ANNEXURE 5

a. An introduction to approximation theory and optimization (MA305)

Objectives: Approximation theory and optimization techniques are extremely important in tackling real world problems. This course is expected to familiarize the students with the basics of this field of study.To have a general understanding of approximations and optimization, with an emphasis on computational algorithms

Prerequisites: Basic knowledge on projections, inner products and norms

Course Contents: Basic concepts related to best approximation and best coapproximation (in R^n and possibly in other important mathematical structures including matrices), their relations with orthogonality, elementary geometric visualizations of these concepts and their applications to some relevant real world problems from the perspective of optimization, basic computations related to best (co)approximations, including the problem of existence and uniqueness.

References:

1. Introduction to optimization by Pablo Pedregal, Springer, 1st Edition, 2004.
2. Approximation Theory and Approximation Practises, SIAM, 1st Edition, 2017.

b. Deep Learning with Graphs [3 credits]

How does the disease spread nationwide? How can we predict traffic or weather? Answering these questions requires massive amounts of data. Complex data can be represented as a graph of object relationships and interactions. Graph data structures can be ingested by algorithms such as neural networks to perform classification, clustering, and regression tasks.

Objectives

1) Course explores the computational, algorithmic, and modeling challenges of analyzing massive graphs from network science and deep learning perspectives.

2) By studying underlying graph structures, we will master machine learning and network science techniques that can improve prediction and reveal insights into massive networks' structural and dynamic properties.

By the end of this course, students will be able to:

· Distinguish between traditional deep neural networks and deep neural networks with graphs

· Identify opportunities in solving real world problems using Graph neural networks

· Implementation of Graph Neural networks for real-world data sets using PyTorch

Prerequisites

Linear algebra, probability, calculus, differential equations, and Python programming is necessary.

Course contents

Section 1: Graph theory, Basic concepts and definitions; Diameter, Path length, Clustering, Centrality metrics; Structure of real networks, Degree distribution, Power-laws.

Section 2: Models of network formation; The Erdos-Renyi random model, Scale-free model; Clustered models; Models of network growth, Preferential attachment; Small-world networks, community detection, Diffusion, Percolation, epidemic process on networks, dynamical systems

Section 3: Deep Neural Networks basics, Convolution Neural Networks, node embedding, Knowledge Graph Embedding

Section 4: Traditional Methods for ML on Graphs, Graph neural networks, applications of graph neural networks, theory of Graph Neural Networks, Difference between deep neural networks and Graph neural networks, Deep Generative Models for Graphs,

Section 5: Implementation of Graph Neural networks using PyTorch

Section 6: Case study on epidemic spreading and stock market time series data sets.

Tools: Cytoscape, Gephi, NetworkX, PyTorch, PyG: The ultimate library for Graph Neural Networks

References

Together with several research papers, we will cover specific chapters from the following textbooks:

- A-L. Barabási, Network Science, available online, 2015.
- M.E.J. Newman, Networks - An introduction, Oxford Univ Press, 2010.
- A. Barrat, M. Barthelemy and A. Vespignani, Dynamical Processes on Complex Networks, Cambridge Univ Press, 2008.
- Aaron Courville, Ian Goodfellow, and Yoshua Bengio, Deep Learning
- CS224W: Machine Learning with Graphs, Stanford University

c. Introduction to Quantum Machine Learning [3 credits]

The pace of development in quantum computing mirrors the rapid advances made in machine learning and artificial intelligence. It is natural to ask whether quantum technologies could boost learning algorithms: this field of inquiry is called quantum-enhanced machine learning. This course aims to show what benefits current and future quantum technologies can provide to machine learning, focusing on algorithms that are challenging with classical digital computers. We strongly emphasize implementing the protocols using open-source frameworks in Qiskit on Real Quantum Computers.

Objectives:

1) Understand the notion of quantum states and their evolution in closed/open systems and quantum measurements as a form of sampling.

2) Contrast quantum computing paradigms and implementations. Recognize the limitations of current and near-future quantum technologies and the kind of tasks where they outperform or are expected to outperform classical computers. Explain variational circuits.

3) Describe and implement classical-quantum hybrid learning algorithms. Encode classical information in quantum systems. Perform discrete optimization in ensembles and unsupervised machine learning with different quantum computing paradigms.

4) Summarize quantum Fourier transformation, quantum phase estimation, and quantum matrix, and implement these algorithms using Qiskit

By the end of this course, students will be able to:

· Distinguish between quantum computing paradigms relevant to machine learning

· Identify opportunities in machine learning for using quantum resources

· Implement learning algorithms on real quantum computers using Qiskit.

Prerequisites:

Linear algebra, probability theory, complex numbers, Python, and basic knowledge of machine learning will be advantageous for this course.

Course contents

Section 1: Classical Probability, Linear algebra, concepts of Bra-Ket and matrix notations, unitary matrix, Basics of Quantum Mechanics: Axioms of quantum mechanics, Quantum States, Mixed states, Evolution in Closed Quantum Systems, Open Quantum Systems, Tensor products of Hilbert space, Observables, Measurements (Projective Measurements), Dynamics.

Section 2: The Qubits, Multiple Qubits (Geometric representation of Qubits-Bloch Sphere), Bipartite quantum systems, Entanglement, Quantum logic gates and Quantum Circuit diagrams, Quantum Fourior transformation, Quantum error correction. Models of quantum computing (Gate-Model, Adiabatic Quantum Computing, Quantum Annealing)

Section 3: Basics of Machine learning, Quantum Fourier transform, Quantum Phase estimation, The HHL Algorithm, Quantum Linear Regression and Classification, Variational quantum circuits for machine learning

Section 4: Qiskit/Pennylane (Optimization purposes), Quantum Walks, Parameterized Quantum Circuit, Quantum neural networks

Section 5: Quantum machine learning projects using Qiskit/Pennylane

References

[1] Michael A. Nielsen and Isaac L. Chuang, Quantum Computation and Quantum Information, (http://mmrc.amss.cas.cn/tlb/201702/W020170224608149940643.pdf)

[2] John Preskill Lecture notes, https://www.lorentz.leidenuniv.nl/quantumcomputers/literature/preskill_1_to_6.pdf

[3] Quantum Machine Learning using Qiskit, https://learn.qiskit.org/course/machine-learning/parameterized-quantum-circuits

[4] IBM Online notes on Qiskit, https://qiskit.org/textbook/ch-states/introduction.html

[5] Access IBM Quantum Computer, https://quantum-computing.ibm.com/

[6] Quantum Machine Learning using Pennylane, https://pennylane.ai/

(d) Math Tools for Data Science & Machine Learning(MA304)

Prerequisite: Calculus I and II; Linear Algebra; Vector Calculus, An introductory course in Probability and Statisics.

Objective of the course is to provides a rigorous introduction to mathematical tools for the data science drawn from linear algebra, harmonic analysis, probability theory and convex optimization. The main topics are the Singular-value-decomposition (SVD), application of dimensionality reduction, Markov Chains, Random process, Newton's method, Norms, Basis and orthogonal projections. The material is motivated by multiple data-analysis applications including dimensionality reduction, sound and image processing.

Course Contents: **Unit I: Linear Algebra & Vector Calculus**

Vectors and Matrices and Basic operations, Vector spaces, Eigenvalues and Eigenvectors, Singular value decomposition (SVD), and application to dimensionality reduction, Gradient of vector-valued functions, Gradients of matrices, Useful identities for computing Gradients.

Unit II: Probability and Statistics

Basic probability, conditional probability, Bayes' rule, random variables, random vectors, Probability bounds, Markov Chains, Application to web search algorithms, Introduction to Random processes, and Some important random processes.

Unit III: Foundation of Statistical Learning

Basics of statistical learning, models, Linear regression, the curse of dimensionality, overfitting etc., optimization and convexity, Gradient descent, Newton's method.

Unit IV: Analytic Geometry

Norms, Inner Products. Lengths and Distances, Angles and orthogonality, Orthogonal Basis, Orthogonal Complement, Inner Product of functions, Orthogonal Projections.

Unit V: Dimensionality Reduction with PCA

Problem Setting, Projection Perspective, Eigenvector Computation and Low-Rank Approximation, PCA in high Dimensions.

References:

Advanced Engineering Mathematics by Erwin Kreyszig

Introduction to Linear Algebra by Gilbert Strang

Element of Statistical Learning by T. Hastie, Robert Tibshirani and J. Friedman.

Linear Algebra and Optimization for Machine Learning by Charu C Aggarwal.

Machine Learning by Murphy

An introduction to Probability theory and its applications by William Feller.

First Course in Probability by S. Ross.

6 (G) Expansion of a one credit course "Intro. of Probability" to a three-credit course "Intro. of Probability, Statistics and Random Processes".

Proposed Changes: The proposed changes to the course will include the following:

1. Adding additional course materials, such as readings and assignments, to provide students with a more in-depth understanding of the subject matter.
2. Incorporating hands-on activities to provide students with practical experience in the subject matter.
3. Increasing the amount of time sent in class to allow for more in-depth discussions and group work.
4. Increasing the number of credits for the course from 1 to 3.

Benefits: The benefits of expanding the course to a 3 credit will include:

1. Providing students with a more comprehensive understanding of the subject matter.
2. Allowing students to gain practical experience in the subject matter through hands-on activities
3. Giving students more opportunities to engage in in-depth discussions and group work.

IOP(1 credit) course syllabus: Sample space and events, definitions of probability, properties of probability, conditional probability. Random variables: distribution functions, discrete and continuous random variables, moments of random variables, conditional expectation, Chebyshev inequality, and functions of random variables. Special Distributions: Bernoulli, Binomial, Geometric, Pascal, Poisson, Exponential, Uniform, Normal distributions, Limit Theorems: Law of the large number

IOP (3 credits) course syllabus

Basic concepts such as random experiments, probability axioms, conditional probability, and counting methods for Single and multiple random variables (discrete, continuous, and mixed), as well as moment-generating functions, characteristic functions, random vectors, and inequalities, Limit theorems and convergence Introduction to mathematical statistics, in particular, Bayesian and classical statistics Random processes including the processing of random signals, Poisson processes, discrete-time, and continuous-time Markov chains, and Brownian motion.

References:

1. An introduction to Probability theory and its applications by William Feller.
2. First Course in Probability by S. Ross.
3. Introduction to Probabilty by D. Bertsekas. J. Tsitsiklis
4. The signal and the Noise: Why most Predictions Fail but SOme Don't
5. Intoduction to Probability by Joseph K. Blitzstein and Jessica Hwang