Numerical Computations

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Overview

Our goal is to approximate the value of $f'(x)$ based on the given values of $f(x)$ at certain points.

Numerical differentiation

As we know the derivative of the function f at x_0 is:

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

Thus an obvious way to generate an approximation for $f'(x_0)$ is:

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

for small value of h. **It is not very successful due to round-off error**.

Approximation of $f'(x)$

To approximate $f'(x_0)$ suppose that $x_0 \in (a, b)$ and there exists $f''(x_0)$ on (a, b) .We construct the first Lagrange polynomial $P_1(x)$ for x_0 and $x_1 = x_0 + h$:

$$P_1(x) = \left(\frac{x - x_1}{x_0 - x_1}\right) f(x_0) + \left(\frac{x - x_0}{x_1 - x_0}\right) f(x_1)$$

$$= \left(\frac{x - x_0 - h}{-h}\right) f(x_0) + \left(\frac{x - x_0}{h}\right) f(x_0 + h)$$

Approximation of $f'(x)$ (cont.)

Thus:

$$f(x) = P_1(x) + \frac{(x-x_0)(x-x_1)}{2!} f''(\eta(x))$$

$$= \left(\frac{x-x_0-h}{-h}\right) f(x_0) + \left(\frac{x-x_0}{h}\right) f(x_0+h) + \frac{(x-x_0)(x-x_0-h)}{2!} f''(\eta(x))$$

for some $\eta(x)$ between x_0 and x_2.

Approximation of $f'(x)$ (cont.)

Thus:

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} + D_x\left[\frac{(x-x_0)(x-x_0-h)}{2!} f''(\eta(x))\right]$$

$$= \frac{f(x_0+h) - f(x_0)}{h} + \frac{2(x-x_0)-h}{2} f''(\eta(x)) + \frac{(x-x_0)(x-x_0-h)}{2!} D_x(f''(\eta(x)))$$

Approximation of $f'(x)$ (cont.)

So by deleting the terms involving $f''(\eta(x))$ (**round-off error**.) we obtain:

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

which may not be small enough.

Also, we have no information about $D_x(f''(\eta(x))$, so that when x is $x_0, D_x(f''(\eta(x)) = 0$. Thus:

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

Approximation of $f'(x)$ (cont.)

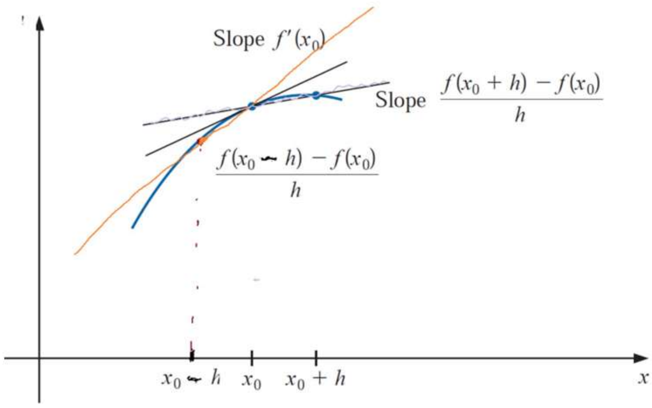
Assume M is a bound on $|f''(x)|$ for x between x_0 and $x_0 + h$ then for small values of h, $f'(x_0)$ can be approximated by

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

with an error bounded by $\frac{M|h|}{2}$.

This is called forward difference formula if $h > 0$ and the backward difference formula if $h < 0$.

Approximation of $f'(x)$ (cont.)



Approximation of $f'(x)$ (cont.)

Example. Approximate the derivative of $f(x) = lnx$ at $x_0 = 1.8$ where $h = 0.1, h = 0.05,$ and $h = 0.01$ by using the forward difference formula. Then determine bounds for the approximation errors.

Approximation of $f'(x)$ (cont.)

Solution. The forward-difference formula

$$\frac{f(1.8+h)-f(1.8)}{h}.$$

Let $h = 0.1$, thus

$$\frac{f(1.8+h)-f(1.8)}{h} = \frac{ln1.9 - ln1.8}{0.1}$$
$$= \frac{0.64185389 - 0.58778667}{0.1} = 0.5406722.$$

Since $f'' = \frac{-1}{x^2}$ and $1.8 < \eta < 1.9$, we have

$$\frac{|hf''(x)|}{2} = \frac{|h|}{2\eta^2} \leq \frac{0.1}{2(1.8)^2} = 0.0154321$$

Approximation of $f'(x)$ (cont.)

Approximation values and error bound for $h = 0.01$ and $h = 0.05$:

h	$f(1.8+h)$	$\frac{f(1.8+h)-f(1.8)}{h}$	$\frac{\lvert h\rvert}{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.0154321
0.05	0.61518564	0.5479795	0.0077160
0.01	0.59332685	0.5540180	0.0015432

Approximation of $f'(x)$ and $(n+1)$-point Formula

Now, suppose that the value of $f(x)$ are given at $n+1$ distinct points $x_0, x_1 \dots, x_n$ in an interval I and there exists $f^{n+1}(x)$ on I. By using Lagrange polynomial and its error, we have

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{(x-x_0)(x-x_1)\dots\cdot(x-x_n)}{(n+1)!} f^{n+1}(\eta(x))$$

for some $\eta(x) \in I$.

Approximation of $f'(x)$ and $(n+1)$-point Formula (cont'd)

Thus,

$$f'(x) = \sum_{k=0}^{n} f(x_k)L_k{}'(x)$$

$$+ D_x\left[\frac{(x-x_0)(x-x_1)\cdots(x-x_n)}{(n+1)!}\right] f^{n+1}(\eta(x))$$

$$+ \frac{(x-x_0)(x-x_1)\dots\cdot(x-x_n)}{(n+1)!} D_x[f^{n+1}(\eta(x))]$$

Approximation of $f'(x)$ and $(n+1)$-point Formula (cont'd)

Again we have a estimation problem with $D_x(f^{n+1}(\eta(x)))$ unless

we choose one of points $x_0, x_1 \dots, x_n$ in which the term

$D_x(f^{n+1}(\eta(x))) = 0$ and

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L_k'(x_j) + \frac{f^{(n+1)}\left(\eta(x_j)\right)}{(n+1)!} \prod_{k=0,k\neq j}^{n} (x_j - x_k)$$

The above formula is called an $(n+1)$-point formula to

approximate $f'(x_j)$.

Three-Point Formula

In this section we explain three point formulas and aspect of their errors. We have

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \to L_0{}'(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

Similarly:

$$L_1{}'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)},$$

$$L_2{}'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}$$

Three-Point Formula (cont.)

Thus we obtain for j=0,1,2

$$f'(x_j)=\frac{(2x_j-x_1-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0)+\frac{(2x_j-x_0-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1)+\frac{(2x_j-x_1-x_0)}{(x_2-x_0)(x_2-x_1)}f(x_2)+\frac{1}{6}f^3(x_j)\prod_{k=0 and k\neq J}^{2}(x_j-x_k)$$

Three-Point Formula (cont.)

Note that the notation y_j is dependent to x_j.

Now we suppose that the points are equally special that means $x_1=x_0$+h and $x_2=x_1$+h for some = $h\neq 0$.

By this assumption

$$f'(x_0)=\frac{1}{h}[-\frac{3}{2}f(x_0)+2f(x_1)-\frac{1}{2}f(x_2)]+\frac{h^2}{3}f^3(y_0)$$

$$f'(x_1)=\frac{1}{h}[-\frac{1}{2}f(x_0)+\frac{1}{2}f(x_2)]-\frac{h^2}{6}f^3(y_1)$$

$$f'(x_2)=\frac{1}{h}[\frac{1}{2}f(x_0)-2f(x_1)+\frac{3}{2}f(x_2)]+\frac{h^2}{3}f^3(y_2)$$

Three-Point Formula (cont.)

Thus:

$f'(x_0)=\frac{1}{2h}[-3f(x_0)+4f(x_0+h)-f(x_0+2h)]+\frac{h^2}{3}f^3(y_0)$

$f'(x_0+h)=\frac{1}{2h}[-f(x_0)+2f(x_0+2h)]-\frac{h^2}{6}f^3(y_1)$

$f'(x_0+2h)=\frac{1}{2h}[f(x_0)\text{-}4\,2f(x_0+h)+3f(x_0+2h)]+\frac{h^2}{3}f^3(y_2)$

The Similar Formula Based on Different Methods

As we remember we find to formulation for $f'(x_0)$ when we use the lagrange polynomial with first order called forward-difference formula (h>0) and backward difference formula (h<0) by the three above formulation we have similar situation when we use second order Lagrange polynomial

$f'(x_0)=\frac{1}{2h}[-3f(x_0)+4f(x_0+h)-f(x_0+2h)]+\frac{h^2}{3}f^3(y_0)$

$f'(x_0-h+h)=\frac{1}{2h}[-f(x_0-h)+2f(x_0+2h-h)]-\frac{h^2}{6}f^3(y_1)$

$f'(x_0+2h-2h)=\frac{1}{2h}[f(x_0-2h)\text{-}4\,2f(x_0+h-2h)+3f(x_0+2h-2h)]+\frac{h^2}{3}f^3(y_2)$

The Similar Formula Based on Different Methods (cont.)

Where

y_0 lies between x_0 and x_0+2h

y_1 lies between x_0-h and x_0+h

y_2 lies between x_0-2h and x_0

Three Point Endpoint / Midpoint Formula

The formulas

$$f'(x_0)= \frac{1}{2h}[-3f(x_0)+ 4f(x_0+h) - f(x_0+2h)]+ \frac{h^2}{3} f^3(y_0)$$

and

$$f'(x_0+h)= \frac{1}{2h}[-f(x_0)+ 2f(x_0+2h)]- \frac{h^2}{6} f^3(y_1)$$

Are called endpoint formula and midpoint formula respectively.

Three Point Endpoint / Midpoint Formula (cont.)

The error for both of them are O(h^2) although the error of midpoint is approximately half the error of end point this may be because midpoint formula uses data on both sides of x_0 while endpoint formula use data on only one side moreover is midpoint formula the evaluation is done based on only two points while in the endpoint formula, we need to have the data of three points, see the figure

Five Point Formula

Generally , two equations, endpoint and midpoint formulas are called three points with error O(h^2).

Similarly, there are five points formulas in which the data at two additional points are considered in evaluation and relevant error is O(h^4)

Five Point Midpoint Formula

$$f'(x_0)=\frac{1}{12h}[f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)]+\frac{h^4}{30}f^5(y)$$

Where y lies between x_0-2h and x_0+2h

Five Point Endpoint Formula

$$f'(x_0)=\frac{1}{12h}[-25f(x_0)+48f(x_0+h)-36f(x_0+2h)+16f(x_0+3h)-3f(x_0+4h)]+\frac{h^4}{5}f^{(5)}(x)$$

Where y lies between x_0 and x_0+4h

An Example

Value for $f(x) = xe^x$ are given as follows:

Table 4.2

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Use all applicable three-point and five-point formulas to approximate $f'(2.0)$.

Solution

The data in the table permit us to find four different three-point approximations.

We can use the endpoint formula with h=-.01, and we can use the midpoint formula with h=0.1 or with h=0.2.

Using the endpoint formula with h =0.1 gives

$\frac{1}{0.2}[-3f(2.0) + 4f(2.1) - f(2.2)] = 5[-3(14.778112) + 4(17.148957) - 19.855030]$
$= 22.032310$

And with h=-0.1 gives 22.054525.

Solution (cont.)

Using the midpoint formula with h=0.1 gives

$$\frac{1}{0.2}[f(2.1) - f(1.9)] = 5(17.148957 - 12.7703199)$$
$$= 22.228790$$

And with h=0.2 gives 22.414163.

The only five-point formula for which the table gives sufficient data is the midpoint formula with h=0.1. This gives

$$\frac{1}{1.2}[f(1.8) - 8f(1.9) + 8f(2.1) - f(2.2)] = \frac{1}{1.2}[10.889365 - 8(12.703199) + 8(17.148957) - 19.855030]$$
$$= 22.166999$$

Solution (cont.)

If we had no other information we would accept the five-point midpoint approximation using h=0.1 as the most accurate, and expect the true value to be between that approximation and the three-point midpoint approximation that is the interval [22.166,22.229].

Solution (cont.)

The true value in the case is
$f'(2.0) = (2+1)e^2 = 22.167168$, so the approximation errors are actually:

Three-point endpoint with h=0.1: 1.35×10^{-1};
Three-point endpoint with h=-0.1: 1.13×10^{-1};
Three-point midpoint with h=0.1: -6.16×10^{-2};
Three-point midpoint with h=0.2: -2.47×10^{-1};
Five-pint midpoint with h=0.1: 1.69×10^{-4}.

Solution (cont.)

Methods can also be derived to find approximation to higher derivatives of a function using only tabulated values of the function at various points. The derivation is algebraically tedious, however, so only a representative procedure will be presented.

Expand a function f in a third Taylor polynomial x_0 and evaluate at $x_0 + h$ and $x_0 - h$. Then

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\epsilon_1)h^4$$

And

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\epsilon_{-1})h^4$$

Where $x_0 - h < \epsilon_{-1} < x_0 < \epsilon_1 < x_0 + h$.

Solution (cont.)

If we add these equations, the terms involving $f'(x_0)$ and $-f'(x_0)$ cancel, so

$$f(x_0+h)+f(x_0-h)=2f(x_0)+f''(x_0)h^2+\frac{1}{24}[f^{(4)}(\epsilon_1)+f^{(4)}(\epsilon_{-1})]h^4.$$

Solving this equation for $f''(x_0)$ gives

$$f''(x_0)=\frac{1}{12}[f(x_0-h)-2f(x_0)+f(x_0+h)]-\frac{h^2}{24}[f^{(4)}(\epsilon_1)+f^{(4)}(\epsilon_{-1})]$$

Solution (cont.)

Suppose $f^{(4)}$ is continuous $[x_0-h, x_0+h]$.

Since $\frac{1}{2}[f^{(4)}(\epsilon_1)+f^{(4)}(\epsilon_{-1})]$ is between $f^{(4)}(\epsilon_1)$ and $f^{(4)}(\epsilon_{-1})$, the Intermediate Value Theorem implies that a number ϵ exists between ϵ_1 and ϵ_{-1}, and hence in (x_0-h, x_0+h), with

$$f^{(4)}(\epsilon)=\frac{1}{2}[f^{(4)}(\epsilon_1)+f^{(4)}(\epsilon_{-1})].$$

This permits us to rewrite the last equation in its final form.

ANY QUESTIONS?