Numerical Analysis MTH614

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Finite Difference method

Talyor series

Talyor series can provide useful polynomial approximation such as finite difference scheme, interpolations and so on.

• Taylor's Theorem in one variable

Let f(x) be a function with derivatives of all orders in some interval containing a as an interior point. Then

$$f(x) = f(a) + f'(a)(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \frac{f^n(x)}{n!}(x - a)^n + \frac{f^{n+1}(\xi)}{(n+1)!}(x - a)^{n+1}$$

Proof)

We start with the fundamental idea of calculus,

$$f(x_0 + h) = f(x_0) + \int_{x_0}^{x_0 + h} f'(\tau) \, d\tau \tag{1}$$

and we let $d\tau = -d(x_0 + h - \tau)$ (2)

Integrate by parts,

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \int_{x_0}^{x_0 + h} f''(\tau)(x_0 + h - \tau) d\tau$$
(3)

The last term is

$$\int_{x_0}^{x_0+h} f''(\tau)(x_0+h-\tau) d\tau = -\frac{1}{2} \int_{x_0}^{x_0+h} f''(\tau) d(x_0+h-\tau)^2 \tag{4}$$

$$=\frac{1}{2}f''(x_0)h^2 + \frac{1}{2}\int_{x_0}^{x_0+h} f'''(\tau)(x_0+h-\tau)^2\,d\tau \tag{5}$$

Together with the above equation, we have

$$f(x_0+h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{2}\int_{x_0}^{x_0+h} f'''(\tau)(x_0+h\tau)\,d\tau \tag{6}$$

For example, we compare with the first and second Taylor approximations using MATLAB.

If the function $f(x) = e^x + 1$ is evaluated at c = 0 with the Talyor approximation.

Linear equation : f(x) = 2 + x, Quadratic equation: $f(x) = 2 + x + x^2$.

The following is a MATLAB script.

The domain x of the function is equally spaced using "linspace". Plot command draws one line and curve with the same domain x.



• Taylor's Theorem in two variables

Now consider functions of two variables and a point (x_0, y_0) . We would like to derive a similar formula for an approximation of f by a polynomial near (x_0, y_0) . i.e. we approximate $f(x_0 + h, y_0 + k)$, where h and k both small real numbers.

Note that the last term is approximation error.

If we differentiate the function at (x_0, y_0) by the chain rule, then we get for the polynomial of order 2.

$$\begin{aligned} f(x_0 + h, y_0 + k) &= f(x_0, y_0) + \left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right) f(x_0, y_0) \\ &+ \frac{1}{2!} \left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^2 f(x_0, y_0) + \cdots \\ &+ \frac{1}{(n-1)!} \left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^{n-1} f(x_0, y_0) \\ &+ \frac{1}{n!} \left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^n f(x_0 + \theta h, y_0 + \theta k), \quad 0 < \theta < 1 \end{aligned}$$

For example, we compare with the first and second Taylor approximations in two variables. Having a function $f(x, y) = e^{x+y} + 1$, then we can differentiate at $(x_0, y_0) = (0, 0)$, as follows

$$f_x(x,y) = f_y(x,y) = e^{x+y}, f_{xx}(x,y) = f_{yy}(x,y) = f_{xy}(x,y) = e^{x+y},$$

$$f(0,0) = 2,$$

```
mesh(xx,yy,exp(xx+yy)+1)
hold on
mesh(xx,yy,2+xx+yy)
for i=1:20
  for j=1:20
    T(i,j)=2+x(i)+y(j)+0.5*(x(i)^2+2*x(i)*y(j)+y(j)^2);
  end
end
mesh(xx,yy,T)
```



Numerical Differentiation

The derivative of the function f(x) wit respect to the x.

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$
(1)

We define a "forward" difference

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} := D_h f(x)$$
(2)

where h is called the step size. And its error term is given as,

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(\xi) = D_h f(x) - \frac{h}{2}f''(\xi)$$
(3)

(4)

We also denote a "backward" difference approximation $D_h f(x) = \frac{f(x) - f(x - h)}{h}$ Centered difference approximation of the first derivative,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f^{(3)}(x) + O(h^4),$$
(1)

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f^{(3)}(x) + O(h^4).$$
⁽²⁾

We obtain that

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f^{(3)}(x) + O(h^4)$$
(3)

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

The Equation is called a "centered" finite difference representation,

$$D_h f(x) := \frac{f(x+h) - f(x-h)}{2h}$$
(5)

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

Note that the truncation error is of the order $h^2\,$ in contrast to the forward and backward approximation of the order of $\,h\,$.