Syllabus for M. Phil in (Futures Studies) as per 2016 UGC regulations:

Eligibility/Qualification :

Candidates for admission to the M.Phil. course in Futures Studies shall possess Masters degree in Applied Sciences and Technology/Science/Engineering/Applied Sciences/Engineering and Technology. There will be a total intake of 8 students according to the UGC 2016 regulations. Selection Procedure Eligible applicant for admission shall be required to take an entrance test covering objective type questions.

Course Structure:

The course structure will be as follows.

Semester I : Course work. (6 months)

Semester II : Dissertation (6 months)

Two core courses and one elective. The core courses are I:

Paper I: Interdisciplinary Research & Research Methodology (4 Credits)

Paper II: Scientific Computing and Forecasting (4 Credits)

Paper III: Elective. (4 Credits)

Semester II : Dissertation (20 credits)

Core Courses

Paper I : FUS 711: Interdisciplinary Research & Research Methodology

Unit I: Survey of Research Methodologies- Rationalism, Idealism, Positivism, Post Positivism, Introduction to major binaries, Subjectivity vs Objectivity, Realism vs Anti –realism, True vs False, Scientific evolution vs Scientific Revolutions, Continuity vs Discontinuity, Deterministic vs Probabilistic, Linearity vs Non –Linearity, Beyond the binaries

Unit II: Methods: Epistemology, Ontology, Deduction, Induction, Hypothetical Deductive method, Explanation and Prediction, General and Particular, Cause and Effect.

Unit III: History and Philosophy of science, Scientific revolutions, Paradigms, Against Method, Epistemic shift.

Unit IV: Techniques-Quantitative Techniques, Techniques of generating data, Techniques of classification, Techniques of measures, Central Tendency and Dispersion, Measures of

Correspondence/Correlation, Measures of Causal relations/Regression , Techniques of Explanation ANOVA, Time Series Analyis-ARMA, Adaptive Estimation Procedures (Kalman Filters) Techniques of inference , Qualitative – Delphi , PRA , RRA etc.

Unit V: Advanced Techniques- Advanced Statistical Methods for data Analysis, Structural, quantitative, or statistical approaches for the analysis of data, Advances in classification, clustering and pattern recognition methods, Strategies for modeling complex data and mining large data sets, Chaos analysis and its measurement, Methods for the extraction of knowledge from whatever type of data, and Application of advanced methods in specific domains of practice.

UnitVI: Futures Research: Introduction to Futures Research, Interdisciplinary/Multidisciplinary Research, Systems Analysis, Methods/techniques of Futures Research

Recommended Reading and References:

Abraham Kaplan, 1964, Conduct of Inquiry, Chander Publishing Company, California. Ann Majchrzak, 1984, Methods for Policy Research, Sage London Carl G Hempel "The Covering Law Analysis of Scientific Explanation" in Leonard I Krimerman (ed) Catheriner Marsh, 1988, Exploring Data, Polity Press, Cambridge Cohen and Ernest Nagel (ed) 1978, An Introduction to Logic and Scientific Method, Allied, New Delhi Jean-Francois Lyotard, 1986, The Post Modern Condition: A Report on Knowledge, The Manchester University Press, Manchester John Brewer and Albewrt Hunter, Multimethod Research: A synthesis of Styles, Sage Publications, London. John Hughes, 1990, The Philosophy of Social Research, Longman, London Karl R Popper, "The Hypothetical – Deductive Method and the Unity of Social and Natural Science", in Leonard I Krimerman (ed) Keith Lehrer, 1990, Theory of Knowledge, Routledge, London Leonard I Krimerman (ed) The Nature and Scope of Social Science, Apple-Century –Croafts, New York Margolis J Kransz, and Burian R M, (EDS) 1986, Rationality, Relativism and Human Sciences, Nijhoff Publications, Dordrecht. Partha Nath Mukherji, 1998, Methodology in Social Research, Sage, New Delhi Paul Feverabend, 1984, Against Method, Verso, London Pauline V Young, 1988, Scientific Social Survey Research, Mcgraw-Hill Book Company, New York Peter Clough and Cathy Nutbrown, 2002, A Students Guide to Methodology, Sage Publications, London Thomas S Khun, 1970, The Structure of Scientific Revolution, University of Chicago Press, Chicago Olaf Helmer, Looking Forward, Sage, 1979

Paper II: FUS 712: (Scientific Computing and Forecasting)

Introduction to systems modelling: Theoretical *vs.* computational modellingStages of computational modelling, Abstraction of idea – properties of models, Importance of virtual experiments in science and technology.

Numerical methods for scientific computing - Solution of Linear Algebraic Equations,

Interpolation and Extrapolation, Random Number generation, Linear and Nonlinear curve fitting of Data, solution of ODEs and PDEs, Fast Fourier Transform. Programming of these methods using Fortran and C.

Time Series Analysis & Forecasting- Identification, Estimation and Diagnostic Techniques for ARMA and ARIMA Models. Seasonal ARIMA models. Exponential smoothing and ARIMA models. Introduction to spectral anlysis. Transfer function models. State Space models and Kalman filters. Design of Feed Forward and Feed backward Control Schemes.

Introduction to computer algebra systems - Matlab, Scilab and SAGE, Neural networks, Genetic algorithm, Cellular automata and R

References:

Gaston H. Gonnet, Ralf Scholl, Scientific Computation, Cambridge University Press, 2009

Eric F. Van de Velde, Concurrent scientific computing, Springer, 1994

William H. Press, Numerical recipes: The art of scientific computing, Cambridge University Press, 2007

Dietmar P. F. Moeller, Mathematical and computational modeling and simulation: Fundamentals and Case Studies, Springer, 2004

Charles S. Taber, Richard J. Timpone, Computational modeling, SAGE, 1996.

Bovas, A. and Johannes, L (1983), Statistical Methods for Forecasting, John wiley, New York.

Box G.E.P. and Jenkins, G.M. (1976), Time Series Analysis Forecasting and Control, san Francisco.

Paper III: Elective Courses (One elective to be chosen among the list)

List of Electives

Elective 1: FUS 713: Technological Futures, Forecasting and Assessment

The rapidly changing technological scene and the need for competitiveness and economic growth/ development – Role of technology forecasting in development planning - Technology forecasting as a tool for corporate strategy - Technology forecasting as a tool for social strategy - Stage of innovation - Methodologies of Technology forecasting and Futures Problem solving-Computer modelling techniques - Sensitivity analysis for models - Features of technology assessment - Objectives of technology assessment - Distinction between technology assessment and environment impact analysis - Types of technology assessment / environment impact analysis - technology assessment as a map for alternate futures - components of technology assessment - the technology delivery systems - social impact analysis - Limitations of technology forecasts and assessment - case studies of technology forecast and assessment. Future

technological options - environmental friendly technologies - appropriate technology - case studies of technological futures: bio technology, information technology, Nano Science and technology, Bio-Informatics, Energy technology options (source wise) – R and D in technology development

References:

Technological Forecasting for Decision Making, Joseph Martino, Tata McGraw-Hill

Forecasting Technological Innovation. B. Henry, Kluwer

Forecasting & Management of Technology -Alan.L.Porter, Wiley Series

Technology in Context: Technology Assessment for Managers (Management of Technology and Innovation), Ernest Braun, Rutledge

Perspectives on technology assessment- Sherry R. Arnstein, Alexander N. Christakis, Science and Technology Publishers

Elective 2: FUS 714 :Computational Chemistry

Introduction to quantum mechanics, Schrodinger Equation, Quantum mechanics applied to simple problems such as particle in a 1D box, harmonic oscillator, rigid rotor, hydrogen atom solutions, multi-electron systems

Building molecules (3D structures), Stereochemistry, Molecular Symmetry

Empirical and semi-empirical molecular orbital theory : Qualitative and Qualitative MO theory, Hückel method, Semi empirical methods such as AM1, MNDO etc.

Basic ab initio quantum chemistry : Ab initio and semi-empirical methods, Introductory DFT, Basis set, hybrid calculations

Molecular Mechanics and Dynamics : Molecular Potential Energy Functions, Molecular Mechanics, Molecular Mechanics Force Field, Optimisation, Selecting force field, Parameters and other problems with Molecular Mechanics, Molecular Dynamics, Simulated Annealling, Monte Carlo Simulations

References:

Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, John Wiley and Sons, 2004 Errol G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Springer, 2003 David C. Young, Computational chemistry: a practical guide for applying techniques to real world problems John Wiley and Sons, 2001

Elective 3: FUS 715 : Molecular Modeling and Molecular dynamics

Computational Chemistry . concepts of computational chemistry-Born-Oppenheimer approximations, Application of Hartree-Fock equations to molecular systems, approximate molecular orbital theories, semi-emperical methods. Macro-molecular force fields, salvation , long range forces.

Molecular Mechanics: general features, bond stretching, angle bending, improper torsions, out of plane bending, cross terms, non-bonded interactions, Ramachandran diagram point charges, calculation of atomic charges, polarization, van der waals interactions, hydrogen bond interactions, Water models, Force field, all atoms force field and united atom force field.

Energy minimization: Steepest descent, conjugate gradient – Derivatives, First order steepest decent and conjugate gradients. Second order derivatives Newton-Raphson, Minima, maxima saddle points and convergence criteria.-non derivatives minimization methods, the simplex, sequential univariate.

Simulation methods : Newton's equation of motion, equilibrium point, radial distribution function, pair correlation functions, MD methodology, periodic box, Solvent access, Equilibration, cutoffs, algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzmann velocity, time steps, duration of the MD run, Starting structure, analysis of MD job, uses in drug designing, ligand protein interactions. Various methods of MD, Monte Carlo, systematic and random search methods.

Differences between MD and MC, Energy, Pressure, Temperature, Temperature dynamics ,simulation softwares. Various methods of MD, Monte Carlo, systematic and random search methods.

Docking and Drug design : Discovery and design of new drugs, computer representation of molecules, 3d database searching, conformation searches, derving and using the 3d Pharmacophore,- keys constrained systematic search, clique detection techniques, maximum likelihood method, molecular docking, scoring functions, structure based de novo Ligand design, quantitiative structure activity relationship QSAR, QSPRs methodology, various descriptors quantum chemical . use of genetic algorithms, Neural Network and Principle components analysis in QSAR equations. Combinatorial libraries, design of "Drug like" libraries.

References :

Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.

Fenniri, H. "Combinatorial Chemistry – A practical approach", (2000) Oxford University Press, UK.

Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.

Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

Elective 4: FUS 716 :Optimization Techniques

Review- Sets and Sequences in \mathbb{R}^n Sequences and Limites, Subsequences and Limit Points, Cauchy Sequences and Completeness, Suprema, Infima, Maxima, Minima, Monotone Sequence in \mathbb{R} , The Lim Sup and Lim Inf, Open Balls, Open Sets, Closed sets, Bounded sets and Compact Sets, Convex Combinations and Convex Sets, Unions, Intersections and other binary operations, Matrices, Functions, Quadratic forms, Separation Theorems, The intermediate and Mean value theorems, The inverse and implicit function theorems

Optimization problems in R^n , Optimization problems in parametric form, Examples of optimization problems – Utility maximization, expenditure minimization, profit maximization, cost minimization, consumption-leisure choice, portfolio choice, Objectives of optimization theory

Existence of Solutions, The Weierstrass Theorem, Unconstrained Optima

Equality Constraints and the Theorem of Lagrange, Second order conditions, Inequality Constraints and the Theorem of Kuhn and Tucker, Convex Structures in Optimization Theory, Concave and Convex functions, Implications of convexity, Convexity and optimization,

Quasi – Convexity and Optimization, Quasi-convexity as generalization of convexity, Parametric continuity: The maximum theorem, The maximum theorem under convexity, Finite - Horizon Dynamic Programming, Stationary Discounted Dynamic Programming.

Numerical Optimization Techniques- Unconstrained multi-parameter optimisation techniques, Nelder-Mead's sequential simplex method, Powell's conjugate directions method, Fletcher-Reeves' Conjugate Gradient method, Newton's Method, Quasi-Newton Method.

References:

R. K. Sundaram, A First Course in Optimization Theory, Cambridge Uni. Press, 1996.

- C. Mohan , Kusum Deep, Optimization Techniques, New Age Science, 2009
- T. Back, Evolutionary Algorithms in Theory and Practice, Oxford Uni. Press, New York, 1995

D. E. Goldberg, Genetic Algorithms in Search Optimization and Machine Learning, Addison-Wesley, 1989.

J. Nocedal, and S. J. Wright, Numerical Optimization, Springer, 1999.

U. M. Diwekar, Introduction to Applied Optimization, Kluwer Academic Publishers, 2003

Elective 5: FUS 717 : Nonlinear Dynamics and Chaos

Review – Chaos, Fractals and Dynamics, Brief History of Dynamics, One dimensional flows, Fixed points and stability, Bifurcations, Flows on a circle Two dimensional flows, Linear systems, Phase Plane, Limit cycles, Bifurcations Chaos, One dimensional Maps – Fixed points and cobwebs, logistic map, Fractals, cantor set, different dimensions, Strange attractors, Nonlinear time series analysis

References:

Steven H. Stogatz, Nonlinear dynamics and chaos – with applications to Physics, Biology, Chemistry and Engineering., Perseus Books Publishing, 1994

James Gleick, chaos – making of a new science, Penguin, 1987

Katheleen T. Alligood, Tim D. Sauer, james A. Yorke, Chaos: an introduction to dynamical systems, Springer, 1996

Richard Kautz, chaos: The science of predictable random motion, Oxford university press, 2011 Holger Kantz, Thomas Schreiber, Nonlinear Time Series Analysis, Cambridge University Press, 2004

Elective 6: FUS 718: Computational Physics

Introduction to Computational Physics, Classical Physics and statistical mechanics, Stochastic simulations, elctrodynamics and hydrodynamics, Quatom mechanics, Relations between quantum mechanics and classical statistical mechanics

Quantum scattering with spherically symmetric potential, calculations of scattering cross sections

The variational method for the Schrodinger equation, variational calculus, examples of variational calculations, solution of the generalised eigen value problem, perterbation theory and variational calculus

Density function theory, The local density approximation, one and two particle excitations Solving the Schrodinger equation in periodic solids

Classical equilibrium statistical mechanics, Molecular dynamics simulations, Quatum molecular dynamics, The Monte Carlo method Quantum Monte Carlo methods, The finite elements method for partial differential equations

References

J. M. Thijssen, computational Physics, second edition, Cambridge University Press, 2007 D. K. Jha, Computational Physics, Discovery publishing House, 2009 Rubin H. Landau, Manuél José Páez Mejía, Cristian C. Bordeianu -Computational Physics: Problem Solving With Computers - John Wiley & Sons, 2007

Elective 7: FUS 719 :Computational Biology and Bioinformatics

Introduction to molecular biology, Genomics, Proteomics and Bioinformatics. DNA, Proteins,

Genetic code, t-RNA and protein sequences, Metabolic Metabolic Pathways and Analyses, Information retrieval with Entrez and Web browsers.

Human Genome Project, Genome and Sequence Databases, Datamining results of genome projects, Protein Sequence and Motif Databases, Sequence Alignment, Sequence Similarity Search, Multiple Sequence Alignment, Visualization of sequence data; Visualization of structures using Rasmol or SPDB Viewer. Finding protein coding regions, Finding genes

Clustering gene expression pattern, Coordinately Regulated Genes, Discovering Gene Regulatory Signals. Gene Regulatory Modules and Networks, Prediction of macromolecular properties.

Restriction Maps, Multiple Maps, Algorithms for DDP – Approaches to DDP- Simulated annealing, Mapping with real data, Cloning and clone libraries, Physical genome maps, Oceans, Islands and anchors

RNA secondary structure : Combinatorics, counting shapes, minimum energy structures. Trees and sequences: – splits, matrices on trees, distance, parsimony, maximum likehoold trees – Counting time Markov Chains, estimating rate of change, likehood and trees. Hidden Markov Models.

Reference:

Haubold, Bernhard, Wiehe, Thomas, Introduction to Computational Biology: An Evolutionary Approach, Springer, 2006

Michael S. Waterman, Introduction to Computational Biology : Maps, Sequences and genomes, Chapmann & Hall/CRC 1995

Introduction to Computational Biology: An Evolutionary Approach, Bernhard Haubold, Thomas Wiehe, Birkhäuser Basel, 2006.

Richard E. Neapolitan, Probabilistic Methods for Bioinformatics: with an Introduction to Bayesian Networks, Morgan Kaufmann, 2009

Neil C. Jones, Pavel A. Pevzner, An Introduction to Bioinformatics Algorithms, MIT Press, 2004.

Elective 8: FUS 7110 : Operations Research and Decision Theory

Introduction to OR - History, nature, scope and phases - OR and decision theory - Structure of decision strategies - Decision trees -Decision under competitive situation - Theory of games - pure and mixed strategies - Types of models in OR - Guidelines for modelling an OR project - Linear programming – Formulation, Theory and algorithms-Primal and Dual simplex algorithms and Interior point algorithms - post optimality analysis - complications in LP problems and resolutions - Goal programming - Waiting line models and their industrial applications **References:**

Introduction to operations research: a computer-oriented algorithmic approach, Billy E. Gillett, <u>Tata</u> <u>McGraw-Hill</u> Operations Research, Hamdy Taha, PHI Linear programming: theory and extensions 1& 2, George Bernard Dantzig, Mukund Narain Thapa, Springer Integer and Combinatorial Optimization –L.A Woolsey and G.L Nemhauser – John Wiley

Elective 9: FUS 7111 : Discrete Mathematics and Combinatorics (Elective-M.Phil)

Introduction to Combinatorics

Principles of Counting, Properties of the Integers: Mathematical Induction; Relations and Functions, Order (Posets, lattices, Moebius inversion) ; The Principle of Inclusion and Exclusion ; Generating Functions ; Recurrence Relations

Introduction to Graph Theory

Graphs and Simple Graphs- Subgraphs – Graph Isomorphism – Automorphisms – Vertex-Transitivity -The Incidence and Adjacency Matrices – Subgraphs – Vertex Degrees – Paths and Connection – Cycles – Trees and Forests – Planar Graphs - Graphs Invariants – The No-Homomorphism Lemma

The Shortest Path Problem – Sperner's Lemma - Graphs as Models – Paths and Connectedness – Cut nodes and Blocks – Graph Classes and Graph Operations

The Center and Eccentricity – Self-Centered Graphs – The Median – Central Paths – Other Generalized Centers

Connectivity and Edge-Connectivity – Menger's Theorem - Properties of *n*-Connected Graphs – Circulants - Radius – Small Diameter – Diameter – Long Paths and Long Cycles

Graph Representation_- The Adjacency Matrix – The Incidence Matrix – The Distance Matrix

The Eccentric Sequence – Distance Sequences – The Distance Distribution – Path Sequences – Other Sequences -

Algorithms and complexity theory

Polynomial Algorithms and NP-Completeness – Path Algorithms – Maximum Matchings – The Max-Flow Min-Cut Theorem – Minimum Spanning Trees – Travelling Salesman Problem – Shortest Paths – Centers –

Mathematical logic and proof-

Connectives, Tautologies, Valid Arguments, Derivation Rules, Deduction, Quantifiers and Predicates, Validity, Universal Instantiation and Generalization, Existential Instantiation and Generalization.

Textbook: Ralph P. Grimaldi, Discrete and Combinatorial Mathematics, Fifth edition, Addison-Wesley, 2003.

Text Book : Distances in Graphs, Harary and Buckley

Elective 10: FUS 7112 : Econometrics and Economic Forecasting

Module I

Nature and Scope of Econometrics, Statistical Concepts: Normal distribution; chi-sq, t- and Fdistributions; estimation of parameters; properties of estimators; testing of hypotheses, Simple Linear Regression Model: Two Variable Case - Estimation of model by method of ordinary least squares; properties of estimators; goodness of fit; tests of hypotheses; scaling and units of measurement; confidence intervals; Gauss-Markov theorem; forecasting.

Module II

Multiple Linear Regression Model Estimation of parameters; properties of OLS estimators; goodness of fit - R^2 and adjusted R^2 - partial regression coefficients; testing hypotheses - Violations of Classical Assumptions: Consequences, Detection and Remedies Multicollinearity; heteroscedasticity; serial correlation, Specification Analysis - Omission of a relevant variable; inclusion of irrelevant variable; tests of specification errors.

Module III

Dummy variable technique – Use of dummy variables, regression with dummy variables – ANOVA models, ANCOVA models, interaction effects, piecewise regression, deseasonalisation, Logit, probit and Tobit models.

Module IV

Forecasting using Time series models: Smoothing and Extrapolation of Time series – Simple extrapolation models, Smoothing and seasonal adjustment. Properties of stochastic Time series: Introduction to stochastic time series models. Stationary and Non stationary Time series, Linear Timer Series Models. Moving average models, ARIMA Models and Specification of ARIMA models.

Module V

Application of Statistical Packages

Reading List

Christian Gourieroux, Econometric of Qualitative Dependent Variables, Cambridge University Press, 2000. Christopher Dougherty, Introduction to Econometrics, Oxford University Press, 3rd edition, Indian Edition, 2007. Greene, W. H., Econometric Analysis, Prentice Hall.Goldberger, A., A Course in Econometrics, Harvard University Press.
Gujarati, D. N. and D.C. Porter, Essentials of Econometrics, McGraw Hill, 4th edition, International Edition, 2009.
Jan Kmenta, Elements of Econometrics, Indian Reprint, Khosla Publishing House, 2nd edition, 2008
Kerry Patterson, An Introduction to Applied Econometrics: A time series Approach, Macmillan Press, London 2000.
Krishna, K.L. Econometric Applications in India, OUP, New Delhi 1999.
Robert. S.Pindiyck & Daniel Rubinfield, Econometric Models and Economic Forecasts, MacGraw Hill, 1998.
Ruud, P., An Introduction to Classical Econometric Theory, Oxford University Press.
Stock, J.H. and M.W. Watson, Introduction to Econometrics (first edition), Addison-Wesley, 2003 (available at the COOP
Walter Enders, Applied Econometric Time Series, 2nd Edn., Wiley, 2008.
Wooldridge, J.M., Introductory Econometrics, South-Western College Publishing.

Semester II:

FUS 721: Dissertation