

MATLAB Marina: Numerical Differentiation

Student Learning Objectives

After completing this module, one should:

- 1. Be able to use MATLAB to compute numerical derivatives.
- 2. Be able to explain the limitations of numerical differentiation.

Terms

numerical differentiation, forward difference, backwards difference, central difference

MATLAB Functions, Keywords, and Operators

diff

Numerical Differentiation

The derivative of a function f(x) is the rate of change of the function with respect to the

independent variable x, written $\frac{df(x)}{dx}$. Numerical differentiation is typically used when a

formula for the function to differentiate is not available or the derivative would be difficult to determine analytically. Numerical differentiation can yield accurate results if the function is piecewise continuous, relatively smooth, the increment between function points is relatively small, and the data is accurate. Numerical differentiation is very sensitive to inaccuracies in the data (noisy data).

Methods for computing numerical (approximate) derivatives include: backward difference approximation, forward difference approximation, and central or midpoint difference approximation. Given vectors f and x of the same length:

 The backwards difference approximation of the derivative of f(x) is the slope of the line between the current and the previous point computed at each point x_k in x via

$$f'(x_{k}) = \frac{f(x_{k}) - f(x_{k-1})}{x_{k} - x_{k-1}}$$

 The forward difference approximation of the derivative of f(x) is the slope of the line between the current and the next point computed at each point x_k in x via

$$f'(x_k) = \frac{f(x_{k+1}) - f(x_k)}{x_{k+1} - x_k}$$

 The central difference approximation of the derivative of f(x) is the slope of the line between the previous and the next point computed at each point x_k in x via

$$f'(x_k) = \frac{f(x_{k+1}) - f(x_{k-1})}{x_{k+1} - x_{k-1}}$$

Numerical Differentiation using MATLAB

The MATLAB function diff can used to compute approximate derivatives. The diff function when used with a single argument returns a vector length one less than the original of the differences of the adjacent values in the vector. For example, diff(x) returns [x(2) – x(1), x(3) – x(2), ... x(N) – x(N-1)], where N is the length of the vector. Thus given two vectors f and x where f is a function of x, diff(f)./diff(x) computes either the forward (if values are interpreted as being for x(1:end-1)) or backward difference approximation (if values are interpreted as being for x(2:end)).

The MATLAB program of Figure 1a computes the forward and central difference

approximations of $\frac{df(x)}{dx}$ for the polynomial function $f(x) = x^2 + 2x + 1$. The central difference has one less point than the forward difference. Figure 1b shows the polynomial function and the numerical derivative (forward difference) of the function.

```
%% Numerical differentiation of polynomial function
clear; clc; close all;
function f(x) = x^2 + 2x + 1
x = linspace(-5, 5, 100);
f = x.^2 + 2*x + 1;
% analytical derivative of polynomial function
dfdxAn = 2*x + 2;
% numerical derivative of polynomial function
df = diff(f);
dx = diff(x);
% forward difference
dfdx = df./dx;
% central difference
dfdxCen = (df(2:end)+df(1:end-1))./(dx(2:end) + dx(1:end-1));
figure(1)
plot(x, f, 'b-', x(1:end-1), dfdx, 'g-')
xlabel('x'), legend('f(x)', 'numerical derivative of f(x)')
% plot(x,f,'b-',x(2:end-1),dfdxCen,'g-')
```

Figure 1a. MATLAB Program for Numerical Derivative of Polynomial Function

For a backwards difference approximation, the difference dfdx values are interpreted for the x value range of 2 to the end. The plot statement for the forward difference in Figure 1a would be replaced with

plot(x, f, 'b-', x(2:end), dfdx, 'g-')
for a backwards difference.



Figure 1b. Plot of Polynomial Function and Numerical Derivative

The numerical derivative of the second order polynomial function is very close to the analytic derivative for the interval used. The maximum variation between dfdx and dfdxAn is 0.101 over the x range. For 1000 instead of 100 x values over the same range, the maximum variation between dfdx and dfdxAn is 0.010 over the x range.

The numerical derivative is accurate in this example because: the polynomial function is smooth, the function values are accurate, and the independent variable interval used is small relative to how rapidly the function changes.

Typically, one does not have access to the function describing the data like in the example of Figure 1a, but rather one has measured data values for the function. The approximate derivative will be less accurate for functions whose data values are less accurate and for which the interval between measurements is larger relative to how rapidly the function changes.

Additional Information on the diff Function

The diff function can also be used for approximations of higher order derivatives and can be used to take differences along a dimension of a 2D array. For example:

- diff(x, 2) is the 2nd order difference of x and is equivalent to diff(diff(x))
- diff(x, N) is the Nth order difference of x
- diff(X,1,1) is the 1st order difference of x along dimension 1 (difference along columns)
- diff(X, 1, 2) is the 1st order difference of x along dimension 2 (difference along rows)

An approximate second order derivative of the polynomial function $f(x) = x^2 + 2x + 1$ is computed using the MATLAB code of Figure 2.

```
% approximate second order derivative of polynomial function
% function f(x) = x^2 + 2x + 1
x = linspace(-5,5,100);
f = x.^2 + 2*x + 1;
dx = diff(x);
d2ydx2Back = diff(f,2)./(dx(2:end).^2);
```

Figure 2. MATLAB Code for Approximate 2nd Order Derivative

The second difference of f, diff(f, 2), will have one less point than the first difference of x, diff(x). Also note that the approximate second order derivative is not computed using diff(f, 2)./ diff(x, 2)

which would not only be incorrect and but if the interval between the x values was constant like in the example of Figure 2, diff(x, 2) will be a vector of all 0s.

Last modified Thursday, April 8, 2021

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