$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \\ w_7 \\ w_8 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & 1/2 & 0 & \dots & 0 & -1/2 \\ -1/2 & 0 & 1/2 & \dots & 0 & 0 \\ 0 & -1/2 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1/2 \\ 1/2 & 0 & 0 & \dots & -1/2 & 0 \end{bmatrix} \begin{bmatrix} 5 \\ 15 \\ 35 \\ 65 \\ 100 \\ 145 \\ 195 \\ 255 \end{bmatrix}$$

Answer

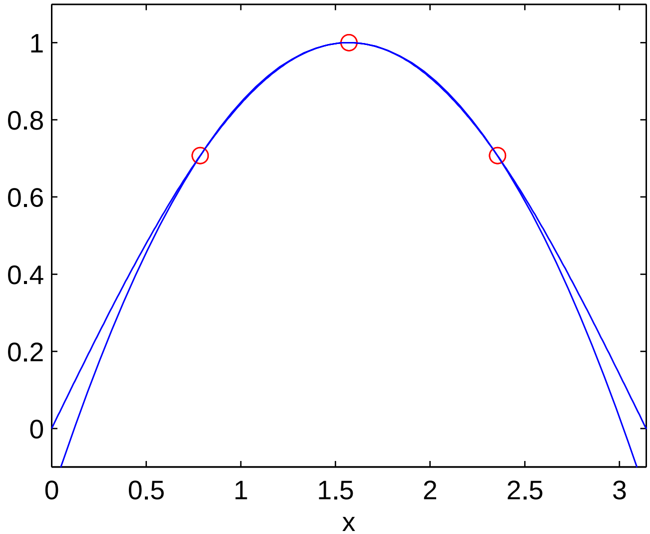
The vector **w** contains the y values of the derivative approximation. The x values are the same as the x values of the points we wanted to take a derivative of.

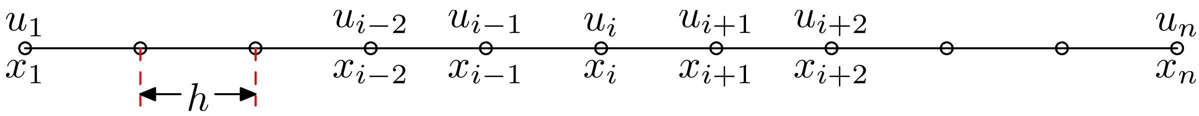
$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \\ w_7 \\ w_8 \end{bmatrix} = \begin{bmatrix} -60 \\ 7.5 \\ 12.5 \\ 16 \\ 20 \\ 23.75 \\ 27.5 \\ -47.5 \end{bmatrix}$$

Graph



Fourth Order Differentiation Matrix





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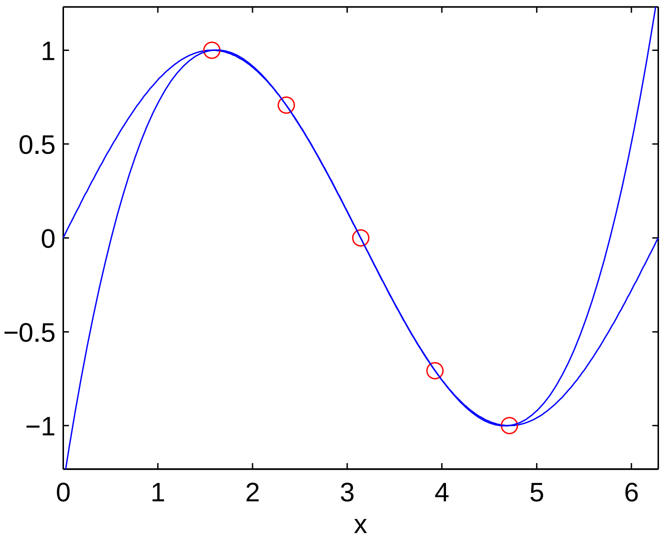
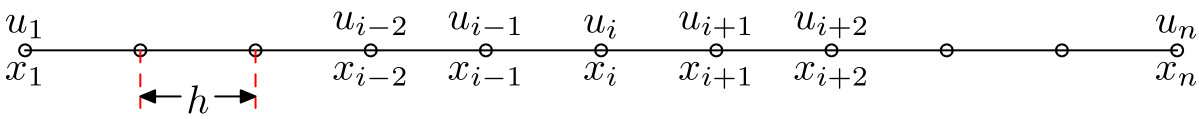
Lagrange Interpolating Polynomial

$$P(x) = \sum_{k=1}^{5} \left(\prod_{\substack{l=1 \\ l \neq k}}^{5} \frac{x - x_l}{x_k - x_l} \right) y_k$$

$$P(x) = \left(\prod_{\substack{l=1 \\ l \neq 1}}^{5} \frac{x - x_l}{x_1 - x_l} \right) y_1 + \left(\prod_{\substack{l=1 \\ l \neq 2}}^{5} \frac{x - x_l}{x_2 - x_l} \right) y_2 + \left(\prod_{\substack{l=1 \\ l \neq 3}}^{5} \frac{x - x_l}{x_3 - x_l} \right) y_3$$
$$+ \left(\prod_{\substack{l=1 \\ l \neq 4}}^{5} \frac{x - x_l}{x_4 - x_l} \right) y_4 + \left(\prod_{\substack{l=1 \\ l \neq 5}}^{5} \frac{x - x_l}{x_5 - x_l} \right) y_5$$

Fitting the Curve





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Fourth Order Polynomial

$$
\begin{aligned}
P_j(x) = &\frac{(x-x_{j-1})(x-x_j)(x-x_{j+1})(x-x_{j+2})}{(x_{j-2}-x_{j-1})(x_{j-2}-x_j)(x_{j-2}-x_{j+1})(x_{j-2}-x_{j+2})}u_{j-2} \\
&+\frac{(x-x_{j-2})(x-x_j)(x-x_{j+1})(x-x_{j+2})}{(x_{j-1}-x_{j-2})(x_{j-1}-x_j)(x_{j-1}-x_{j+1})(x_{j-1}-x_{j+2})}u_{j-1} \\
&+\frac{(x-x_{j-2})(x-x_{j-1})(x-x_{j+1})(x-x_{j+2})}{(x_j-x_{j-2})(x_j-x_{j-1})(x_j-x_{j+1})(x_j-x_{j+2})}u_j \\
&+\frac{(x-x_{j-2})(x-x_{j-1})(x-x_j)(x-x_{j+2})}{(x_{j+1}-x_{j-2})(x_{j+1}-x_{j-1})(x_{j+1}-x_j)(x_{j+1}-x_{j+2})}u_{j+1} \\
&+\frac{(x-x_{j-2})(x-x_{j-1})(x-x_j)(x-x_{j+1})}{(x_{j+2}-x_{j-2})(x_{j+2}-x_{j-1})(x_{j+2}-x_j)(x_{j+2}-x_{j+1})}u_{j+2}
\end{aligned}
$$

Fourth Order Differentiation Equation

$$P_j'(x_j) = \frac{1}{h}\left[\frac{1}{12}u_{j-2} - \frac{2}{3}u_{j-1} + \frac{2}{3}u_{j+1} - \frac{1}{12}u_{j+2}\right]$$

System of Equations

$$w_1 = \frac{1}{h}\left[\frac{1}{12}u_{N-1} - \frac{2}{3}u_N + \frac{2}{3}u_2 - \frac{1}{12}u_3\right]$$

$$w_2 = \frac{1}{h}\left[\frac{1}{12}u_N - \frac{2}{3}u_1 + \frac{2}{3}u_3 - \frac{1}{12}u_4\right]$$

$$w_3 = \frac{1}{h}\left[\frac{1}{12}u_1 - \frac{2}{3}u_2 + \frac{2}{3}u_4 - \frac{1}{12}u_5\right]$$

$$\vdots$$

$$w_{N-1} = \frac{1}{h}\left[\frac{1}{12}u_{N-3} - \frac{2}{3}u_{N-2} + \frac{2}{3}u_N - \frac{1}{12}u_1\right]$$

$$w_N = \frac{1}{h}\left[\frac{1}{12}u_{N-2} - \frac{2}{3}u_{N-1} + \frac{2}{3}u_1 - \frac{1}{12}u_2\right]$$

Fourth Order Differentiation Matrix

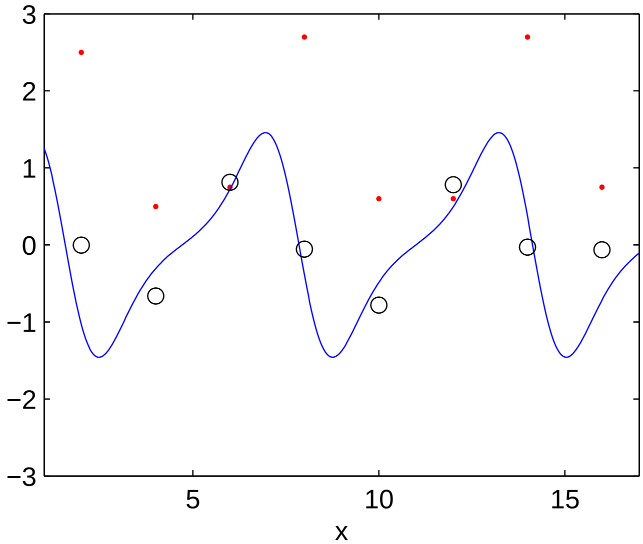
$$
\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ \vdots \\ w_{N-1} \\ w_N \end{bmatrix}
= \frac{1}{h}
\begin{bmatrix}
 & & \ddots & & & 1/12 & -2/3 \\
 & & \ddots & -1/12 & & & 1/12 \\
 & & \ddots & 2/3 & \ddots & & \\
 & & \ddots & 0 & \ddots & & \\
 & & \ddots & -2/3 & \ddots & & \\
-1/12 & & & 1/12 & \ddots & & \\
2/3 & -1/12 & & & \ddots & &
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ \vdots \\ u_{N-1} \\ u_N \end{bmatrix}
$$

Differentiation Using the Fourth Order Matrix

$$(2, 2.5),\ (4, .5),\ (6, .75),\ (8, 2.7),\ (10, .6),\ (12, .6),\ (14, 2.7),\ (16, .75)$$

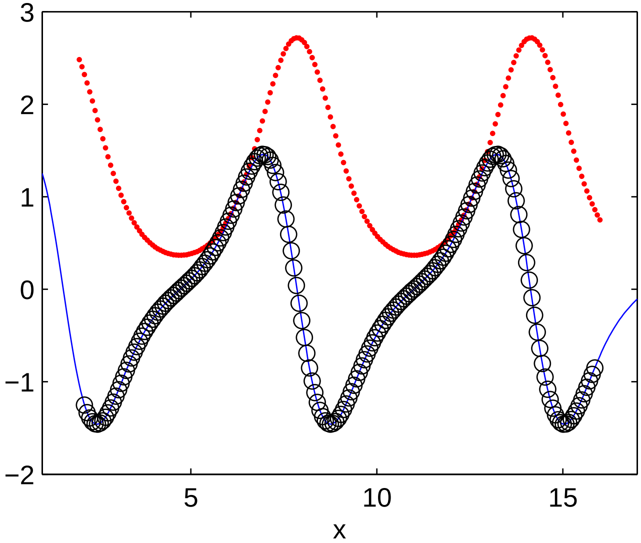
$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \\ w_7 \\ w_8 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} & & \ddots & & & 1/12 & -2/3 \\ & & \ddots & -1/12 & & & 1/12 \\ & & \ddots & 2/3 & \ddots & & \\ & & \ddots & 0 & \ddots & & \\ & & \ddots & -2/3 & \ddots & & \\ -1/12 & & & 1/12 & \ddots & & \\ 2/3 & -1/12 & & & \ddots & & \end{bmatrix} \begin{bmatrix} 2.5 \\ .5 \\ .75 \\ 2.7 \\ .6 \\ .6 \\ 2.7 \\ .75 \end{bmatrix}$$

Plotting Data Points

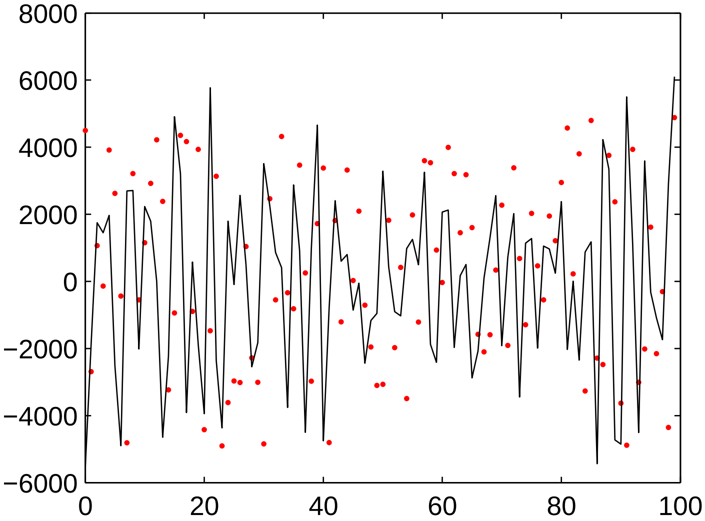


$$y = e^{\sin x} \qquad \text{and} \qquad y' = (\cos x)e^{\sin x}$$

Accuracy Increases with an Increase of Points



Conclusion



References

[1] Loyd N. Trefethen *2000 Spectral Methods in MATLAB.*