The Derivation of Second and Fourth Order Differentiation Matrices.

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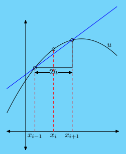
Abstract

The purpose of this document is to describe the derivation of second and fourth order differentiation matrices. This will be done using two different methods. First we will derive a second order differentiation matrix from the Taylor polynomial. Then we will derive second and fourth order differentiation matrices from the Lagrange interpolating polynomial.

1. Introduction

Numerical methods for approximating derivatives are especially important in real world applications. This is because the ability to solve for the rate of change when given a set of data points can be very difficult. You will soon learn how you can easily obtain a good approximation of a derivative that would be difficult or impossible to evaluate symbolically.



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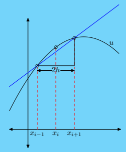

Differentiation matrices are a way to approximate derivatives using methods of Linear Algebra. There are other ways to approximate derivatives, but using a differentiation matrix has its advantages. In a situation where you have a discrete set of points rather than a continuous function. You can obtain the derivative directly. Instead of having to find an interpolating polynomial and then take the derivative of that.

2. Solving For Second Degree Differentiation Matrix:

The following will show how to derive the second degree differentiation matrix using the Taylor series and the Lagrange interpolating polynomial.

2.1. Taylor Series Polynomial:

Notice from the number line in Figure 1 that we will be defining the three distinct points (x_{i-1}, u_{i-1}), (x_i, u_i) and (x_{i+1}, u_{i+1}), where $u(x_i) = u_i$.

We will be using the points x_{i-1} and x_{i+1} to approximate the derivative at x_i. If we denote the approximation of the derivative of our function, $u(x_i)$, as $w_i = u'(x_i)$ then notice from Figure 2 that

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

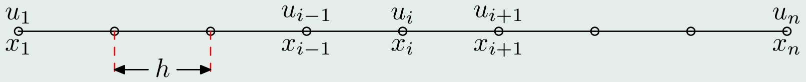

Figure 1: Taylor series number line

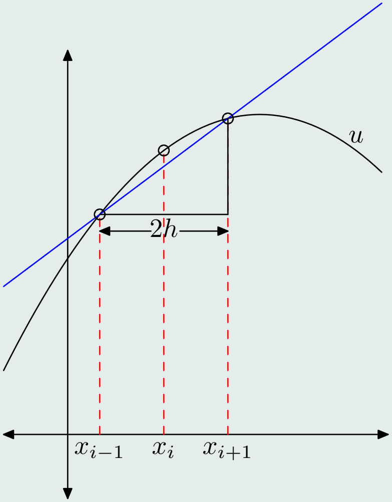

Figure 2: Secant line derivative approximation

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From the Taylor series we know that

$$f(x) = \frac{f(a)(x-a)^0}{0!} + \frac{f'(a)(x-a)^1}{1!} + \frac{f''(a)(x-a)^2}{2!} + \frac{f'''(a)(x-a)^3}{3!} + \cdots \frac{f^{(n)}(a)(x-a)^n}{n!},$$

which can be written more concisely as

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)(x-a)^2}{2!} + \frac{f'''(a)(x-a)^3}{3!} + \cdots.$$

So if we substitute $x = a + h$ where $h = x_{i+1} - x_i$ then we get the following,

$$\begin{aligned} f(a+h) &= f(a) + f'(a)(a+h-a) + \frac{f''(a)(a+h-a)^2}{2!} + \frac{f'''(a)(a+h-a)^3}{3!} + \cdots \\ &= f(a) + f'(a)h + \frac{f''(a)h^2}{2!} + \frac{f'''(a)h^3}{3!} + \cdots. \end{aligned}$$

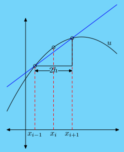
If we say $a = x$, then this can be written as

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \cdots.$$

Then, remembering that our original function is $u(x)$, we can write this as

$$u(x+h) = u(x) + u'(x)h + \frac{u''(x)h^2}{2!} + \frac{u'''(x)h^3}{3!} + \cdots.$$

Since $h = x_{i+1} - x_i$ this means that $x_{i+1} = x_i + h$ and $x_{i-1} = x_i - h$, which gives us



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the two following equations,

$$\begin{aligned}
u(x_{i+1}) &= u(x_{i+h}) \\
&= u(x_i) + u'(x_i)h + \frac{u''(x_i)h^2}{2!} + \frac{u'''(x_i)h^3}{3!} + \cdots \\
u(x_{i-1}) &= u(x_i - h) \\
&= u(x_i) - u'(x_i)h + \frac{u''(x_i)h^2}{2!} - \frac{u'''(x_i)h^3}{3!} + \cdots .
\end{aligned}$$

Subtracting these two equations, we get

$$u(x_{i+1}) - u(x_{i-1}) = 2u'(x_i)h + 2\frac{u'''(x_i)h^3}{3!} + \cdots .$$

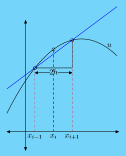
And, since we are only interested in the first derivative, we can drop the higher order terms

$$\begin{aligned}
u(x_{i+1}) - u(x_{i-1}) &= 2u'(x_i)h \\
u'(x_i) &= \frac{u(x_{i+1}) - u(x_{i-1})}{2h}.
\end{aligned}$$

If we again define $w_j = u'(x_i)$, $u_{i+1} = u(x_{i+1})$ and $u_i - 1 = u(x_{i-1})$, then we get the following:

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

Notice that this is the same function that we got from the secant line approximation in equation (1). Now let's solve for the interpolating polynomial.



2.2. Lagrange Interpolating Polynomial

If we start with the same three distinct points (x_{i-1}, u_{i-1}), (x_i, u_i), and (x_{i+1}, u_{i+1}) from our number line in Figure 1, we know that these three points define one specific polynomial. We also know that this polynomial will have at most degree two. The Lagrange interpolating polynomial says that $P(x) = \sum_{k=1}^{N}(\prod_{l\neq k} \frac{x-x_l}{x_k-x_l})y_k$ so using three points we get the following

$$P(x) = \sum_{k=1}^{3}\left(\prod_{\substack{l=1\\ l\neq k}}^{3} \frac{x-x_l}{x_k-x_l}\right) y_k.$$

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

$$P(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)}y_1 + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)}y_2 + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)}y_3.$$

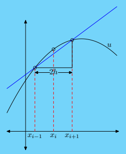
Now, substituting in our points (x_{i-1}, u_{i-1}), (x_i, u_i), and (x_{i+1}, u_{i+1}) for (x_1, y_1), (x_2, y_2), and (x_3, y_3) respectively, we have the following

$$P_i(x) = \frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})}u_{i-1} + \frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})}u_i + \frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}u_{i+1}$$

$$P_i(x) = \frac{(x-x_i)(x-x_{i+1})}{2h^2}u_{i-1} - \frac{(x-x_{i-1})(x-x_{i+1})}{h^2}u_i + \frac{(x-x_{i-1})(x-x_i)}{2h^2}u_{i+1}.$$

Now, taking the derivative of this polynomial, we get

$$P_i'(x) = \frac{(x-x_i)+(x-x_{i+1})}{2h^2}u_{i-1} - \frac{(x-x_{i-1})+(x-x_{i+1})}{h^2}u_i + \frac{(x-x_{i-1})+(x-x_i)}{2h^2}u_{i+1}.$$



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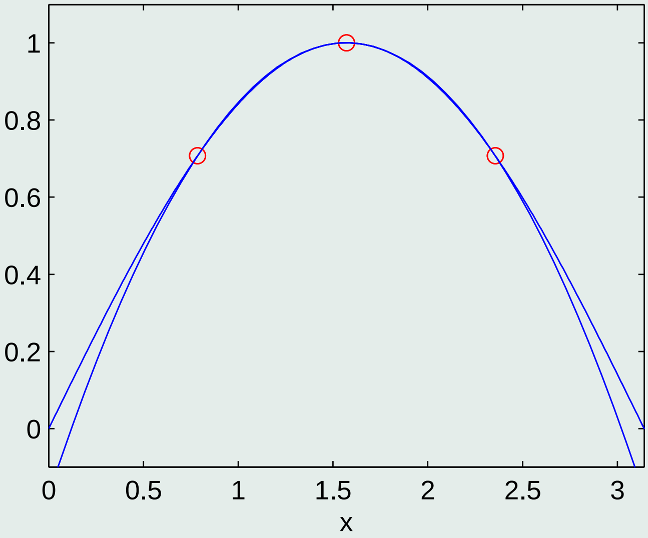


Figure 3: Second degree Lagrange polynomial approximation

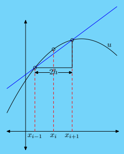
And, evaluating at x_i

$$P_i'(x_i) = \frac{(x_i - x_i) + (x_i - x_{i+1})}{2h^2} u_{i-1} - \frac{(x_i - x_{i-1}) + (x_i - x_{i+1})}{h^2} u_i + \frac{(x_i - x_{i-1}) + (x_i - x_i)}{2h^2} u_{i+1}$$
$$P_i'(x_i) = -\frac{1}{2h} u_{i-1} + \frac{1}{2h} u_{i+1}.$$

If we define $w_i = P'(x_i)$ then we have $w_i = -u_{i+1}/2h + u_{i-1}/2h$ which can be rewritten as $w_i = (u_{i+1} - u_{i-1})/2h$ which is once again equation (1). Notice that we just used a secant line and two separate polynomials to do a second order derivative approximation at the point (x_i, u_i) and came out with the same function. Now in order to write this in matrix form we must solve this function as i goes from 1 to N, we get the following.

$$\begin{aligned}
w_1 &= -\frac{1}{2h} u_0 + \frac{1}{2h} u_2 \\
w_2 &= -\frac{1}{2h} u_1 + \frac{1}{2h} u_3 \\
w_3 &= -\frac{1}{2h} u_2 + \frac{1}{2h} u_4 \\
&\vdots \\
w_{N-1} &= -\frac{1}{2h} u_{N-2} + \frac{1}{2h} u_N \\
w_N &= -\frac{1}{2h} u_{N-1} + \frac{1}{2h} u_{N+1}
\end{aligned}$$

Notice from our number line in Figure 1 that, while we defined u to run from 1 to N, we now have u_0 and u_{N+1} in our system of equations, so we must assume that our



function is periodic and define $u_0 = u_N$ and $u_{N+1} = u_1$. This gives us the following equations which can be written in matrix form.

$$
\begin{aligned}
w_1 &= -\frac{1}{2h}u_N + \frac{1}{2h}u_2 \Rightarrow \frac{1}{h}\left[-\frac{1}{2}u_N + \frac{1}{2}u_2\right]\\
w_2 &= -\frac{1}{2h}u_1 + \frac{1}{2h}u_3 \Rightarrow \frac{1}{h}\left[-\frac{1}{2}u_1 + \frac{1}{2}u_3\right]\\
w_3 &= -\frac{1}{2h}u_2 + \frac{1}{2h}u_4 \Rightarrow \frac{1}{h}\left[-\frac{1}{2}u_2 + \frac{1}{2}u_4\right]\\
&\vdots\\
w_{N-1} &= -\frac{1}{2h}u_{N-2} + \frac{1}{2h}u_N \Rightarrow \frac{1}{h}\left[-\frac{1}{2}u_{N-2} + \frac{1}{2}u_N\right]\\
w_N &= -\frac{1}{2h}u_{N-1} + \frac{1}{2h}u_1 \Rightarrow \frac{1}{h}\left[-\frac{1}{2}u_{N-1} + \frac{1}{2}u_1\right]
\end{aligned}
$$

This gives us the following system.

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

Now remember from Figure 2 that our original equation, equation (1), came from a secant line approximation of the derivative at our point (x_j, u_j). However, we see in

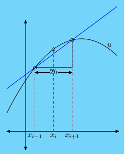


Figure 3 that our second and third derivations of equation (1) came from taking the derivative of a second degree polynomial that passes through our three points. The interesting thing to note here is that both paths take us to exactly the same matrix.

3. Solving for the Fourth Degree Differentiation Matrix

Since we saw that both the Taylor series and the Lagrange interpolating polynomial both have the same result, in this section we will just use the Lagrange interpolating Polynomial to solve for the fourth degree differentiation matrix.

3.1. Lagrange Interpolating Polynomial

If we start with five distinct points this time (x_{j-2}, u_{j-2}), (x_{j-1}, u_{j-1}), (x_j, u_j), (x_{j+1}, u_{j+1}), and (x_{j+2}, u_{j+2}) we know that these five points define one specific polynomial. We also know that this polynomial will have at most degree four. Remember that the Lagrange interpolating polynomial says that

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

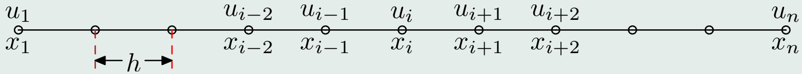
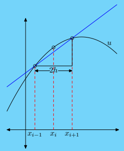


Figure 4: Fourth degree differentiation matrix number line



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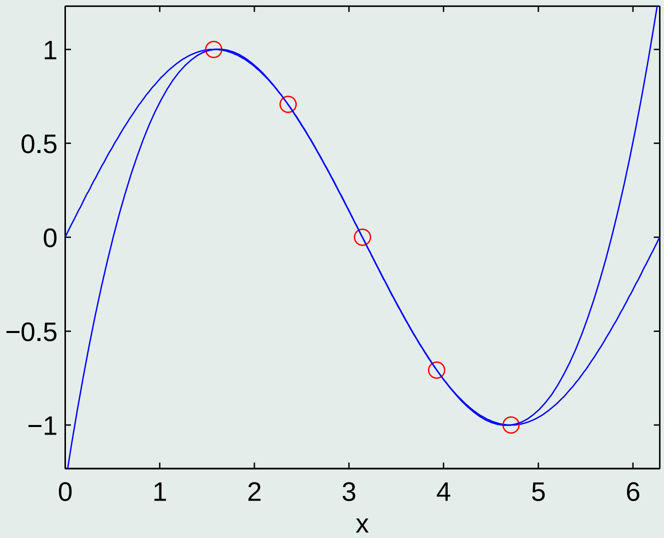
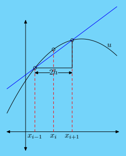


Figure 5: Fourth degree Lagrange polynomial



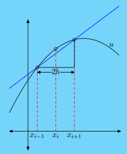
Notice from Figure 5 that with the Lagrange polynomial we will be using a polynomial that passes through our given points and taking the derivative of that specific polynomial to estimate the derivative at the point (x_j, u_j). So using five points we get the following.

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

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

$$\begin{aligned} P(x) = {} & \frac{(x - x_2)(x - x_3)(x - x_4)(x - x_5)}{(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)(x_1 - x_5)} y_1 + \frac{(x - x_1)(x - x_3)(x - x_4)(x - x_5)}{(x_2 - x_1)(x_2 - x_3)(x_2 - x_4)(x_2 - x_5)} y_2 \\ & + \frac{(x - x_1)(x - x_2)(x - x_4)(x - x_5)}{(x_3 - x_1)(x_3 - x_2)(x_3 - x_4)(x_3 - x_5)} y_3 + \frac{(x - x_1)(x - x_2)(x - x_3)(x - x_5)}{(x_4 - x_1)(x_4 - x_2)(x_4 - x_3)(x_4 - x_5)} y_4 \\ & + \frac{(x - x_1)(x - x_2)(x - x_3)(x - x_4)}{(x_5 - x_1)(x_5 - x_2)(x_5 - x_3)(x_5 - x_4)} y_5. \end{aligned}$$

Now substituting in our points (x_{j-2}, u_{j-2}), (x_{j-1}, u_{j-1}), (x_j, u_j), (x_{j+1}, u_{j+1}), and (x_{j+2}, u_{j+2}) for (x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4) and (x_5, y_5), respectively, we have the following:



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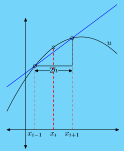
$$
\begin{aligned}
P_j(x) = {} & \frac{(x-x_{j-1})(x-x_j)(x-x_{j+1})(x-x_{j+2})}{(x_{j-2}-x_{j-1})(x_{j-2}-x_j)(x_{j-2}-x_{j+1})(x_{j-2}-x_{j+2})}u_{j-2} \\
& + \frac{(x-x_{j-2})(x-x_j)(x-x_{j+1})(x-x_{j+2})}{(x_{j-1}-x_{j-2})(x_{j-1}-x_j)(x_{j-1}-x_{j+1})(x_{j-1}-x_{j+2}}u_{j-1} \\
& + \frac{(x-x_{j-2})(x-x_{j-1})(x-x_{j+1})(x-x_{j+2})}{(x_j-x_{j-2})(x_j-x_{j-1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

We notice that the denominator can be rewritten as follows:

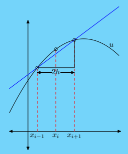
$$
\begin{aligned}
P_j(x) = {} & \frac{(x-x_{j-1})(x-x_j)(x-x_{j+1})(x-x_{j+2})}{24h^4}u_{j-2} \\
& - \frac{(x-x_{j-2})(x-x_j)(x-x_{j+1})(x-x_{j+2})}{6h^4}u_{j-1} \\
& + \frac{(x-x_{j-2})(x-x_{j-1})(x-x_{j+1})(x-x_{j+2})}{4h^4}u_j \\
& - \frac{(x-x_{j-2})(x-x_{j-1})(x-x_j)(x-x_{j+2})}{6h^4}u_{j+1} \\
& + \frac{(x-x_{j-2})(x-x_{j-1})(x-x_j)(x-x_{j+1})}{24h^4}u_{j+2}.
\end{aligned}
$$

Taking the derivative of this polynomial we get



$$\begin{aligned}
P_j'(x) = {} & \frac{(x-x_{j-1})(x-x_j)(x-x_{j+1}) + (x-x_{j-1})(x-x_j)(x-x_{j+2})}{24h^4}u_{j-2} \\
& + \frac{(x-x_{j-1})(x-x_{j+1})(x-x_{j+2}) + (x-x_j)(x-x_{j+1})(x-x_{j+2})}{24h^4}u_{j-2} \\
& - \frac{(x-x_{j-2})(x-x_j)(x-x_{j+1}) + (x-x_{j-2})(x-x_j)(x-x_{j+2})}{6h^4}u_{j-1} \\
& - \frac{(x-x_{j-2})(x-x_{j+1})(x-x_{j+2}) + (x-x_j)(x-x_{j+1})(x-x_{j+2})}{6h^4}u_{j-1} \\
& + \frac{(x-x_{j-2})(x-x_{j-1})(x-x_{j+1}) + (x-x_{j-2})(x-x_{j-1})(x-x_{j+2})}{4h^4}u_j \\
& + \frac{(x-x_{j-2})(x-x_{j+1})(x-x_{j+2}) + (x-x_{j-1})(x-x_{j+1})(x-x_{j+2})}{4h^4}u_j \\
& - \frac{(x-x_{j-2})(x-x_{j-1})(x-x_j) + (x-x_{j-2})(x-x_{j-1})(x-x_{j+2})}{6h^4}u_{j+1} \\
& - \frac{(x-x_{j-2})(x-x_j)(x-x_{j+2}) + (x-x_{j-1})(x-x_j)(x-x_{j+2})}{6h^4}u_{j+1} \\
& + \frac{(x-x_{j-2})(x-x_{j-1})(x-x_j) + (x-x_{j-2})(x-x_{j-1})(x-x_{j+2})}{24h^4}u_{j+2} \\
& + \frac{(x-x_{j-2})(x-x_j)(x-x_{j+2}) + (x-x_{j-1})(x-x_j)(x-x_{j+2})}{24h^4}u_{j+2}.
\end{aligned}$$

While this equation looks very unruly and hard to manipulate, when we evaluate it at x_j it becomes much easier to work with



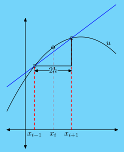
$$\begin{aligned}
P_j'(x_j) = {} & \frac{(x_j - x_{j-1})(x_j - x_{j+1})(x_j - x_{j+2})}{24h^4} u_{j-2} - \frac{(x_j - x_{j-2})(x_j - x_{j+1})(x_j - x_{j+2})}{6h^4} u_{j-1} \\
& + \frac{(x_j - x_{j-2})(x_j - x_{j-1})(x_j - x_{j+1}) + (x_j - x_{j-2})(x_j - x_{j-1})(x_j - x_{j+2})}{4h^4} u_j \\
& + \frac{(x_j - x_{j-2})(x_j - x_{j+1})(x_j - x_{j+2}) + (x_j - x_{j-1})(x_j - x_{j+1})(x_j - x_{j+2})}{4h^4} u_j \\
& - \frac{(x_j - x_{j-2})(x_j - x_{j-1})(x_j - x_{j+2})}{6h^4} u_{j+1} + \frac{(x_j - x_{j-2})(x_j - x_{j-1})(x_j - x_{j+1})}{24h^4} u_{j+2}
\end{aligned}$$

Notice that the numerators can be written in terms of h

$$\begin{aligned}
P_j'(x_j) &= \frac{2h^3}{24h^4} u_{j-2} - \frac{4h^3}{6h^4} u_{j-1} + \frac{4h^3}{6h^4} u_{j+1} - \frac{2h^3}{24h^4} u_{j+2} + \frac{0}{4h^4} u_j \\
P_j'(x_j) &= \frac{1}{12h} u_{j-2} - \frac{2}{3h} u_{j-1} + \frac{2}{3h} u_{j+1} - \frac{1}{12h} u_{j+2} \\
P_j'(x_j) &= \frac{1}{h} \left[\frac{1}{12} u_{j-2} - \frac{2}{3} u_{j-1} + \frac{2}{3} u_{j+1} - \frac{1}{12} u_{j+2} \right].
\end{aligned}$$

If we once again define $w_j = P'(x_j)$ then we have

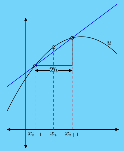
$$w_j = \frac{1}{h} \left[\frac{1}{12} u_{j-2} - \frac{2}{3} u_{j-1} + \frac{2}{3} u_{j+1} - \frac{1}{12} u_{j+2} \right].$$



If we solve each of these for j, as j goes from 1 to N, we get the following result.

$$
\begin{aligned}
w_1 &= \frac{1}{h}\left[\frac{1}{12}u_{-1} - \frac{2}{3}u_0 + \frac{2}{3}u_2 - \frac{1}{12}u_3\right] \\
w_2 &= \frac{1}{h}\left[\frac{1}{12}u_0 - \frac{2}{3}u_1 + \frac{2}{3}u_3 - \frac{1}{12}u_4\right] \\
w_3 &= \frac{1}{h}\left[\frac{1}{12}u_1 - \frac{2}{3}u_2 + \frac{2}{3}u_4 - \frac{1}{12}u_5\right] \\
&\vdots \\
w_{N-1} &= \frac{1}{h}\left[\frac{1}{12}u_{N-3} - \frac{2}{3}u_{N-2} + \frac{2}{3}u_N - \frac{1}{12}u_{N+1}\right] \\
w_N &= \frac{1}{h}\left[\frac{1}{12}u_{N-2} - \frac{2}{3}u_{N-1} + \frac{2}{3}u_{N+1} - \frac{1}{12}u_{N+2}\right]
\end{aligned}
$$

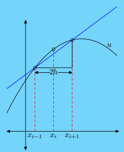
Once again notice from the number line in Figure 4 that, while we defined u to run from 1 to N, we now have u_{-1}, u_0, u_{N+1} and u_{N+2} in our system of equations so we must again assume periodicity and define $u_{-1} = u_{N-1}$, $u_0 = u_N$, $u_{N+1} = u_1$ and $u_{N+2} = u_2$.



This gives us the following equations which can be written in matrix form again

$$
\begin{aligned}
w_1 &= \frac{1}{h}\left[\frac{1}{12}u_{N-1} - \frac{2}{3}u_N + \frac{2}{3}u_2 - \frac{1}{12}u_3\right] \\
w_2 &= \frac{1}{h}\left[\frac{1}{12}u_{N} - \frac{2}{3}u_1 + \frac{2}{3}u_3 - \frac{1}{12}u_4\right] \\
w_3 &= \frac{1}{h}\left[\frac{1}{12}u_{1} - \frac{2}{3}u_2 + \frac{2}{3}u_4 - \frac{1}{12}u_5\right] \\
&\vdots \\
w_{N-1} &= \frac{1}{h}\left[\frac{1}{12}u_{N-3} - \frac{2}{3}u_{N-2} + \frac{2}{3}u_N - \frac{1}{12}u_1\right] \\
w_N &= \frac{1}{h}\left[\frac{1}{12}u_{N-2} - \frac{2}{3}u_{N-1} + \frac{2}{3}u_1 - \frac{1}{12}u_2\right]
\end{aligned}
$$

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



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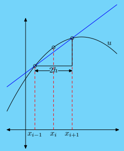
4. Differentiation

Now that we have found our second and fourth degree differentiation matrices, what can we do with them? Well certainly we could obtain a graph like that in Figure 6. This graph is of the function $f(x) = \sin x$ and the approximation of $f'(x)$ on the interval $0 \leq x < 2\pi$. Looking at the graph it appears that the approximation is almost exactly right. Notice that the interval is closed on the left and open on the right. Since we earlier assumed that our function was periodic it makes sense that a periodic function would be correctly approximated. However notice that if we run on a non-periodic interval like $0 \leq x < \frac{3\pi}{2}$ we get a graph like that in Figure 7. Notice how the end points are substantially off in Figure 7. The end points being substantially wrong is completely anticipated on a non-periodic interval though, since we had to assume periodicity in order to derive our differentiation matrix.

We also would get a similar error if we hadn't left the interval open, an open interval is necessary in a periodic function to get the proper endpoints. However, notice that even on our non-periodic interval, the points away from the endpoints are very accurate. This is why matrix differentiation is so useful to analyzing data points instead of functions. For the fourth order differentiation matrix, from the matrix in equation (3), you would expect an error on the last two points and the first two points, but all derivatives in between should be a close approximation. Similarly, for the second order differentiation matrix, from equation (2), there will be two error points, one on each end, but the middle points will have a smaller degree of accuracy.

Let's consider the eight points $(2, 5)$, $(4, 15)$, $(6, 35)$, $(8, 65)$, $(10, 100)$, $(12, 145)$ $(14, 195)$, and $(16, 255)$. If we evaluate the derivative at each point with our differentiation matrix we get the following result.



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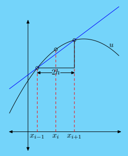


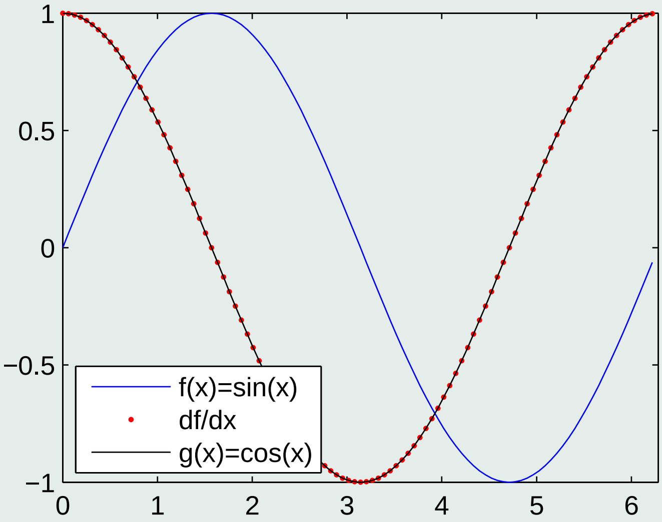


Figure 6: Graph of $\sin x$ and derivative approximation

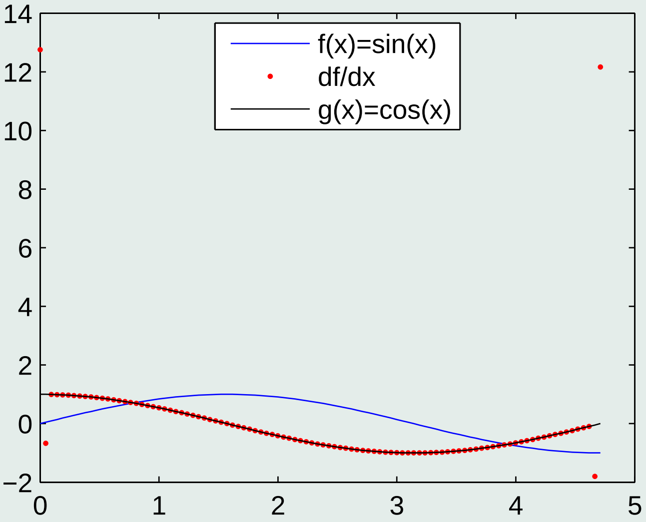


Figure 7: Graph of $\sin x$ and derivative approximation

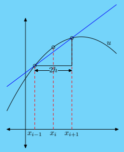
$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \\ w_7 \\ w_8 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & -1/2 \\ -1/2 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/2 & 0 & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1/2 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1/2 & 0 & 1/2 & 0 & 0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

thus,

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

Remembering that **u** is a vector containing the y coordinates we are evaluating, and **w** is a vector containing the y co-ordinates of the derivatives, we can plot the vector **x**, a vector consisting of all the x values, verses both **u** and **w**. This yields Figure 8. Notice how closely the points (x_i, w_i) (where x_i and w_i are corresponding elements of **x** and **w**) are approximating the line $y = 2x$. Then notice how closely our original data points are to fitting the curve $y = x^2$ which of course has the derivative $y = 2x$

A similar graph is produced when we use the fourth order differentiation matrix and the eight points $(2, 2.5)$, $(4, .5)$, $(6, .75)$, $(8, 2.7)$, $(10, .6)$, $(12, .6)$, $(14, 2.7)$, $(16, .75)$ Notice that this produces the following system.



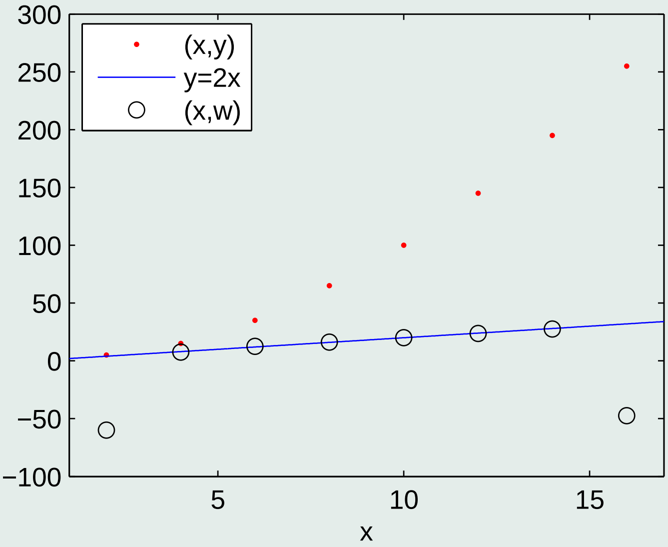


Figure 8: Data points and Derivatives

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

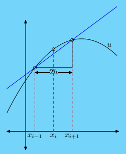
that is,

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \\ w_7 \\ w_8 \end{bmatrix} = \begin{bmatrix} -1/480 \\ -319/480 \\ 13/16 \\ -13/240 \\ -25/32 \\ 25/32 \\ -7/240 \\ -1/16 \end{bmatrix}.$$

Notice in Figure 9 that our data points fall very close to the curve $y = \cos x(e^{\sin x})$. It is a decent approximation of the derivatives at our given points on the curve $y = e^{\sin x}$. It is, however, not completely accurate. Though as you can see in Figure 10 that an increase in the number of data points greatly increases the accuracy.

5. Conclusion

You have seen the derivation and usage of the second and fourth order differentiation matrices. These matrices can be used to approximate derivatives of data points either



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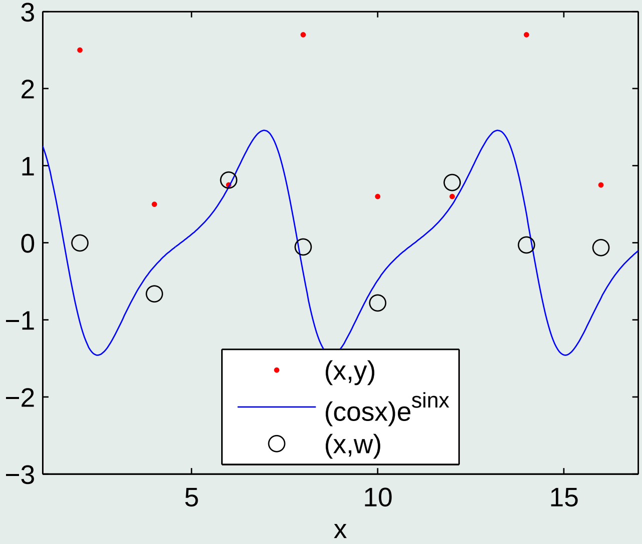
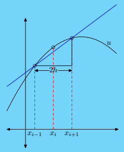


Figure 9: Fourth order data points and Derivatives



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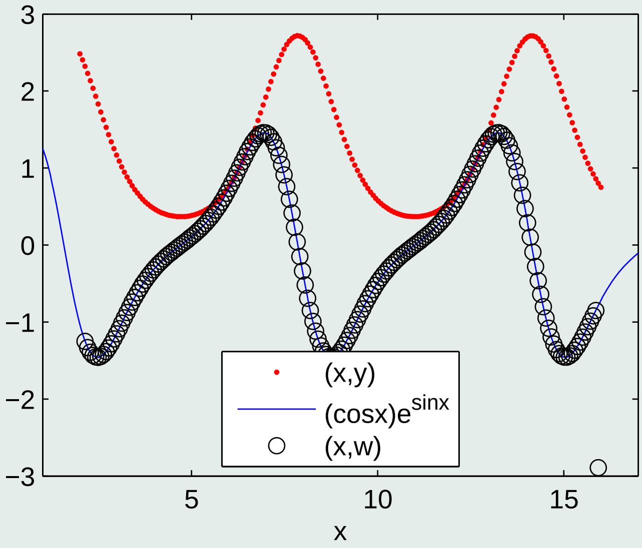
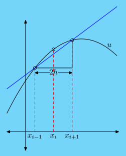


Figure 10: Fourth order multi-data points and Derivatives



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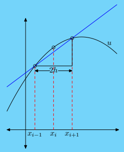
from a curve, lab data and other sources. In order to help demonstrate the accuracy of the matrices, only data points from curves were shown here, but hopefully it can be seen that whether solving for the rate of change of the growth of bacteria, or for the speed of a moving particle, these matrices have many real world applications, and can greatly save time and energy spent in trying to differentiate data points.

References

[1] Trefethen, Loyd N. *Spectral Methods in MATLAB. Philadelphia: Siam, 2000.*

[2] Moler, Cleve *Numerical Computing with Matlab. Philadelphia: Siam, 2004.*



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