MECH3750 PBL Content Summary

Week 1

Content:

- Taylor Series
- Finite Differences
- Newton's Method

Upcoming assessment:

- Problem Sheet 1 **not** submitted/assessed this week
- Quiz 1 (Week 3)

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1 Taylor Series

Taylor series expansions are used to represent any analytic function, $f(x)$, as a power series about a fixed point a,

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

where the last term is called the remainder, and $a < \zeta < x$. This makes the Taylor series exact.

It can also be written with higher order terms grouped:

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + H.O.T.$$

In this course, Taylor series are especially useful for:

1. obtaining simplified approximations to analytic functions near a point;
2. obtaining finite difference approximations; and
3. studying the error of finite difference approximations.

1.1 Multidimensional Taylor Series

For a two-dimensional function $f(x, y)$, the Taylor series about the point (a, b) is:

$$\begin{aligned} f(x,y) = f(a,b) + f_x(a,b)(x-a) + f_y(a,b)(y-b) + \\ \frac{1}{2}\left[f_{xx}(a,b)(x-a)^2 + 2f_{xy}(a,b)(x-a)(y-b) + f_{yy}(a,b)(y-b)^2\right] + H.O.T \end{aligned}$$

Recall f_x and f_{xx} are shorthand notation for the first and second derivatives, respectively.

2 Finite Differences

Finite difference approximations are used to approximate derivatives of complex functions to which no analytical solution exists.

The 2nd part of the course exclusively applies these approximations to solve PDEs.

2.1 First derivatives

An approximation to the first derivative at a point x can be obtained by considering a finite step h. This step can be taken above, below, or to both sides of x to calculate the gradient, yielding the following common finite difference formulas.

Forward difference (1st order accurate):

$$u'(x) \approx \frac{u(x+h) - u(x)}{h}$$

Backward difference (1st order accurate):

$$u'(x) \approx \frac{u(x) - u(x-h)}{h}$$

Central difference (2nd order accurate):

$$u'(x) \approx \frac{u(x+h) - u(x-h)}{2h}$$

Other approximations can be obtained using the method of undetermined coefficients.

2.2 Second derivatives

The common second derivative central difference approximation (2nd order accurate) can be obtained using finite difference approximations of the first derivative.

$$u''(x) \approx \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

Taylor series can also be used to obtain the central difference approximation as well as higher order approximations, by taking an expansion of a function's value at $(x+h)$, $(x-h)$, $(x+2h)$, $(x+2h)$, and so on, about a point x, and performing algebraic manipulation of the resulting series.

3 Newton's Method

Newton's method is an iterative approach to solving systems of non-linear functions.

3.1 Single-variable

Consider a single-variable function, which we want to find the roots of:

$$f(x) = 0$$

Taking a linear Taylor series approximation (where $x^{(0)}$ is our first guess):

$$f(x^{(0)} + h) \approx f(x^{(0)}) + f'(x^{(0)})h$$

Letting the next approximate solution $x^{(1)} = x^{(0)} + h$ be a root, i.e., $f(x^{(0)} + h) = 0$, we obtain:

$$f'(x^{(0)})h = -f(x^{(0)})$$

$$h = -\frac{f(x^{(0)})}{f'(x^{(0)})}$$

Therefore, our updated approximate solution is:

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

Repeat iteration of the above update rule until $f(x^{(n)}) \approx 0$.

3.2 Multi-variable

For sets of equations with multiple variables $\mathbf{x} = (x_1, x_2, x_3, ...)$,

$$\boldsymbol{f}(\boldsymbol{x}) = 0$$

$$\boldsymbol{f}'(\boldsymbol{x}) = \nabla \boldsymbol{f}'(\boldsymbol{x}) = J$$

where,

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ \vdots \\ f_m(\mathbf{x}) \end{bmatrix}$$

and J is the Jacobian:

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots \\ \frac{\partial f_2}{\partial x_1} & \ddots & \vdots \\ \vdots & \cdots & \frac{\partial f_m}{\partial x_m} \end{bmatrix}$$

We then obtain the formula:

$$\mathbf{f}(\mathbf{x}^{(n)} + \mathbf{h}) \approx \mathbf{f}(\mathbf{x}^{(n)}) + J\mathbf{h}$$

from which the general update rule is:

$$\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} - J^{-1}\mathbf{f}(\mathbf{x}^{(n)})$$