MECH70045

Advanced Numerical Methods for Engineers

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Mathematical Preliminaries and Error Analysis

Review of important results from calculus, round off errors and computer arithmetic, algorithms, and convergence.

Geometry and Mesh Generation

Geometric modelling of surfaces and volumes, structured and unstructured mesh methods such as algebraic mesh generation, PDE approaches, multiblock and Delaunay/Advancing front algorithms.

Linear Algebra and Algebraic Matrix Solvers

Review of linear algebra, direct and iterative matrix solution algorithms including eigenvalue solvers (e.g., power iteration). This will focus on both symmetric and non-symmetric methods as well as storage schemes (e.g., compressed row storage – CRS, compressed column storage, block storage etc). Methods will encompass conjugate gradient (CG) solvers, bi-conjugate gradient (BCG), pre-conditioners (e.g., Gauss-Seidel, SSOR, ILU, multigrid) and Krylov subspace methods for non-symmetric solvers (e.g., GMRES).

Ordinary Differential Equations

Review of numerical methods for boundary value and initial value problems (e.g., Euler methods, Runge-Kutta, stiff ODES, systems of ODEs). There will be a focus on applications of the methods to practical problems involving coupled systems of ODES. This differentiates from the second-year course due to the focus on practical problems.

Partial Differential Equations

Numerical methods for boundary value problems and initial values problems. Spatial discretisation methods will encompass finite difference (FD), finite volume (FV), finite element (FE), spectral element (SE) and isogeometric analysis (IGA) methods for elliptic, parabolic, and hyperbolic PDEs. Emphasis will be placed upon the relationship between the different methods using the genera weighted residual method for general elliptic, parabolic and hyperbolic PDEs (e.g., point collocation, subdomain collocation, Bubnov-Galerkin, Petrov-Galerkin, discontinuous Galerkin schemes) and how they are related to variational schemes for certain classes of PDEs such as elliptic PDEs. Also discussed will be the properties of the schemes (e.g., convergence, consistency, stability and verification and validation using techniques such as the method of manufactured solutions). Examples will be taken from heat transfer, radiation transport and fluid mechanics. Initial value PDE problems will use theta time-discretisation methods (i.e., Euler and Crank-Nicholson).

Random Examples

Definition 5.0.1: Limit of Sequence in \mathbb{R}

Let $\{s_n\}$ be a sequence in \mathbb{R} . We say

$$\lim_{n\to\infty}s_n=s$$

where $s \in \mathbb{R}$ if \forall real numbers $\varepsilon > 0$ \exists natural number N such that for n > N

$$s - \epsilon < s_n < s + \epsilon \text{ i.e. } |s - s_n| < \epsilon$$

Question 1

Is the set x-axis \Origin a closed set

Solution: We have to take its complement and check whether that set is a open set i.e. if it is a union of open balls

Note:-

We will do topology in Normed Linear Space (Mainly \mathbb{R}^n and occasionally \mathbb{C}^n)using the language of Metric Space

Claim 5.0.1 Topology

Topology is cool

Example 5.0.1 (Open Set and Close Set)

Open Set: $\bullet \phi$

• $_{x \in X} B_r(x)$ (Any r > 0 will do)

• $B_r(x)$ is open

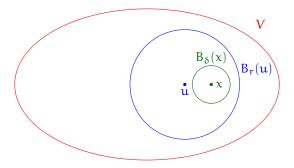
Closed Set: • X, φ

 $\bullet \frac{X, \ \varphi}{B_{r}(x)}$

x-axis $\cup y$ -axis

Theorem 5.0.1

If $x \in \text{open set } V \text{ then } \exists \ \delta > 0 \text{ such that } B_{\delta}(x) \subset V$



Given $x \in B_r(u) \subset V$, we want $\delta > 0$ such that $x \in B_\delta(x) \subset B_r(u) \subset V$. Let d = d(u,x). Choose δ such that $d + \delta < r$ (e.g. $\delta < \frac{r-d}{2}$)

If $y \in B_{\delta}(x)$ we will be done by showing that d(u, y) < r but

$$d(u,y) \leqslant d(u,x) + d(x,y) < d + \delta < r$$

(3)

Corollary 5.0.1

By the result of the proof, we can then show...

Lenma 5.0.1

Suppose $v_1, ..., v_n \in \mathbb{R}^n$ is subspace of \mathbb{R}^n .

Proposition 5.0.1

1 + 1 = 2.

Random

Definition 5.0.2: Normed Linear Space and Norm || · ||

Let V be a vector space over \mathbb{R} (or C). A norm on V is function $\|\cdot\| V \to \mathbb{R}_{\geqslant 0}$ satisfying

- $(1) ||x|| = 0 \iff x = 0 \ \forall \ x \in V$
- ② $\|\lambda x\| = |\lambda| \|x\| \ \forall \ \lambda \in \mathbb{R} (\text{or } \mathbb{C}), \ x \in V$
- (3) $||x+y|| \le ||x|| + ||y|| \ \forall \ x,y \in V$ (Triangle Inequality/Subadditivity)

And V is called a normed linear space.

• Same definition works with V a vector space over $\mathbb C$ (again $\|\cdot\| \to \mathbb R_{\geqslant 0}$) where ② becomes $\|\lambda x\| = |\lambda| \|x\|$ $\forall \ \lambda \in \mathbb C$, $x \in V$, where for $\lambda = \alpha + \mathrm{i} b$, $|\lambda| = \sqrt{\alpha^2 + b^2}$

Example 5.0.2 (p-Norm)

 $V = \mathbb{R}^m$, $p \in \mathbb{R}_{\geq 0}$. Define for $x = (x_1, x_2, \dots, x_m) \in \mathbb{R}^m$

$$\|x\|_p = (|x_1|^p + |x_2|^p + \dots + |x_m|^p)^{\frac{1}{p}}$$

(In school p = 2)

Special Case p = 1: $||x||_1 = |x_1| + |x_2| + \cdots + |x_m|$ is clearly a norm by usual triangle inequality.

 $\textbf{Special Case p} \rightarrow \infty \ (\mathbb{R}^m \ \textbf{with} \ \| \cdot \|_{\infty}) \colon \|x\|_{\infty} = max\{|x_1|,|x_2|,\cdots,|x_m|\}$ For m = 1 these p-norms are nothing but |x|. Now exercise

Question 2

Prove that triangle inequality is true if $p \ge 1$ for p—norms. (What goes wrong for p < 1?)

Solution: For Property (3) for norm-2

When field is \mathbb{R} :

We have to show

$$_{i}(x_{i}+y_{i})^{2} \leq \left(\sqrt{_{i}}x_{i}^{2}+\sqrt{_{i}}y_{i}^{2}\right)^{2}$$

$$\Longrightarrow _{i}(x_{i}^{2}+2x_{i}y_{i}+y_{i}^{2}) \leq _{i}x_{i}^{2}+2\sqrt{\left[_{i}x_{i}^{2}\right]\left[_{i}y_{i}^{2}\right]}+_{i}y_{i}^{2}$$

$$\Longrightarrow \left[_{i}x_{i}y_{i}\right]^{2} \leq \left[_{i}x_{i}^{2}\right]\left[_{i}y_{i}^{2}\right]$$

So in other words prove $\langle x, y \rangle^2 \le \langle x, x \rangle \langle y, y \rangle$ where

$$\langle x, y \rangle = x_i y_i$$

- Note:- $\|x\|^2 = \langle x, x \rangle$
- $\langle x, y \rangle = \langle y, x \rangle$
- $\langle \cdot, \cdot \rangle$ is \mathbb{R} —linear in each slot i.e.

 $\langle rx + x', y \rangle = r \langle x, y \rangle + \langle x', y \rangle$ and similarly for second slot

Here in $\langle x, y \rangle$ x is in first slot and y is in second slot.

Now the statement is just the Cauchy-Schwartz Inequality. For proof

$$\langle x, y \rangle^2 \le \langle x, x \rangle \langle y, y \rangle$$

expand everything of $\langle x - \lambda y, x - \lambda y \rangle$ which is going to give a quadratic equation in variable λ

$$\begin{split} \langle x - \lambda y, x - \lambda y \rangle &= \langle x, x - \lambda y \rangle - \lambda \langle y, x - \lambda y \rangle \\ &= \langle x, x \rangle - \lambda \langle x, y \rangle - \lambda \langle y, x \rangle + \lambda^2 \langle y, y \rangle \\ &= \langle x, x \rangle - 2\lambda \langle x, y \rangle + \lambda^2 \langle y, y \rangle \end{split}$$

Now unless $x = \lambda y$ we have $\langle x - \lambda y, x - \lambda y \rangle > 0$ Hence the quadratic equation has no root therefore the discriminant is greater than zero.

When field is \mathbb{C} :

Modify the definition by

$$\langle x, y \rangle = \overline{x_i} \overline{y_i}$$

Then we still have $\langle x, x \rangle \ge 0$

Algorithms

```
Algorithm 1: what
   Input: This is some input
   Output: This is some output
   /* This is a comment */
 1 some code here;
_{2} \chi\leftarrow0;
 y \leftarrow 0;
 4 if x > 5 then
 5 | x is greater than 5;
                                                                                         // This is also a comment
 _7 x is less than or equal to 5;
8 end
9 foreach y in 0..5 do
10 y \leftarrow y + 1;
11 end
12 for y in 0..5 do
13 y \leftarrow y - 1;
14 end
15 while x > 5 do
16 x \leftarrow x - 1;
17 end
18 return Return something here;
```