# Supplementary Notes 6

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**Abstract**

In this tutorial we discuss numerical differentiation.

## Contents



# 1 Numerical differentiation

Numerical differentiation is the method used to estimate derivatives of a function using values of the function. We know from Calculus that the derivative of a function $f$ at $x_0$ is

$$f'(x_0) = \lim_{h\to 0} \frac{f(x_0+h)-f(x_0)}{h}.$$

This gives us a way to estimate the derivative of $f$ at $x_0$:

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$$

for small values of $h$. This approach doesn't tell us however anything about the error and it can't be generalized. In the following sections we discuss two difference approaches to obtain formulas for the approximation of the derivatives of a function $f$ and how to compute their error. Throughout these notes, we always assume $f$ to be sufficiently smooth.

## 1.1 Lagrange interpolation approach

The first approach we discuss consists in using Lagrange interpolation.

**Example 1.1.** *Let $L_2(x)$ be the Lagrange interpolation polynomial of $f$ at nodes $x_0$ and $x_1 := x_0 + h$ with $h > 0$. Then using Newton's divided difference formula*

$$L_2(x) = f(x_0)f[x_0, x_1](x - x_0) = f(x_0) + \frac{f(x_0+h)-f(x_0)}{h}(x - x - x_0)$$

*Moreover, for any $x \in [x_0, x_0 + h]$*

$$f(x) = L_2(x) + f''(\xi)\frac{(x-x_0)(x-(x_0+h))}{2}.$$

*where $\xi \in (x_0, x_0 + h)$. (To simplify the notation we dropped the dependence of $\xi$ in terms of $x$.) Taking the derivative with respect to $x$ leads to*

$$f'(x) = \frac{f(x_0+h)-f(x_0)}{h} + \frac{2(x-x_0)-h}{2}f''(\xi(x)) + \frac{(x-x_0)(x-x_0-h)}{2}D_x\left(f''(\xi(x))\right).$$

*Now, we take $x = x_0$ and get*

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(\xi)$$

*where $\xi \in (x_0, x_0 + h)$. We have obtained the forward finite difference formula for the first derivative*

$$D_h^+ f(x_0) = \frac{f(x_0+h) - f(x_0)}{h}$$

*which has an error given by*

$$error = f'(x_0) - D_h^+ f(x_0) = -\frac{h}{2} f''(\xi)$$

*where $\xi \in (x_0, x_0 + h)$. We obtained the same formula as the one provided by the limit definition of derivative, but know we have information about the error. Likewise, we could have considered instead $x_1 = x_0 - h$ which would lead to the backward finite difference formula*

$$D_h^- f(x_0) = \frac{f(x_0) - f(x_0-h)}{h}$$

*which has an error given by*

$$error = f'(x_0) - D_h^- f(x_0) = \frac{h}{2} f''(\xi)$$

*where $\xi \in (x_0 - h, x_0)$.*

In general suppose that we have nodes $\{x_0, \dots, x_n\}$ and $f \in C^{n+1}$. Then

$$f(x) = \sum_{k=0}^{n} l_k(x) f(x_k) + f^{(n+1)}(\xi(x)) \frac{(x-x_0)\dots(x-x_n)}{(n+1)!}$$

where the $l_k$ denote the Lagrange basis polynomials. Taking the derivative with respect to $x$, leads to

$$f(x) = \sum_{k=0}^{n} l_k'(x) f(x_k) + D_x \left[ f^{(n+1)}(\xi(x)) \right] \frac{(x-x_0)\dots(x-x_n)}{(n+1)!} + f^{(n+1)}(\xi(x)) \frac{D_x\left[(x-x_0)\dots(x-x_n)\right]}{(n+1)!}.$$

Then by taking $x = x_i$ for some $i \in \{0, \dots, n\}$ we get

$$f'(x_i) = \sum_{k=}^{n} l_k'(x_i) f(x_k) + \frac{f^{(n+1)}(\xi(x_i))}{(n+1)!} \prod_{\substack{k=0 \\ k \neq i}}^{n} (x_i - x_k). \tag{1}$$

This is called an $(n+1)$-point formula to approximate $f'(x_i)$. In general using more points produces greater accuracy, although the number of function evaluations and growth of round-off error discourages this. The most common formulas are those involving three and five evaluation points.

**Example 1.2** (three-point endpoint formula)**.**

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} + \frac{h^2}{3} f^{(3)}(\xi) \tag{2}$$

*where $\xi \in (x_0, x_0 + 2h)$.*

**Example 1.3** (three-point midpoint formula)**.**

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi) \tag{3}$$

*where $\xi \in (x_0 - h, x_0 + h)$.*

**Remark 1.1.** *Note that both errors are $\mathcal{O}(h^2)$. However the error in* (3) *is half the error in* (2) *and requires one less function evaluation. The approximation* (2) *is useful near the ends of an interval because information about $f$ outside the interval may not be available.*

**Exercise 1.1.** *Derive the three-point formulas and respective errors.*

**Solution:** We have

$$l_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad \text{with} \quad l_0'(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}.$$

Similarly,

$$l_1'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)} \quad \text{and} \quad l_2'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}.$$

Hence, by using formula (1) we get

$$\begin{aligned} f'(x_i) =& f(x_0)\frac{2x_j-x_1-x_2}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{2x_j-x_0-x_2}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{2x_j-x_0-x_1}{(x_2-x_0)(x_2-x_1)} \\ &+ \frac{1}{6}f^{(3)}(\xi_j)\prod_{\substack{k=0\\k\neq i}}^{2}(x_i-x_k) \end{aligned}$$

where $\xi_i = \xi(x_i)$.

To derive the three-point endpoint formula we take $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$ for some $h > 0$ and we pick $x_i = x_0$. We obtain

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} + \frac{h^2}{3}f^{(3)}(\xi)$$

where $\xi \in (x_0, x_0+2h)$. To derive the three-point midpoint formula we take $x_1 = x_0 + h$ and $x_2 = x_0 - h$ for some $h > 0$ and we pick $x_i = x_0$. We obtain

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6}f^{(3)}(\xi)$$

where $\xi \in (x_0-h, x_0+h)$.

## 1.2 Degree of accuracy approach

Another method to find a finite difference approximation for a derivative of $f$ is based on making it exact for a class of polynomials. We introduce the notion of degree of accuracy to make the discussion easier. We will use $Df$ to denote the exact derivative of the function $f$ and $D_hf$ the approximate derivative of $f$.

**Definition 1.2.** *We say that $D_hf$ has degree of accuracy of $p$ if $p$ is the largest positive integer with $D(x^i) = D_h(x^i)$ for any $x$ and $i = 0, 1, \ldots, p$.*

**Exercise 1.2.** *Find $a$, $b$, $c$ so that the finite difference of the second derivative*

$$D_h^2 f(x_0) = af(x_0+h) + bf(x_0) + cf(x_0-h)$$

*has the highest degree of accuracy possible. State this degree.*

**Solution:** The idea is for the formula to be exact to the highest degree polynomial possible. Hence, taking $f(x) = 1$ we get

$$D_h^2 f(x_0) = D^2 f(x_0) \iff a + b + c = 0.$$

With $f(x) = x$ we obtain

$$\begin{aligned} D_h^2 f(x_0) = D^2 f(x_0) &\iff a\,(x_0 - h) + bx_0 + c(x_0 + h) = 0 \\ &\iff x_0(a + b + c) + h(-a + c) = 0 \\ &\implies -a + c = 0, \end{aligned}$$

where we used the first equation. Finally, for $f(x) = x^2$, we get

$$\begin{aligned} D_h^2 f(x_0) = D^2 f(x_0) &\iff a\,(x_0 - h)^2 + bx_0^2 + c(x_0 + h)^2 = 2 \\ &\iff (a + b + c)x_0^2 + 2x_0 h(-a + c) + h^2(a + c) = 2 \\ &\implies a + c = \frac{2}{h^2}, \end{aligned}$$

where we used the second equation. We thus have

$$\begin{cases} a + b + c = 0 \\ -a + c = 0 \\ a + c = \frac{2}{h^2} \end{cases} \iff \begin{cases} a = \frac{1}{h^2} \\ b = -\frac{2}{h^2} \\ c = \frac{1}{h^2} \end{cases}$$

We then have

$$D_h^2 f(x_0) = \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2}.$$

Take now $f(x) = x^3$. Then

$$D_h^2 f(x_0) = \frac{1}{h^2}(x_0 + h)^3 - \frac{2}{h^2}x_0^3 + \frac{1}{h^2}(x_0 - h)^3 = 6x_0 = D^2 f(x_0).$$

With $f(x) = x^4$ we get

$$D_h^2 f(x_0) = \frac{1}{h^2}(x_0 + h)^4 - \frac{2}{h^2}x_0^4 + \frac{1}{h^2}(x_0 - h)^4 = 2h^2 + 12x_0^2$$

and

$$D^2 f(x_0) = 12x_0^2.$$

Therefore the degree of accuracy is 3.

## 1.3 Error in finite difference formulas

We now discuss how to obtain formulas for the error of finite difference approximations. The idea is to use the Taylor expansion. The next exercise illustrates this.

**Exercise 1.3.** *Use the Taylor expansion to find a formula for the error of*

$$D_h^2 f(x_0) = \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2}.$$

**Solution:** The idea is to Taylor expand all the function evaluations of the finite difference formula. The Taylor expansion tells that

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x-x_0)^2}{2}f''(x_0) + \frac{(x-x_0)^3}{6}f'''(x_0) + \frac{(x-x_0)^4}{24}f^{(4)}(\xi(x))$$

where $\xi(x)$ is in between $x$, $x_0$. Taking $x = x_0 + h$ and $x = x_0 - h$ leads to

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f^{(4)}(\xi_+)$$

and

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f^{(4)}(\xi_-)$$

where $\xi_- \in (x_0 - h, x_0)$ and $\xi_+ \in (x_0, x_0 + h)$. Adding these equations, the terms with $f'(x_0)$ $f^{(4)}(x_0)$ cancel and we obtain

$$f(x_0 + h) + f(x_0 - h) = 2f(x_0) + h^2 f''(x_0) + \frac{h^4}{24}\left(f^{(4)}(\xi_+) + f^{(4)}(\xi_-)\right).$$

Therefore

$$D_h^2 f(x_0) = f''(x_0) + \frac{h^2}{24}\left(f^{(4)}(\xi_+) + f^{(4)}(\xi_-)\right).$$

By the Intermediate Value Theorem there is $\xi$ between $\xi_+$ and $\xi_-$ (and hence in $(x_0 - h, x_0 + h)$) such that

$$f^{(4)}(\xi) = \frac{\left(f^{(4)}(\xi_+) + f^{(4)}(\xi_-)\right)}{2}$$

since $\frac{\left(f^{(4)}(\xi_+)+f^{(4)}(\xi_-)\right)}{2}$ lies between $f^{(4)}(\xi_+)$ and $f^{(4)}(\xi_-)$. This allows us to write

$$D_h^2 f(x_0) = f''(x_0) + \frac{h^2}{12}f^{(4)}(\xi)$$

where $\xi \in (x_0 - h, x_0 + h)$. The error is then given by

$$error = f''(x_0) - D_h^2 f(x_0) = -\frac{h^2}{12}f^{(4)}(\xi)$$

where $\xi \in (x_0 - h, x_0 + h)$. Notice that the error term is proportional to $f^{(4)}$ which is consistent with $D_h^2 f$ having degree of accuracy 3.

# References


[1] R. L. Burden and J. D. Faires. *Numerical Analysis.* $9^{th}$ edition. Brookes/Cole, 2004.

[2] A. Quarteroni, R. Sacco and F. Saleri. *Numerical Mathematics.* $2^{nd}$ edition. Springer, 2006.

[3] Tutorial notes written by Jan Feys