Federal State Autonomous Educational Institution of Higher Education "Moscow Institute of Physics and Technology (National Research University)"

APPROVED
Head of Landau Phystech-School of Physics & Research
A.V. Rogachev

Work program of the course (training module)

course:	Machine Learning for Quantum and Statistical Physics/Машинное обучение для квантовой и статистической физики
major:	Photonics and Optical Informatics
specialization:	Photonics, Quantum Technologies & 2D Materials/Фотоника, квантовые технологии и двумерные материалы
	Landau Phystech-School of Physics & Research
	Chair of the Russian Quantum Centre
term:	1
qualification:	Master

Semester, form of interim assessment: 2 (spring) - Grading test

Academic hours: 30 AH in total, including:
- lectures: 30 AH.
- seminars: 0 AH.
- laboratory practical: 0 AH.

Independent work: 60 AH.

In total: 90 AH, credits in total: 2

Authors of the program:

A.E. Ulanov, candidate of physics and mathematical sciences
E.S. Tiunov

The program was discussed at the Chair of the Russian Quantum Centre 21.05.2021

Annotation

The purpose of the discipline is to give a brief introduction to the methods of modern deep machine learning in quantum physics. The course consists of two parts.

The first part provides a general idea of the subject of deep learning. The explanation is based on two problems: the problem of classification and the regression problems. To solve these problems, it is suggested to study various types of artificial neural networks (fully connected, convolutional, and recurrent).

The second part of the course is aimed at solving problems of quantum physics using machine learning. A variation method in neural network paradigm for quantum tomography and search of the ground state of multiparticle Hamiltonians will be considered. Various sampling methods will also be discussed in context of application of the variational approach for large-dimensional Hilbert spaces.

All classes of the course are organized as a set of pairs: lecture-seminar. The lectures will cover the theoretical foundations of the topics described above. Seminars consist of solving practical problems in Python on the topics of lectures. While solving problems, students will be given a basic idea of the Numpy and Pytorch libraries. The criterion for successful completion of the course is the delivery of the project. Basic Python programming skills are required for successful completion of the course.

1. Study objective

Purpose of the course

to give a brief introduction to the methods of modern deep machine learning, to give an overview of the existing approaches of machine learning tools utilization for experimental quantum physics and statistical physics.

Tasks of the course

provide to students with the necessary knowledge and skills for independent interdisciplinary research at the intersection of machine learning and physics.

2. List of the planned results of the course (training module), correlated with the planned results of the mastering the educational program

Mastering the discipline is aimed at the formation of the following competencies:

Code and the name of the competence	Competency indicators
UC-1 Use a systematic approach to critically analyze a problem and develop an action plan	UC-1.1 Systematically analyze the problem situation, identify its components and the relations between them
	UC-1.2 Search for solutions by using available sources
	UC-1.3 Develop a step-by-step strategy for achieving a goal, foresee the result of each step, evaluate the overall impact on the planned activity and its participants
UC-2 Manage all stages of a research project	UC-2.2 Forecast the project outcomes, plan necessary steps to achieve the outcomes, chart the project schedule and monitoring plan
	UC-2.4 Publicly present the project results (or results of its stages) via reports, articles, presentations at scientific conferences, seminars, and similar events
UC-4 Use modern communication tools in the academic and professional fields, including those in a foreign language	UC-4.3 Present the results of academic and professional activities in various academic events, including international conferences
Gen.Pro.C-1 Gain fundamental scientific knowledge in the field of physical and mathematical sciences	Gen.Pro.C-1.1 Apply fundamental scientific knowledge in the field of physical and mathematical sciences
	Gen.Pro.C-1.3 Understands the interdisciplinary links in mathematics and physics and is able to apply them to problems in photonics and opto-informatics
Gen.Pro.C-2 Acquire an understanding of current scientific and technological challenges in professional settings, and scientifically formulate professional objectives	Gen.Pro.C-2.3 Understand professional terminology used in modern scientific and technical literature and present scientific results in oral and written form within professional communication

Gen.Pro.C-3 Select and/or develop approaches to professional problem-solving with consideration to the limitations and specifics of different solution methods	Gen.Pro.C-3.1 Analyze problems, plan research strategy to achieve solution(s), propose, and combine solution approaches
	Gen.Pro.C-3.3 Gain knowledge of analytical and computational methods of problem-solving, understand the limitations for applying the obtained solutions in practice
Gen.Pro.C-4 Successfully perform a task, analyze the results and present conclusions, apply knowledge and skills in the field of physical and mathematical sciences and ICTs	Gen.Pro.C-4.1 Apply ICT knowledge and skills to find and study scientific literature and use software products
	Gen.Pro.C-4.2 Apply knowledge in the field of physical and mathematical sciences to solve problems, make conclusions, and evaluate the obtained results
Pro.C-1 Assign, formalize, and solve tasks, develop and research mathematical models of the studied phenomena and processes, systematically analyze scientific problems and obtain new scientific results	Pro.C-1.2 Make hypotheses, build mathematical models of the studied phenomena and processes, evaluate the quality of the developed model
Pro.C-3 Professionally use research and testing equipment (devices and installations, specialized software) in a selected subject field	Pro.C-3.1 Understand the operating principles of the equipment and specialized software
	Pro.C-3.2 Conduct an experiment (simulation), using research equipment (software)
	Pro.C-3.3 Evaluate the accuracy of the experimental (numerical) results

3. List of the planned results of the course (training module)

As a result of studying the course the student should:

know:

the basic methods of deep machine learning and existing methods of their application for research in the field of modern quantum technologies.

be able to:

select appropriate machine learning tools for experimental and theoretical research in the field of quantum physics and statistical physics, navigate in modern research at the intersection of quantum technology and machine learning.

master:

basic technologies and algorithms of deep machine learning, and methods for using them as tools for research in various fields of quantum physics and statistical physics.

4. Content of the course (training module), structured by topics (sections), indicating the number of allocated academic hours and types of training sessions

4.1. The sections of the course (training module) and the complexity of the types of training sessions

№	Topic (section) of the course	Types of training sessions, including independent work			
		Lectures	Seminars	Laboratory practical	Independent work
1	Introduction.	3			5
2	Linear classification and fully-connected neural networks.	3			5
3	Diagnosing quality of trained models.	3			5
4	Convolutional neural networks.	3			5
5	Recurrent neural networks.	3			5
6	Boltzmann machines for statistical physics.	3			5

7	Boltzmann machines for quantum state tomography.	3			5
8	Sampling methods	3			5
9	Variational autoregressive neural networks for statistical physics.	3			5
10	Overwiev of recent advance.	1			5
11	Final project.	2			10
AH in total		30			60
Exam preparation		0 AH.			
Total complexity		90 AH., credits in total 2			

4.2. Content of the course (training module), structured by topics (sections)

Semester: 2 (Spring)

1. Introduction.

Introductory lecture. Overview of modern methods of machine learning. Course overview.

2. Linear classification and fully-connected neural networks.

Linear classification, optimization objective, gradient descent, deep neural networks, forward and back propagation. Methods of automatic differentiation.

3. Diagnosing quality of trained models.

Diagnosing quality of trained models. Quality metrics of training, diagnosing overfitting and underfitting. Regularization.

4. Convolutional neural networks.

Convolutional neural networks. Examples of convolutions, stride, pooling, padding. Examples of convolutional neural network architectures.

5. Recurrent neural networks.

Recurrent neural networks. Different types of recurrent architectures. Backward propagation. Gradient vanishing and explosion. Gated Recurrent Unit (GRU), Long Short Term Memory (LSTM). Bidirectional recurrent networks.

6. Boltzmann machines for statistical physics.

Boltzmann machines for problems of statistical physics. Description of the Boltzmann machine, definition, problem statement, optimization functional, gradient derivation and gradient descent. Utilization for classification and statistical physics tasks.

7. Boltzmann machines for quantum state tomography.

Boltzmann machines for quantum state tomography. Tomography of pure and mixed quantum states. Maximum Likelihood Method. Utilization of Boltzmann machines for tomography. Comparison of methods.

8. Sampling methods

Two sampling algorithms from an arbitrary distribution are discussed: the Gibbs algorithm and Metropolis algorithm. These algorithms are used to train a Boltzmann machine.

9. Variational autoregressive neural networks for statistical physics.

Variational autoregressive neural networks for statistical physics and many-body physics. Problem statement, optimization objective derivation, method of model training, overview of possible neural network architectures. Possible applications for other tasks.

10. Overwiev of recent advance.

Overwiev of recent advance in machine learning.

11. Final project.

Presentation of the independent research projects of students.

5. Description of the material and technical facilities that are necessary for the implementation of the educational process of the course (training module)

A classroom equipped with a board, multimedia-projector, and projection screen. Students will also need personal computers.

6. List of the main and additional literature, that is necessary for the course (training module) mastering

Main literature

Ian Goodfellow, Yoshua Bengio, Aaron Courville. Deep Learning, MIT Press, 2016. (available online)

Additional literature

A. I. Lvovsky and M. G. Raymer, Continuous-variable optical quantum-state tomography. Reviews of Modern Physics 81, 299–332 (2009).
G. Carleo and M. Troyer, Solving the quantum many-body problem with artificial neural networks. Science 355, 602–606 (2017).
G. Torlai, G. Mazzola, J. Carrasquilla, M. Troyer, R. Melko and G. Carleo, Neural-network quantum state tomography. Nature Physics 1 (2018).
E. S. Tiunov, V. V. Tiunova, A. E. Ulanov, A. I. Lvovsky and A. K. Fedorov, Experimental quantum homodyne tomography via machine learning. (2019).
M. Benedetti, J. Realpe-Gómez, R. Biswas and A. Perdomo-Ortiz, Quantum-Assisted Learning of Hardware-Embedded Probabilistic Graphical Models. Physical Review X 7, 041052 (2017).
D. Wu, L. Wang and P. Zhang, Solving Statistical Mechanics Using Variational Autoregressive Networks. Physical Review Letters 122, 080602 (2019).

7. List of web resources that are necessary for the course (training module) mastering

https://github.com/yandexdataschool/Practical_DL

8. List of information technologies used for implementation of the educational process, including a list of software and information reference systems (if necessary)

All students must have the Anaconda software package and the Pytorch library installed.

9. Guidelines for students to master the course

Students should learn the basic concepts of machine learning for quantum and statistical physics, as well as how to apply their theoretical knowledge in practice.

For the successful assimilation of the course, in addition to attending classes, students are required to perform homework whose amount in hours should be not less than the number of hours specified in the curricula of the faculties. Studying at home includes:

- reading the recomended literature and making notes;
- processing and analysis of lecture materials (using notes, textbooks and scientific articles), answering questions, proving some statements;
- solving problems given on lectures and seminars for self-study;
- preparing for the tests and exams.

SUPPLEMENT

Assessment funds for course (training module)

major:	Photonics and Optical Informatics
specialization:	Photonics, Quantum Technologies & 2D Materials/Фотоника, квантовые технологии и двумерные материалы
	Landau Phystech-School of Physics & Research
	Chair of the Russian Quantum Centre
term:	1
qualification:	Master

Semester, form of interim assessment: 2 (spring) - Grading test

Authors:

A.E. Ulanov, candidate of physics and mathematical sciences
E.S. Tiunov

1. Competencies formed during the process of studying the course

Code and the name of the competence	Competency indicators
UC-1 Use a systematic approach to critically analyze a problem and develop an action plan	UC-1.1 Systematically analyze the problem situation, identify its components and the relations between them
	UC-1.2 Search for solutions by using available sources
	UC-1.3 Develop a step-by-step strategy for achieving a goal, foresee the result of each step, evaluate the overall impact on the planned activity and its participants
UC-2 Manage all stages of a research project	UC-2.2 Forecast the project outcomes, plan necessary steps to achieve the outcomes, chart the project schedule and monitoring plan
	UC-2.4 Publicly present the project results (or results of its stages) via reports, articles, presentations at scientific conferences, seminars, and similar events
UC-4 Use modern communication tools in the academic and professional fields, including those in a foreign language	UC-4.3 Present the results of academic and professional activities in various academic events, including international conferences
Gen.Pro.C-1 Gain fundamental scientific knowledge in the field of physical and mathematical sciences	Gen.Pro.C-1.1 Apply fundamental scientific knowledge in the field of physical and mathematical sciences
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Gen.Pro.C-2 Acquire an understanding of current scientific and technological challenges in professional settings, and scientifically formulate professional objectives	Gen.Pro.C-2.3 Understand professional terminology used in modern scientific and technical literature and present scientific results in oral and written form within professional communication
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	Gen.Pro.C-3.3 Gain knowledge of analytical and computational methods of problem-solving, understand the limitations for applying the obtained solutions in practice
Gen.Pro.C-4 Successfully perform a task, analyze the results and present conclusions, apply knowledge and skills in the field of physical and mathematical sciences and ICTs	Gen.Pro.C-4.1 Apply ICT knowledge and skills to find and study scientific literature and use software products
	Gen.Pro.C-4.2 Apply knowledge in the field of physical and mathematical sciences to solve problems, make conclusions, and evaluate the obtained results
Pro.C-1 Assign, formalize, and solve tasks, develop and research mathematical models of the studied phenomena and processes, systematically analyze scientific problems and obtain new scientific results	Pro.C-1.2 Make hypotheses, build mathematical models of the studied phenomena and processes, evaluate the quality of the developed model
Pro.C-3 Professionally use research and testing equipment (devices and installations, specialized software) in a selected subject field	Pro.C-3.1 Understand the operating principles of the equipment and specialized software
	Pro.C-3.2 Conduct an experiment (simulation), using research equipment (software)
	Pro.C-3.3 Evaluate the accuracy of the experimental (numerical) results

2. Competency assessment indicators

As a result of studying the course the student should:

know:

the basic methods of deep machine learning and existing methods of their application for research in the field of modern quantum technologies.

be able to:

select appropriate machine learning tools for experimental and theoretical research in the field of quantum physics and statistical physics, navigate in modern research at the intersection of quantum technology and machine learning.

master:

basic technologies and algorithms of deep machine learning, and methods for using them as tools for research in various fields of quantum physics and statistical physics.

3. List of typical control tasks used to evaluate knowledge and skills

Examples of control tasks

1. Solve the problem of nonlinear logistic regression
2. Solve the problem of image classification using a multi-layer perceptron in MNIST database
3. Analyze the learning curves and apply regularization methods to improve the quality of the model
4. Solve the problem of image classification using a deep convolutional network in MNIST database
5. Evaluate numerically the correlation functions in the Ising model using different sampling methods and compare the results with the exact solution

4. Evaluation criteria

Examples of checking questions:

1. Obtain the shape of the focusing surface separating two media with different refractive indices using a neural network
2. Using Helium as an example, apply several variation ansats to search for the energy of the ground state
3. Train a limited Boltzmann machine by sampling
4. Train a fully connected Boltzmann machine with a single hidden layer of sampling
5. Find the ground state of a multiparticle Hamiltonian using a neural network anzac
6. Observe the phase transition in this system by changing the parameters of the Hamiltonian
7. Create a neural network that predicts the wave function in the coordinate representation
8. Solve the problem of tomography of the state of a quantum harmonic oscillator
9. Develop a method for solving differential equations using neural networks
10. Predict the dynamics of a physical system by minimizing the action integral on a neural network.

Examples of examination questions:

Card 1.

1. Obtain the shape of the focusing surface separating two media with different refractive indices using a neural network
2. Using Helium as an example, apply several variation ansats to search for the energy of the ground state

Card 2.

1. Train a limited Boltzmann machine by sampling
2. Train a fully connected Boltzmann machine with a single hidden layer of sampling

Assessment "excellent (10)" is given to a student who has displayed comprehensive, systematic and deep knowledge of the educational program material, has independently performed all the tasks stipulated by the program, has deeply studied the basic and additional literature recommended by the program, has been actively working in the classroom, and understands the basic scientific concepts on studied discipline, who showed creativity and scientific approach in understanding and presenting educational program material, whose answer is characterized by using rich and adequate terms, and by the consistent and logical presentation of the material;

Assessment “excellent (9)” is given to a student who has displayed comprehensive, systematic knowledge of the educational program material, has independently performed all the tasks provided by the program, has deeply mastered the basic literature and is familiar with the additional literature recommended by the program, has been actively working in the classroom, has shown the systematic nature of knowledge on discipline sufficient for further study, as well as the ability to amplify it on one’s own, whose answer is distinguished by the accuracy of the terms used, and the presentation of the material in it is consistent and logical;

Assessment “excellent (8)” is given to a student who has displayed complete knowledge of the educational program material, does not allow significant inaccuracies in his answer, has independently performed all the tasks stipulated by the program, studied the basic literature recommended by the program, worked actively in the classroom, showed systematic character of his knowledge of the discipline, which is sufficient for further study, as well as the ability to amplify it on his own;

Assessment “good (7)” is given to a student who has displayed a sufficiently complete knowledge of the educational program material, does not allow significant inaccuracies in the answer, has independently performed all the tasks provided by the program, studied the basic literature recommended by the program, worked actively in the classroom, showed systematic character of his knowledge of the discipline, which is sufficient for further study, as well as the ability to amplify it on his own;

Assessment “good (6)” is given to a student who has displayed a sufficiently complete knowledge of the educational program material, does not allow significant inaccuracies in his answer, has independently carried out the main tasks stipulated by the program, studied the basic literature recommended by the program, showed systematic character of his knowledge of the discipline, which is sufficient for further study;

Assessment “good (5)” is given to a student who has displayed knowledge of the basic educational program material in the amount necessary for further study and future work in the profession, who while not being sufficiently active in the classroom, has nevertheless independently carried out the main tasks stipulated by the program, mastered the basic literature recommended by the program, made some errors in their implementation and in his answer during the test, but has the necessary knowledge for correcting these errors by himself;

Assessment “satisfactory (4)” is given to a student who has discovered knowledge of the basic educational program material in the amount necessary for further study and future work in the profession, who while not being sufficiently active in the classroom, has nevertheless independently carried out the main tasks stipulated by the program, learned the main literature but allowed some errors in their implementation and in his answer during the test, but has the necessary knowledge for correcting these errors under the guidance of a teacher;

Assessment “satisfactory (3)” is given to a student who has displayed knowledge of the basic educational program material in the amount necessary for further study and future work in the profession, not showed activity in the classroom, independently fulfilled the main tasks envisaged by the program, but allowed errors in their implementation and in the answer during the test, but possessing necessary knowledge for elimination under the guidance of the teacher of the most essential errors;

Assessment “unsatisfactory (2)” is given to a student who showed gaps in knowledge or lack of knowledge on a significant part of the basic educational program material, who has not performed independently the main tasks demanded by the program, made fundamental errors in the fulfillment of the tasks stipulated by the program, who is not able to continue his studies or start professional activities without additional training in the discipline in question;

Assessment “unsatisfactory (1)” is given to a student when there is no answer (refusal to answer), or when the submitted answer does not correspond at all to the essence of the questions contained in the task.

5. Methodological materials defining the procedures for the assessment of knowledge, skills, abilities and/or experience

The grade is assigned based on the results of the final written test. Students will be provided with two questions. During the test, the student is given 30 minutes to prepare. The student's questionning should not exceed one astronomical hour.