UNIVERSITY of MISKOLC
Faculty of Materials Science and Engineering

Antal Kerpely Doctoral School of Materials Science & Technology

Modern artificial intelligence and material science application

Dr. Pál Tóth

COURSE DESCRIPTION

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Author: Dr. Pál Tóth

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Lecturer

Dr. Pál Tóth, assoc. professor, Institute of Physical Metallurgy, Metalforming and Nanotechnology.

room: B1 gr fl. 3 mail: femvali@uni-miskolc.hu, tel: 1545, 302183699,
http://www.matsci.uni-miskolc.hu/mertinger.htm

Recommendation

This course is recommended for students interested in the methods and achievements of modern artificial intelligence and machine learning.

Language

Hungarian or English.

Scope

The objective of this course is to introduce students to the history, milestones, mathematical concepts and methods of modern artificial intelligence.

Methodology

Course material is communicated through lectures, one-on-one consultation and online courses (either live or recorded). During the course, obligatory homework will be assigned. Independent study and research will be required to solve homework assignments.

Topics

1. Linear algebra
2. Statistical inference
3. Concepts, definitions and objectives of machine learning
4. Convex optimization
5. Gradient-free optimization (random search, genetic algorithms, etc.)
6. Gradient-based optimization (gradient descent, momentum, Nesterov momentum, etc.)
7. Automatic differentiation, frameworks
8. Neural networks in the context of statistical inference: Ordinary Least Squares Regression – Multiple Linear Regression – Multivariate Regression – Logistic Regression – Multilayer Perceptron
9. Network initialization, activation functions, optimizers
10. Convolutional Neural Networks
11. Recurrent Neural Networks
12. Variational and Bayes Neural Networks

13. Milestones: Batchnorm, Dropout, Residual Learning, important architectures: VGG, Inception, ResNet, DenseNet, MobileNet…
14. Outlook

References

1. Ian Goodfellow, Yoshua Bengio, Aaron Courville: Deep Learning. MIT Press, 2016
2. Christopher Bishop: Pattern Recognition and Machine Learning. Springer, 2006

Exam

Evaluation will be through graded homework assignments and an oral final examination.

Complex exam questions

1. Derive the equations of backpropagation and give an update rule for the weights of a Multilayer Perceptron.
2. Write an update rule for the weights of a convolutional neural kernel. In the context of convolutional neural networks, give a list of useful convolutional operations. What are the tasks, advantages and disadvantages of these?
3. Write an update rule for the weights of a recurrent neural network. How can you solve the vanishing gradient problem in recurrent neural networks?
4. Starting from the appropriate statistical distributions, derive the following error functions: mean squared error, binary crossentropy, categorical crossentropy.
5. Implement a gradient-free optimization algorithm of choice. Use your algorithm to optimize the cost of a material recipe given constraints. Give the optimal recipe.
6. Propose modern solutions for the following problems: point cloud classification, set regression with varying-length sets, classification of 3D (voxel) data, data-driven cellular automata.
7. Propose modern solutions for the following problems: segmentation of grains in optical micrographs, measurement of interlayer spacing in transmission electron micrographs, demarcation of grain boundaries in CT voxel data, fast deconvolution of XRD spectra.