Advanced Numerical Analysis - Web course

COURSE OUTLINE

This course on Numerical Analysis has been designed with the following learning objectives in mind

- Clearly bring out role of approximation theory in the process of developing a *numerical recipe* for solving an engineering problem
- Introduce geometric ideas associated with the development of numerical schemes
- Familiarize the student with ideas of convergence analysis of numerical methods and other analytical aspects associated with numerical computation

It is shown that majority of problems can be converted to computable forms (discretized) using three fundamental ideas in the approximation theory, namely Taylor series expansion, polynomial interpolation and least square approximation. In addition, the student is expected to clearly understand role of the following four fundamental tools

- Linear Algebraic Equation
- Nonlinear Algebraic Equations
- Ordinary Differential Equations- Initial Value Problem
- Optimization

which are most often used for creating a *numerical recipe* tocompute numerical solutions.

COURSE DETAIL

Lecture	**Contents**	
(*1 hr*)	(*Sections from a module, which are relevant for each lecture, are indicated in the last column*)	
	Module 1: Equation Forms in Process Modeling	**Sections**
1	Introduction and Motivation, Linear and Nonlinear Algebraic Equation	1,2.12.2
2	Optimization based Formulations, ODE-IVPs and Differential Algebraic Equations	2.3,2.4, 3
3	ODE-BVPs and PDEs	4
4	ODE-BVPs and PDEs, Abstract model forms	4,5
	Module 2: Fundamentals of Vector Spaces	**Sections**
5	Generalized concepts of vector space, sub-space, linear dependence	1,2
6	Concept of basis, dimension, norms defined on general vector spaces	2
7	Examples of norms defined on different vector spaces, Cauchy sequence and convergence, introduction to concept of completeness and Banach spaces	3

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Chemical Engineering

Pre-requisites:

- Basic courses on Engineering Mathematics covering fundamentals of calculus, linear algebra and ordinary differential equations
- Familiarity with mathematical models used in engineering problems

Additional Reading:

- Linz, P.; *Theoretical Numerical Analysis*, Dover, New York, (1979).
- Gilbert Strang , *Introduction to Applied Mathematics*, Wellesley Cambridge Press (2009)

Hyperlinks:

(Provide Link to NPTEL Lecture course on Advanced Numerical Analysis by Prof. Sachin Patwardhan)

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8	Inner product in a general vector space, Inner-product spaces and their examples,	4
9	Cauchy-Schwartz inequality and orthogonal sets	4
10	Gram-Schmidt process and generation of orthogonal basis, well known orthogonal basis	5
11	Matrix norms	6
	Module 3: Problem Discretization Using Approximation Theory	**Sections**
12	Transformations and unified view of problems through the concept of transformations, classification of problems in numerical analysis, Problem discretization using approximation theory	1,2
13	Weierstrass theorem and polynomial approximations, Taylor series approximation	2, 3.1
14	Finite difference method for solving ODE-BVPs with examples	3.2
15	Finite difference method for solving PDEs with examples	3.3
16	Newton's Method for solving nonlinear algebraic equation as an application of multivariable Taylor series, Introduction to polynomial interpolation	3.4
17	Polynomial and function interpolations, Orthogonal Collocations method for solving ODE-BVPs	4.1,4.2,4.3
18	Orthogonal Collocations method for solving ODE-BVPs with examples	4.4
19	Orthogonal Collocations method for solving PDEs with examples	4.5
20	Necessary and sufficient conditions for unconstrained multivariate optimization, Least square approximations	8
21	Formulation and derivation of weighted linear least square estimation, Geormtraic interpretation of least squares	5.1,5.2
22	Projections and least square solution, Function approximations and normal equation in any inner product space	5.3
23	Model Parameter Estimation using linear least squares method, Gauss Newton Method	5.4
24	Method of least squares for solving ODE-BVP	5.5
	Gelarkin's method and generic equation forms arising in problem	

25	discretization	5.5
26	Errors in Discretization, Generaic equation forms in transformed problems	6,7
	Module 4: Solving Linear Algebraic Equations	**Sections**
27	System of linear algebraic equations, conditions for existence of solution - geometric interpretations (row picture and column picture), review of concepts of rank and fundamental theorem of linear algebra	1,2
28	Classification of solution approaches as direct and iterative, review of Gaussian elimination	3
29	Introduction to methods for solving sparse linear systems: Thomas algorithm for tridiagonal and block tridiagonal matrices	4
30	Block-diagonal, triangular and block-triangular systems, solution by matrix decomposition	4
31	Iterative methods: Derivation of Jacobi, Gauss-Siedel and successive over-relaxation methods	5.1
32	Convergence of iterative solution schemes: analysis of asymptotic behavior of linear difference equations using eigen values	9
33	Convergence of iterative solution schemes with examples	5.2
34	Convergence of iterative solution schemes, Optimization based solution of linear algebraic equations	
35	Matrix conditioning, examples of well conditioned and ill-conditioned linear systems	7
	Module 5: Solving Nonlinear Algebraic Equations	**Sections**
36	Method of successive substitutions derivative free iterative solution approaches	1,2
37	Secant method, regula falsi method and Wegsteine iterations	3.1,3.2
38	Modified Newton’s method and qausi-Newton method with Broyden’s update	3.3, 3.4, 3.5
39	Optimization based formulations and Leverberg-Marquardt method	4
40	*Contraction mapping principle and introduction to convergence analysis* (*Optional lecture*)	6

	Module 6: Solving Ordinary Differential Equations – Initial Value Problems (ODE-IVPs)	Sections
39	Introduction, Existence of Solutions (optional topic),	
40	Analytical Solutions of Linear ODE-IVPs	3
41	Analytical Solutions of Linear ODE-IVPs (contd.), Basic concepts in numerical solutions of ODE-IVP: step size and marching, concept of implicit and explicit methods	4
42	Taylor series based and Runge-Kutta methods: derivation and examples	5
43	Runge-Kutta methods	5
44	Multi-step (predictor-corrector) approaches: derivations and examples	6.1
45	Multi-step (predictor-corrector) approaches: derivations and examples	6.1
46	Stability of ODE-IVP solvers, choice of step size and stability envelopes	7.1,7.2
47	Stability of ODE-IVP solvers (contd.), stiffness and variable step size implementation	7.3,7.4
48	Introduction to solution methods for differential algebraic equations (DAEs)	8
49	Single shooting method for solving ODE-BVPs	9
50	Review	

References:

- Gilbert Strang, *Linear Algebra and Its Applications* (*4th Ed.*), Wellesley Cambridge Press (2009).
- Philips, G. M.,Taylor, P. J. ; Theory and Applications of Numerical Analysis (2nd Ed.), Academic Press, 1996.
- Gourdin, A. and M Boumhrat; Applied Numerical Methods. Prentice Hall India, New Delhi, (2000).
- Gupta, S. K.; Numerical Methods for Engineers. Wiley Eastern, New Delhi, 1995.