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# *Journal of Applicable Chemistry*

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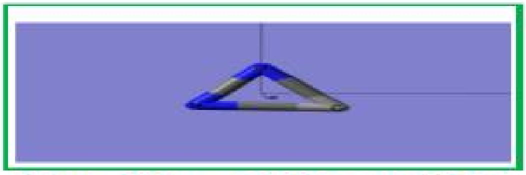
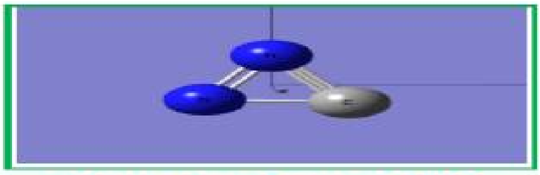
## New Chemistry News

$^-N=C=N^-$



New News of Chem (NNC)



ChemNewsNew (CNN)

| | |
|---|---|
| **Artificial Intelligence (AI)** | **Part 2(a) AI. Medicine (Aim)**<br>**Part 2(b) AI. Games(Ag)**<br>**Part 2(c) AI. Neocognitron** |

# Part 2(a) AI. Medicine (Aim)

Reach:REading and Assembling Contextual and Holistic mechanisms from text

Output:

- + Automated, large-scale machine reading system for biomedical papers
- + Extracts mechanistic descriptions of biological processes
- + Relatively high precision
- + High throughput

Future:

- ! To identify/explain signaling pathways in cancer types
- ! Human-curated 'big mechanisms' + extracted 'big data' → understanding causal factors in cellular processes

| | |
|---|---|
| Large-scale automated machine reading discovers new cancer-driving mechanisms | Database, 2018, 1–14<br>doi: 10.1093/database/bay098 |
| Marco A. Valenzuela-Escárcega, Özgün Babur, Gus Hahn-Powell, Dane Bell, Thomas Hicks, Enrique Noriega-Atala, Xia Wang, Mihai Surdeanu, Emek Demir and Clayton T. Morrison | |

**AI.Med — AI.Med — AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.MedAI.Med**

| | |
|---|---|
| Dartmouth AI conference objectives | To explore ways to make a machine that could<br>o Reason like a human<br>o Capable of abstract thought<br>o problem-solving<br>o Self-improvement |

| DENDRAL | Expert system (AI) |
|---|---|
| Joshua Lederberg | Geneticist |
| Edward Feigenbaum | Computer scientist |
| Carl Djerassi | Organic chemist |
| Bruce Buchanan | Philosopher-of-science |

| | |
|---|---|
| Data. Instrument | Mass-spectra |
| Method | o Production rules<br>o To encode chemists' knowledge<br>o Clever algorithms |
| Output | Likely chemical structures of organic compounds |

Influencing factors in Artificial Intelligence in Medicine (AIM) research

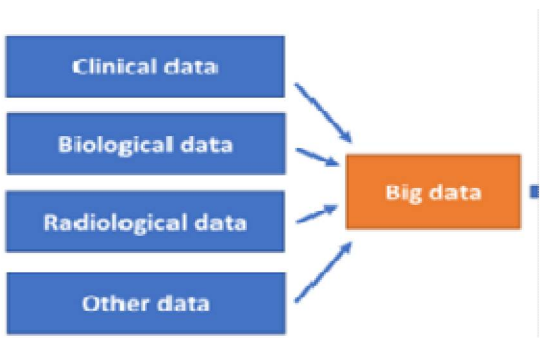
+ Evolution of computer science, hardware
+ Technology, communications, biomedicine

| | |
|---|---|
| Artificial Intelligence in Medicine: Weighing the Accomplishments, Hype, and Promise | IMIA Yearbook of Medical Informatics 2019, http://dx.doi.org/10.1055/s-0039-1677891 |
| Edward H. Shortliffe | |

**AI.Med — AI.Med — AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.MedAI.Med**

Sources of Medical (Med.) Big Data

- o Clinical data
  - o Public or private health insurance
  - o Cohorts
  - o Digital traces
- o Keywords put in a web server
- o Images (millions of pixels)
- o Biological data
- o Omics approaches




Big Data. Short comings in practice

- Lack of expertise of researchers in this emerging field
- Massive collection of data does not guarantee their quality, stability or consistency
- Data may not be collected in the same way within each source

| | |
|---|---|
| | - Big data is extremely vast, dynamic and constantly evolving<br>- Analysis: inappropriate use of these specialized methods →<br>- Lead to erroneous results due to unexpected relationships between factors without conformed causal relationship |
| **Remedial Measures: bilateral** | |
| | 🕮 Close collaboration and upgradation/exchange of knowledge between clinicians and data scientists specializing in Big Data |

| | |
|---|---|
| Big Data | Sjögren project consortium<br>o International collaboration<br>o Common database to 22 countries on 5 continents |
| Disease | Sjögren syndrome |
| Data Type | Clinical, biological, histological data<br>10,500 subjects |
| Goal | o To deepen knowledge about Sjögren's syndrome<br>o To improve its management around the world |
| Outcome | o Confirmed influence of immunological markers on the clinical phenotype of primary Sjögren's syndrome<br>o Greater correlation between systemic manifestations and hypocomplementemia<br>o Cryoglobulinemia rather than with anti-nuclear and anti-Ro/La antibodies |

| | |
|---|---|
| Disease | Arthritis |
| Task | Correlation between rheumatoid arthritis or spondyloarthritis versus physical activity |
| Data | Number of steps per minute recorded in real time using a physical activity tracer (bracelet)<br>224,952 hours data |
| Method | o Machine learning algorithm<br>o Prediction model for flares based on the steps |
| Outcome | o Mean sensitivity 96%, mean specificity 97% |
| Future scope | o Remote monitoring of disease activity<br>+ High accuracy and minimal burden on the patient |
| | |
| Disease | ▪ Diabetic retinopathy |
| Data Type | ▪ Fundus images |
| Task | o Automated detection of diabetic retinopathy |
| Method | o Convolutional neural networks |
| Output | o Simultaneous detection of exudates, haemorrhages and microaneurysms automatically<br>o Sensitivity of 85 to 96% |

| | |
|---|---|
| Disease | ▪ Myositis |
| Data Type | ▪ Ultrasound osteoarticular imaging |
| Task | o Automated diagnosis of myositis |
| Method | o Convolutional NNs |
| Output FOM | o Sensitivity 66 to 82%<br>o Specificity 65 to 92% |

| Big Data and Artificial Intelligence: Will they change our practice? | Joint Bone Spine (2019), doi.org/10.1016/j.jbspin.2019.09.001 |
|---|---|
| Joanna Kedra Laure Gossec | |

AI.Med — AI.Med — AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.MedAI.Med

| | |
|---|---|
| Disease | ▪ Ventricular dysfunction (ejection fraction ≤ 35%,) |
| Data | ▪ Electrocardiogram(ECG)<br>▪ Transthoracic echocardiogram (TTE) Using paired 12-lead ECG<br>▪ Echocardiogram data |
| Patients | o 44,959 at the Mayo Clinic<br>o Mean age : 61.8 ± 16.5 years |
| Method | o Convolutional NN |
| Unique advantage | o ECG +AI<br>+ Ubiquitous, low-cost test<br>+ Permits ECG to screening tool to identify ALVD |

| Screening for cardiac contractile dysfunction using an artificial intelligence–enabled electrocardiogram | Nature Medicine , VOL 25, JANUARY 2019, 70–74 |
|---|---|
| Zachi I. Attia, Suraj Kapa, Francisco Lopez-Jimenez, Paul M. McKie , Dorothy J. Ladewig, Gaurav Satam, Patricia A. Pellikka , Maurice Enriquez-Sarano, Peter A. Noseworthy , Thomas M. Munger, Samuel J. Asirvatham, Christopher G. Scott, Rickey E. Carter and Paul A. Friedman | |

AI.Med — AI.Med — AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.MedAI.Med

| | |
|---|---|
| Discipline | o Orthopedic surgery |
| Task | o Detection and prediction of osteoarthritis (OA)<br>o Spine pathology detection<br>▪ Bone and cartilage image segmentation |
| Data | ▪ Medical images |
| Method | o Support vector machines<br>o Neural networks |

| | |
|---|---|
| Discipline | ▪ Arthroplasty |
| Data | ▪ Preoperative patient data |
| Task | o Identify risk factors for complications |
| Method | o Heuristic AI; machine learning, deep neural nets<br>o Validation for tasks, data in diagnosis, treatment, surgery, patient management |

| Artificial Intelligence and Machine Learning in Lower Extremity Arthroplasty: A Review | The Journal of Arthroplasty 34 (2019) 2201-2203, https://doi.org/10.1016/j.arth.2019.05.055 |
|---|---|

Heather S. Haeberle, James M. Helm, Sergio M. Navarro, MBA,Jaret M. Karnuta, MS, Jonathan L. Schaffer, MD, MBA, John J. Callaghan, MD,Michael A. Mont, MD, Atul F. Kamath, MD, Viktor E. Krebs, MD,
Prem N. Ramkumar, MD, MBA

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| | |
|---|---|
| Task | ▪ Detection and conformation of a disease |
| Data Type | ▪ Slides, images |
| Yesteryears | o Pathologists share digital slide images for clinical use |
| Now | o Computer-aided diagnostic techniques + Large database of slides + AI → image diagnosis for cancer |

| | |
|---|---|
| Digital pathology and artificial intelligence | www.thelancet.com/oncology, 20, 2019 |
| Muhammad Khalid Khan Niazi, Anil V Parwani, Metin N Gurcan | |

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| | |
|---|---|
| Disease | ▪ Sepsis |
| Task | o Early identification<br>o Assistance of treatment |
| Output | o improved performance |

| Method. AI | | |
|---|---|---|
| 🕮 Machine Learning<br>🕮 Deep Learning Model<br>🕮 Neural Network<br>🕮 Causal Probabilistic Network | 🕮 Random Forest Model<br>🕮 Stochastic Gradient Boosting<br>🕮 Gradient-boosted tree model<br>🕮 Long short-term memory | 🕮 SVM<br>🕮 Fuzzy Logic<br>🕮 Cox proportional hazards model<br>🕮 Elastic Net logistic classifier |

Major risks of models.Medical data

- Bias (diagnosis criteria are part of the predictor variables like blood pressure)
- Poor generalizability due to overfitting
- Lack of standardized protocols in construction/validation → large gap between the AI embedded algorithms and their implementation in clinical practice

| | |
|---|---|
| Clinical applications of artificial intelligence in sepsis: A narrative review | Computers in Biology and Medicine115(2019)103488, https://doi.org/10.1016/j.compbiomed.2019.103488 |
| M. Schinkel, K. Paranjape, R.S. Nannan Panday, N. Skyttberg, P.W.B. Nanayakkara | |

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| | | | |
|---|---|---|---|
| Disease | ▪ LVD | | |
| Data Type | ▪ 12-lead electrocardiogram | Patients | 40,000 |
| Task | o To predict the risk for LVD on a different cohorts of 50,000 subjects | | |
| Method | o CNN<br>o Sensitivity: 86.3%, Specificity: 85.7%, Accuracy: 85.7%. | | |
| Uniqueness | o CNN classified positively some patients who do not have clinical LVD noticed later during follow-upthat these subjects were at 4 times the risk for developing LVD compared with other patients | | |

| | |
|---|---|
| Method | o Deep convoluted NN |
| Architecture | o The input layer is divided into small regions called local receptive fields → adjacent input values together<br>o Each local receptive field is connected to a single neuron in next convolutional layer.<br>o Convolutional layers comprise one or more feature maps<br>o Each feature map can only detect one input pattern<br>o For each input pattern, corresponding number of feature maps are created inside the convolutional layer<br>o The pooling layer creates a condensed feature map for each feature map of the convolutional layer → reduces further the number of neurons in the network<br>o Several sets of associating a convolutional layer and a pooling layer are used consecutively<br>o Output neurons classify the inputs into one of the output categories |

| | |
|---|---|
| Artificial Intelligence in Nephrology: Core Concepts, Clinical Applications, and Perspectives | Am J Kidney Dis. 1-8. doi: 10.1053/j.ajkd.2019.05.020 |
| Olivier Niel and Paul Bastard | |

**AI.Med — AI.Med — AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.MedAI.Med**

| | |
|---|---|
| AI | Visual orientated diagnosis<br>o Radiology, Pathology, Ophthalmology, Dermatology |
| Disease | 14 subcategories<br>▪ Emphysema, pulmonary nodules<br>▪ Pneumonia etc. |
| Data Type | ▪ National Institutes of Health (chestx-ray14)<br>▪ 112,120 radiographs<br>▪ 30,805 unique patients |
| Comparison | o Four radiologists<br>o One thoracic subspecialist<br>o Three generalists |

| | |
|---|---|
| Artificial Intelligence in Medicine:Where Are We Now? | Academic Radiology, 2019, https://doi.org/10.1016/j.acra.2019.10.001 |
| Sagar Kulkarni, MBBS, BSc, Nuran Seneviratne, MBBS, MA, Mirza ShaheerBaig, MBBS, BSc, Ameer Hamid Ahmed Khan, MBBS, BSc | |

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| | |
|---|---|
| Patient care | Centralised patient care<br>▪ Increased precision healthcare<br>▪ Less invasiveness<br>▪ Hospital length of stay yielding a cost-effective approach<br>▪ Prediction of clinical outcomes and death |
| Surgery | ▪ Ascending aortic aneurysm → optimizes patient and<br>▪ surgeon clinical outcomes and expectations |
| Method | ▪ Human intelligence +AI |
| AI Unique features | ✓ AI manifests in different shapes and forms |

| | |
|---|---|
| | ✓ Combines ability of computation with input and experiences<br>✓ Self-learning<br>✓ Ability to adapt for change<br>✓ Resemblance to human thought process<br>o Selective thinking |

| | |
|---|---|
| ArtiÞcial Intelligence in Aortic Surgery: The Rise of the Machine | Seminars in Thoracic and Cardiovascular Surgery (2019), https://doi.org/10.1053/j.semtcvs.2019.05.040 |
| Mohamad Bashir , Amer Harky | |

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| | |
|---|---|
| Patient care | ▪ Planning patient management |
| Software | DXplain<br>▪ Developed by computer science professionals at Massachusetts General Hospital during 1980s<br>o Assists in clinical decision-making and establishing diagnoses |
| Diagnosisassistance | AI + image recognition<br>✓ Automated electroencephalogram interpretation<br>✓ Electrocardiography analyses<br>✓ Facial recognition technology |

| | |
|---|---|
| Disease | ▪ Mitral valve (MV) disease |
| Type | ▪ Intraoperative 3D-transesophageal echocardiography |
| Data size | ▪ Four patients |
| Task | o Analysis with AI |

| | |
|---|---|
| Artificial Intelligence in Mitral Valve Analysis | Annals of Cardiac Anaesthesia,20, 2,2017, DOI: 10.4103/aca.ACA_243_16 |
| JelliffeJeganathan,ZiyadKnio, Yannis Amador, Ting Hai, ArashKhamooshian, Robina Matyal, Kamal R Khabbaz, Feroze Mahmood | |

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| | |
|---|---|
| Disease | Diabetes mellitus (dysfunction of glucose homeostasis)<br>▪ Type 1 diabetes (T1D)<br>▪ Type 2 diabetes (T2D)<br>▪ Gestational diabetes (GDM) |
| | 🕮 Blood glucose prediction<br>🕮 Blood glucose control strategies<br>🕮 Detection of adverse glycemic events<br>🕮 Insulin bolus calculators -- advisory systems<br>🕮 Risk and patient personalization<br>🕮 Lifestyle<br>▪ Detection of meals, exercise, faults<br>🕮 Daily-life support |

| | |
|---|---|
| Methods | ▪ Blood glucose prediction<br>o ANN, SVM, SR, KERNEL,DT, EAN, KNN, RF, EA, Naïve Bayes.<br>▪ Detection of adverse glycemic events<br>o PSO, Decision tree, PR |
| long-term complications- | ▪ Nephropathy<br>▪ Retinopathy<br>▪ Diabetic foot<br>▪ Cardiovascular disease or stroke |

#Publications: 1849 during years 2010 to 2018

| | |
|---|---|
| 🕮 Artificial intelligence (186) | 🕮 Computational intelligence (179) |
| 🕮 Machine learning (88) | 🕮 Deep learning (3) |
| 🕮 K-means (9) | 🕮 Fuzzy logic (24) |
| 🕮 Bayes (19) | 🕮 Heuristic (10) |
| 🕮 Clustering analysis (281) | 🕮 Decision tree (67) |
| 🕮 Clustering (510) | 🕮 Random forest (21) |
| 🕮 Particle swarm optimization (7) | 🕮 Pattern recognition (31) |
| 🕮 Genetic algorithm (43) | 🕮 Supervised algorithm (14) |
| 🕮 Unsupervised algorithm (9) | 🕮 Knowledge-based (14) |
| 🕮 Self-organizing map (4) | 🕮 Evolutionary computation (2) |
| 🕮 Neural network (72) | 🕮 Natural language processing (34) |
| 🕮 Case-based reasoning (11) | 🕮 Decision support system (71) |
| 🕮 Reinforcement learning (6) | 🕮 Support Vector machine (23) |
| 🕮 Data mining (111) | |

▶ Filtered to 141 in this review

| | |
|---|---|
| Artificial Intelligence for Diabetes Management and Decision Support: Literature Review | J Med Internet Res 2018;20(5):e10775) doi: 10.2196/10775 |
| Ivan Contreras, PhD; Josep Vehi1, PhD | |

**AI.Med — AI.Med — AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.MedAI.Med**

| | |
|---|---|
| Disease | ▪ Atrial fibrillation (A fib )<br>▪ Atrial flutter (A fl)<br>▪ Ventricular fibrillation (V fib ) |
| Data | ▪ Different ECG segments; input samples; 500; 1250 |
| Task | o Automatic detection & classification |
| Method | Deep.CNN<br>o Eleven-layers<br>o output layer (four neurons) |
| Hardware | o Workstation<br>o Two Intel Xeon 2.40 GHz (E5620) processors<br>o 24GB RAM |
| Unique advantages of DeepNN | o No need to experiment with<br>o Different features extraction techniques<br>o Choice of classifier methods |

| | |
|---|---|
| Future research | ! Improving performance of model by<br>o Increase of samples in each class<br>o Data augmentation<br>o Using bagging algorithm<br>! Exploring feasibility to diagnose<br>o Myocardial infarction<br>o Coronary artery diseases.<br>! Automatic classification ECG signals using CNN without performing any noise filtering |

| | |
|---|---|
| Automated detection of arrhythmias using different intervals of tachycardia ECG segments with convolutional neural network | Information Sciences 405 (2017) 81–90, http://dx.doi.org/10.1016/j.ins.2017.04.012 |
| U. Rajendra Acharya, Hamido Fujita, Oh Shu Lih, Yuki Hagiwara, Jen Hong Tan, Muhammad Adam | |

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| | |
|---|---|
| Disease | ▪ Ventricular Arrhythmias |
| Data Type | 2sec ECG: Episodes; Non-shockable: 48, 095; Shockable: 6,001 |
| Method | Deep CNN |

| 2sec ECG | Episodes |
|---|---|
| Non-shockable | 48, 095 |
| Shockable | 6,001 |

| Layer | TF |
|---|---|
| 1,3,5,7,9,10 | Leaky rectifier linear unit (LReLU) |
| 11 | SoftMax |
| Biases of each layer set to 1.0 | |

| Layers | Operation | # neurons in OL |
|---|---|---|
| 0 to 1 | Convolution | 496x3 |
| 1-2 | Max pooling | 248x3 |
| 2-3 | Convolution | 244x5 |
| 3-4 | Max pooling | 122x5 |
| 4-5 | Convolution | 118x10 |

| | |
|---|---|
| Automated identification of shockable and non-shockable life-threatening ventricular arrhythmias using convolutional neural network | Future Generation Computer Systems, 2017, http://dx.doi.org/10.1016/j.future.2017.08.039 |
| U Rajendra Acharya, Hamido Fujita, Shu Lih Oh, U Raghavendra, Jen Hong Tan, Muhammad Adam, Arkadiusz Gertych, Yuki Hagiwara | |

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| | |
|---|---|
| Disease | MI |
| Data Type | ECG beats (with noise and without noise) |
| FOM | Average accuracy<br>93.53% with noise<br>95.22% after noise removal |

| Method | Deep CNN |
|---|---|

| Layers | Type | #neurons (Output Layer) | Kernel size |
|---|---|---|---|
| 0–1 | Convolution | 550 ×3 | 102 |
| 1–2 | Max-pooling | 275 ×3 | 2 |
| 2–3 | Convolution | 252 ×10 | 24 |
| 3–4 | Max-pooling | 126 ×10 | 2 |
| 4–5 | Convolution | 116 ×10 | 11 |
| 5–6 | Max-pooling | 58 ×10 | 2 |
| 6–7 | Convolution | 50 ×10 | 9 |
| 7–8 | Max-pooling | 25 ×10 | 2 |
| 8–9 | Fully-connected | 30 | – |
| 9–10 | Fully-connected | 10 | – |
| 10–11 | Fully-connected | 2 | – |

| | |
|---|---|
| Regularization | To prevent overfitting of the data |
| Momentum | To control how fast or slow the network learn during training |
| Learning rate | To help in the convergence |

| Confusion matrix of ECG beats | | |
|---|---|---|
| | Normal | MI |
| Normal | 9933 | 613 |
| MI | 1814 | 38 ,368 |

| Application of deep convolutional neural network for automated detection of myocardial infarction using ECG signals | Information Sciences 415–416 (2017) 190–198, http://dx.doi.org/10.1016/j.ins.2017.06.027 |
|---|---|
| U. Rajendra Acharya, Hamido Fujita, ShuLih Oh, Yuki Hagiwara, Jen Hong Tan, Muhammad Adam | |

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**CDSS (Clinical Decision Support System)**

Requires
- Rigorous evidence of system's safety
- Reliability as well as scientific evidence for each advice outputted
- Should be similar to or better than the standard practice
- Not perfect tools ; have failures.
  - Future remedies: fail-safe designs; harm free

Built based on
- Linkages between clinical data and gold standards
  - Eg, biopsies, autopsies, biomolecular markers, or surgical findings)

Therapeutic support system
- No gold standard
- Disagreement, even among experts

**If** a therapeutic advice by system and an expert clinician reach different conclusions

**Then** difficult to manage a specific case, [as it is not clear which is "correct"]

AI-med-04-Rev

Applications of machine learning in medicine

- Assessing risk of onset of the disease
- Estimating treatment success
- Managing or alleviating complications
- Ongoing patient care
- Ongoing pathology
- Treatment efficacy research

| | | |
|---|---|---|
| MYCIN | Infectious diseases<br>o Diagnosis<br>o Recommend treatment | Dosage of drug for serious infections |
| GUIDON | Intelligent computer-aided instruction program | Teaching infectious disease diagnosis to medical students |
| Analysis of hand movements of expert/ novice surgeons | AI-based measure | o Provides feedback on surgeons' current skill levels<br>o Used to inform areas of improvement |
| INTERNIST-1 | Assists health care professionals in patient diagnosis | Knowledge database of 570 diseases |

| | |
|---|---|
| CASNET | Glaucoma care |
| EXPERT | Models for reasoning in<br>o Rheumatology, Endocrinology |
| Prediction of risk of congenital heart disease (CHD) in pregnant women | Machine learning |
| Prediction of conventional risk factors in mitral valve analysis | Three-dimensional cardiac motion |
| Prediction of individuals at high risk for colorectal cancer | Electronic medical records |
| Identification of depression from human speech patterns | Neural network models |
| o Emergency room visit<br>o Hospital outcome | IBM Research (Yorktown Heights, NY, USA) and Google (Mountain View), CA |
| Automated diagnosing congenital heart disease | 1035 patients |

| | |
|---|---|
| Diagnosis<br>o Melanoma<br>o Dementia<br>o Diabetic retinopathy | Predicting the outcome<br>▪ Radiation therapy<br>▪ Acute respiratory disease events<br>▪ Mortality in smokers |

- Tuberculosis
- Glaucoma

Prediction of
- Breast cancer prognosis
- Depression in breast cancer patients
- Neurosurgical outcomes in focal epilepsy patients
- Ischemic stroke
- Thromboembolism in patients with atrial fibrillation
- Cardiovascular risk factors from retinal fundus images

- Success of substance abuse disorder treatment
- Onset of diabetes
- HIV transmission patterns
- Prolonged postoperative ventilation in patients undergoing coronary artery bypass grafting

| Artificial intelligence in medicine: What is it doing for us today? | Health Policy and Technology 8 (2019) 198–205, https://doi.org/10.1016/j.hlpt.2019.03.004 |
|---|---|

Aliza Becker

AI.Med — AI.Med — AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.MedAI.Med

Guidelines for clinicians in
- AI supported diagnostic tools
- Feature selection
- General medicine
- Cardiology + AI + machine learning
- Frequent pitfalls Ex.: improper dichotomization

| Artificial Intelligence in Cardiology | Journal of the American College Of Cardiology, 71(23)(2018) 2 6 6 8 – 7 9 doi.org/10.1016/j.jacc.2018.03.521 |
|---|---|

Kipp W. Johnson, BS, Jessica Torres Soto, MS,c, Benjamin S. Glicksberg, PHD, Khader Shameer, PHD, Riccardo Miotto, PHD, Mohsin Ali, MPHIL, Euan Ashley, MBCHB, DPHIL, Joel T. Dudley, PHD

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PD (Parkinson's Disease) diagnosis
- Yesteryears
  - High dimensionality in multimodal MRI data
  - Traditional mathematical analysis
  - Could not effectively extract the huge information in them →
  - Accuracy of PD diagnosis in large sample size is still unsatisfying

**Remedy**: AI [varieties of statistical models + machine learning algorithms]

| Data & Images | |
|---|---|
| rsfMRI | Resting state functional MRI |
| sMRI | Structural MRI |
| DTI | Diffusion tensor imaging |
| PIGD | Postural instability and gait difficulty |

| | |
|---|---|
| Use of Magnetic Resonance Imaging and Artificial Intelligence inStudies of Diagnosis of Parkinson's Disease | ACS Chem. Neurosci. 2019, 10, 2658−2667, DOI: 10.1021/acschemneuro.9b00207 |
| Jingjing Xu and Minming Zhang | |

**AI.Med — AI.Med — AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.Med— AI.Med — AI.MedAI.Med**

AI + MachLrn
- Diagnostic support
- Neurodegenerative movement disorders of parkinsonian type

Monitoring disease

| Machine learning algorithms | |
|---|---|
| SVM | Tree-based algorithms |
| k-Nearest Neighbors | Decision Trees |
| Naïve Bayes | AdaBoost DT |
| Artificial Neural Networks | Random Forest |
| Linear Discriminant Analysis | Random Trees |

| | |
|---|---|
| Artificial intelligence for assisting diagnostics and assessment of Parkinson's disease—A review | Clinical Neurology and Neurosurgery 184 (2019) 105442, |
| MinjaBelić, VladislavaBobić, MilicaBadža, Nikola Šolaja, MilicaĐurić-Jovičić, Vladimir S. Kostic | |

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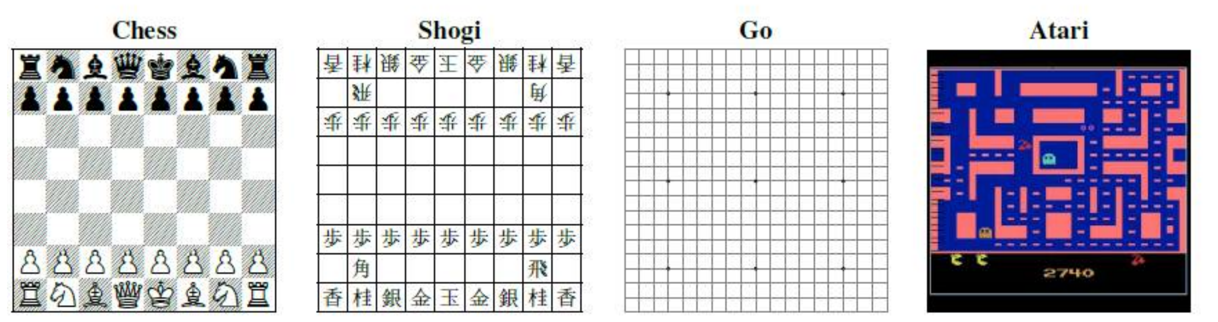
|---|---|
| Computational intelligence techniques for medical diagnosis and prognosis: Problems and currentdevelopments | Biocybernetics and biomedical engineering 39( 2019)638-672, https://doi.org/10.1016/j.bbe.2019.05.010 |
| Afzal Hussain Shahid, M.P. Singh | |

| | |
|---|---|
| Computational intelligence approaches for classification of medical data: State-of-the-art, future challenges and research directions | Neurocomputing 276 (2018) 2–22, https://doi.org/10.1016/j.neucom.2017.01.126 |
| Ali Kalantari ,AmirrudinKamsin, ShahaboddinShamshirband, Abdullah Gani, Hamid Alinejad-Rokny, Anthony T. Chronopoulos | |

# Part 2(b) AI. Games (Ag)



MuZero algorithm: Tree-based search + Learned model

- Achieves superhuman performance
- Without any knowledge of underlying dynamics of system
  - 57 different Atari games
  - Go, Chess, Shogi

| Muzero-arxiv | |
|---|---|
| Mastering Atari, Go, Chess and Shogi by Planning with a Learned Model | arXiv:1911.08265v1 [cs.LG] 19 Nov,2019 |
| Julian Schrittwieser, IoannisAntonoglou, Thomas Hubert, Karen Simonyan, Laurent Sifre, Simon Schmitt, Arthur Guez, Edward Lockhart, Demis Hassabis, Thore Graepel, Timothy Lillicrap, David Silver | |

**IBM ventures in Games**

| | |
|---|---|
| **Deep Blue** | Solves (complex, strategic) chess game |
| Applications. Of DeepBlue | Discovery of medical drugs<br>Financial modeling→<br>to identify trends;<br>do risk analysis;<br>Large database searches<br>Massive calculations<br>in many fields of science<br>To explore/understand limits of massively parallel processing |
| Life cycle | Deep Blue was retired to Smithsonian Museum in Washington, DC |

| | |
|---|---|
| Deep Blue | 200 million possible chess positions per second<br>( IBMers knew power of machine) |

Deep Blue versus human grandmaster

| #Game. chess | Winning partner |
|---|---|
| 1 | ✓ grandmaster won |
| 2 | ✓ Deep Blue won |
| 3,4,5 | ▪ Draw between two players |
| 6, end match | ✓ Deep Blue made a crushing defeat of the champion |

- Match's outcome made headlines worldwide
- Helped a broad audience better understand high-powered computing

| | |
|---|---|
| **IBM Blue Gene** | Applications in<br>▪ Gene science |

| | |
|---|---|
| **IBM Watson** | Substantial step forward from Deep Blue<br>Software for natural language processing (NLP)<br>Relies on the massive supply of information poured into machine<br>Demonstrated whole new generation of human - machine interactions |

| | |
|---|---|
| GO game | o Search algorithm : Monte Carlo simulation + value and policy networks. →<br>o Alphago program achieved 99.8% winning rate against other Go programs<br>o Defeated human European Go champion by 5 games to 0. |

| | |
|---|---|
| Mastering the game of Go with deepneural networks and tree search | Nature, 529(2016)484 |
| David Silver, Aja Huang, Chris J. Maddison, Arthur Guez, Laurent Sifre, George van den Driessche, Julian Schrittwieser, IoannisAntonoglou, Veda Panneershelvam, Marc Lanctot, Sander Dieleman, DominikGrewe,John Nham, NalKalchbrenner, Ilya Sutskever, Timothy Lillicrap, Madeleine Leach, KorayKavukcuoglu,ThoreGraepe&Demis Hassabis | |

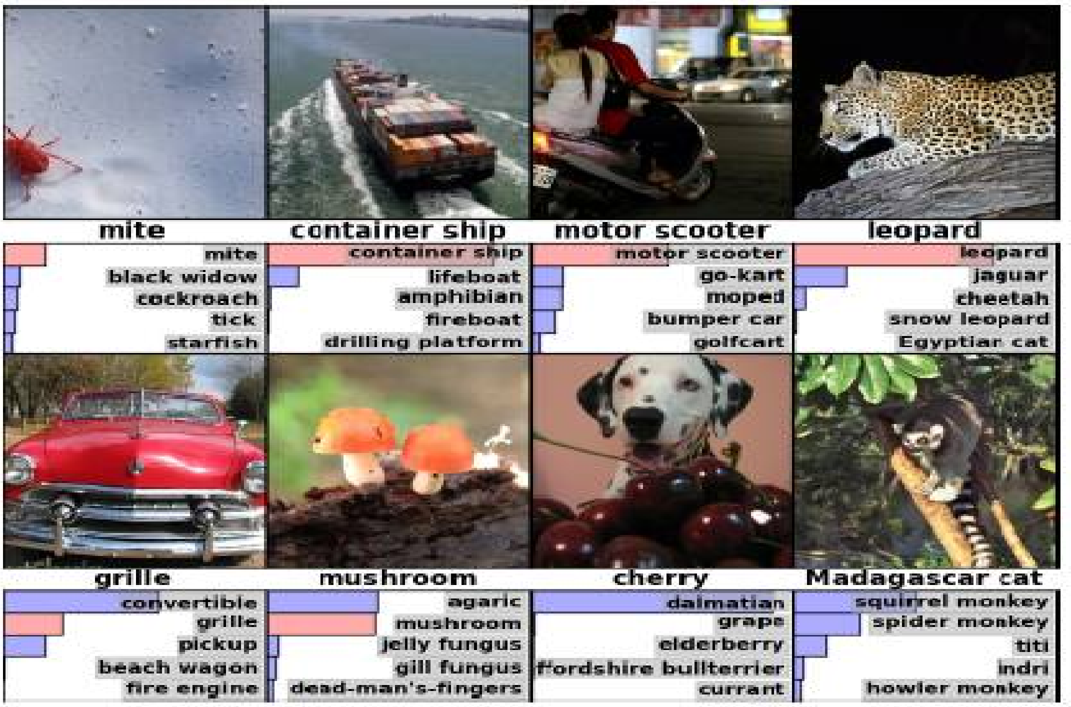
- ! AlphaGo
- ! AlphaGo Zero
- ! AlphaGo Master
- ! AlphaGo Lee
- ! AlphaGo Fan

| | |
|---|---|
| | **AlphaGo** |
| | First program to defeat a world champion in game of Go |
| Tree Search | Evaluated positions and selected moves using deep neural networks |
| Training Algs | ☞ Supervised learning from human expert moves<br>☞ Reinforcement learning from self-play |
| | 🕮 Solely on reinforcement learning<br>🕮 Only game rules<br>🕮 No human data<br>🕮 No guidance<br>🕮 No domain knowledge<br>→<br>🕮 AlphaGo becomes its own teacher |

| | |
|---|---|
| AlphaGo Zero program | o Achieved superhuman performance in the game of Go within 24 hours<br>Work (Method) flow<br>o Starts with random play<br>o<br>o Learning from self-play games + Tabula Rasa Reinforcement<br>o Games of chess ; shogi (Japanese chess)<br>o Defeated a World-champion program in each case |
| | o Input: game rules<br>o No domain knowledge |
| | 🕮 Achieved superhuman performance<br>🕮 Winning 100–0 against previously published, champion-defeating AlphaGo |

| | |
|---|---|
| | 🕮 Head to head against AlphaGo Master in a 100-game match with 2-h time controls won by 89 games to 11 |

| | |
|---|---|
| Mastering the game of Go without human knowledge | N at u r e, 550, 2017, doi:10.1038/nature24270 |
| David Silver, Julian Schrittwieser, Karen Simonyan, IoannisAntonoglou, Aja Huang, Arthur Guez,Thomas Hubert, Lucas Baker, Matthew Lai, Adrian Bolton, Yutian Chen, Timothy Lillicrap, Fan Hui, Laurent Sifre,George van den Driessche, Thore Graepel &Demis Hassabis | |




- ILSVRC-2010 test images
- Correct label under each image

Courtesy of Communications of the ACMMay 2017 https://doi.org/10.1145/3065386
Vol 60, NO 6; 84-90

| Contest | LSVRC-2010 |
|---|---|
| Task | Classification |
| Database | ▪ ImageNet<br>▪ 1.2 million high-resolution images |
| # Classes | ▪ 1000 |
| Error rates | ▪ Top-1 (37.5%)<br>▪ top-5 (17.0%)<br>▪ Better compared to previous |

| Parameters | 🕮 60 million |
|---|---|
| Neurons | 🕮 650,000 |
| Architecture (Layers & connections) | 🕮 Five convolutional layers<br>🕮 Three fully-connected layers<br>🕮 non-saturating neurons |
| TFs | 🕮 1000-way softmax |

| | |
|---|---|
| | state-of-the-art NNs |

| | |
|---|---|
| Processors | 🕮 GPUs<br>🕮 To implement,convolution operation |
| Regularization method | 🕮 Dropout<br>o Reduces overfitting in fully-connected layers |

☞ First column: test images (Five) ILSVRC-2010
☞ 2 to 7 Columns: training images in the last hidden layer

| | |
|---|---|
| ImageNet Classification with Deep Convolutional Neural Networks | Communications of the ACM Vol 60, NO 6; 2017, 84-90<br>doi.org/10.1145/3065386 |

Alex Krizhevsky, Ilya Sutskever, Geoffrey E. Hinton

| | |
|---|---|
| Contest | ILSVRC-2012 |
| Error rates (winning) | 🕮 test error rate<br>🕮 top-5(15.3%)<br>🕮 second-best entry (26.2%) |

| | |
|---|---|
| Processors | GPUs<br>🕮 Highly-optimized implementation of 2D convolution<br>🕮 All operations in training Convol-NN |
| ImageNet | Full data set :<br>🕮 Over 15 million labeled high-resolution images<br>🕮 22,000 categories |

| | |
|---|---|
| Small databases of image | |
| Tens of thousands of images | ☞ NORB<br>☞ Caltech-101/256<br>☞ CIFAR-10/100 |
| Current best error rate on the MNIST digit- | ✓ Recognition task (<0.3%)<br>✓ Approaches human performance |
| Larger datasets | LabelMe<br>hundreds of thousands of fully-segmented images |

| | |
|---|---|
| Game of checkers | o Machine learns within a short period of time 18<br>o Input: rules of the game + a sense of direction |

| | |
|---|---|
| Strongest programs for Chess | o Sophisticated search techniques +<br>o Domain-specific adaptations +<br>o Handcrafted evaluation functions<br>o →<br>o Refined by human experts over several decades |

| | |
|---|---|
| Mastering Chess and Shogi by Self-Play with aGeneral Reinforcement Learning Algorithm | arXiv:1712.01815 [cs.AI] , 2017 Dec 5 |
| David Silver, Thomas Hubert, Julian Schrittwieser, IoannisAntonoglou, Matthew Lai, Arthur Guez, Marc Lanctot,<br>Laurent Sifre, Dharshan Kumaran, ThoreGraepel,TimothyLillicrap, Karen Simonyan, Demis Hassabis | |

# Part 2(c) AI. Neocognitron

| | |
|---|---|
| NN | Neocognitron |
| Learning rule | Add-if-silent |

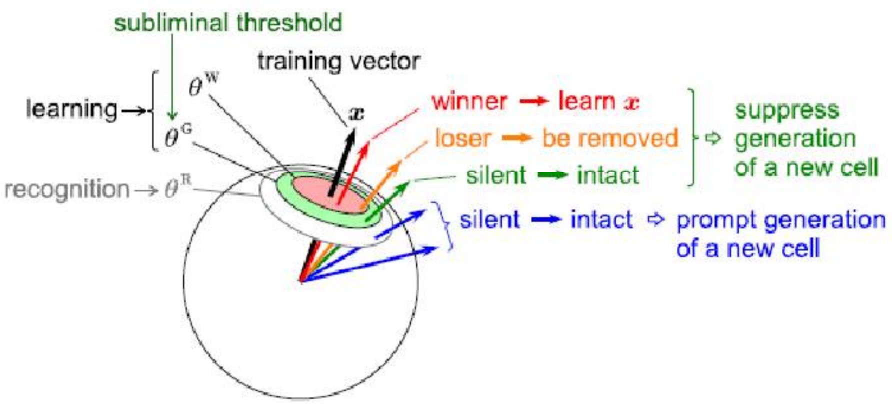
| | |
|---|---|
| | Learning process<br>+ Much simpler<br>+ More stable |

| | |
|---|---|
| Artificial vision by multi-layered neural networks: Neocognitron and its advances | Neural Networks 37 (2013) 103–119, doi:10.1016/j.neunet.2012.09.016 |
| Kunihiko Fukushima | |

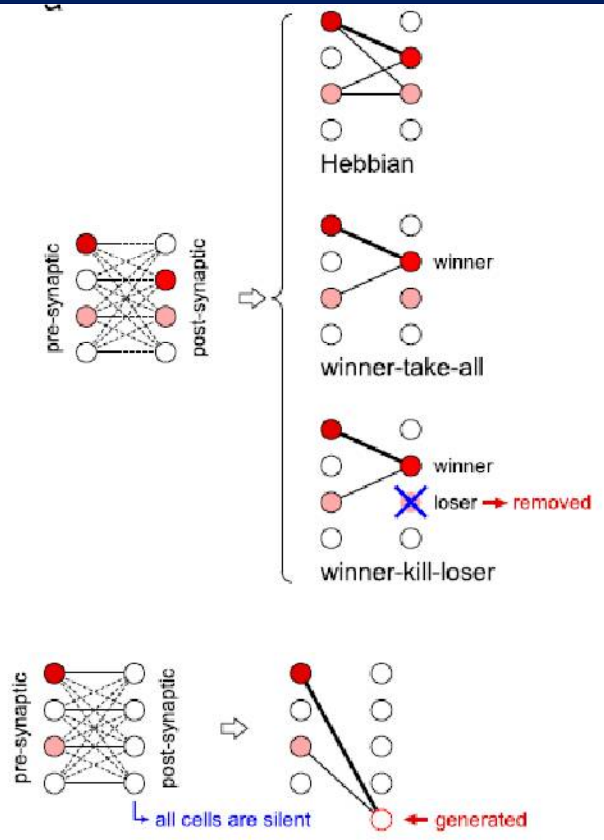
**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI—**

| | |
|---|---|
| NN | Neocognitron |
| Learning rule | o Winner-kill-loser triple threshold competitive learning rule |
| | Learning process more stable. In particular, a high recognition rate can be obtained with a smaller network |
| Application task | Character recognition |
| | Outperform standard winner-take-all learning |

| | |
|---|---|
| Improvements. Neocognitron | 🕮 Disinhibition to the inhibitory surround in the connections to C-cells (or complex cells) from S-cells (or simple cells);<br><br>🕮 Square root shaped saturation in the input-to-output characteristics of C-cells. |
| | + Large increase in recognition rate |




| | dual threshold | triple threshold | |
|---|---|---|---|
| learning phase | $\theta^L$ | $\theta^W$ | for choosing a winner & losers |
| | | $\theta^G$ | for generating a new cell-plane |
| recognition phase | $\theta^R$ | $\theta^R$ | |




| | |
|---|---|
| Neocognitrontrainedbywinner-kill-loserwithtriplethreshold | Neurocomputing129(2014)78–84, http://dx.doi.org/10.1016/j.neucom.2012.05.038 |
| KunihikoFukushima, IsaoHayashi, JasminLéveillé | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI—**

| NN | Neocognitron |
|---|---|
| Learning rule | winner-kill-loser |

| | |
|---|---|
| **If** | all cells are silent |
| **Then** | new cell is generated |

| | |
|---|---|
| Neocognitron trained with winner-kill-loser rule | Neural Networks 23 (2010) 926-938, doi:10.1016/j.neunet.2010.04.008 |
| KunihikoFukushima | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI--**

| NN | Neocognitron |
|---|---|
| Learning rule | o Add-if-silent<br>Learning process<br>+ Computational cost largely reduced |

| | |
|---|---|
| | + High recognition rate without increasing the scale of the network<br>+ Simpler<br>+ More stable |
| Application task | Handwritten digitsrecognition |

| | |
|---|---|
| Training multi-layered neural network neocognitron | Neural Networks 40 (2013) 18–31, doi:10.1016/j.neunet.2013.01.001 |
| KunihikoFukushima | |

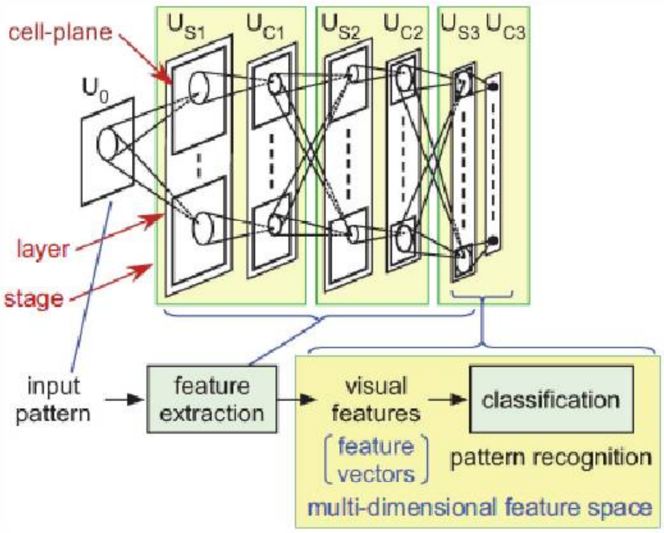
**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI--**

| | |
|---|---|
| NN | Neocognitron |
| Learning rule | o Add-if-silent |
| Task | Regression problem |
| Application | Image patternrecognition |
| Intermediate function | RBF |
| Dataset | Bike Sharing |

| | |
|---|---|
| AI-Neocog-19 | |
| Training multi-layered neural network neocognitron | Neural Networks 40 (2013) 18–31, 2013. doi:10.1016/j.neunet.2013.01.001 |
| KunihikoFukushima | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI--**

| | |
|---|---|
| NN | Neocognitron |
| Deepest(highest) Layer | o Interpolating-Vector→ |
| Search | o Search the nearest planeamong trios containing nearest referencevectors |
| | o Reference vectors for each class are created from a set of training vectors.<br>o To recognize an input vector, distances based on similarities measured between the input vector and planes that are spanned by every trio of reference vectors of the same class |
| | Creation of compact set of reference vectors<br>o Step 1: Reference vectors chosen from training set<br>o Step 2:Reference vectors modified after enough number of reference vectors have been chosen |
| Application | Simulated Hand-written digits |

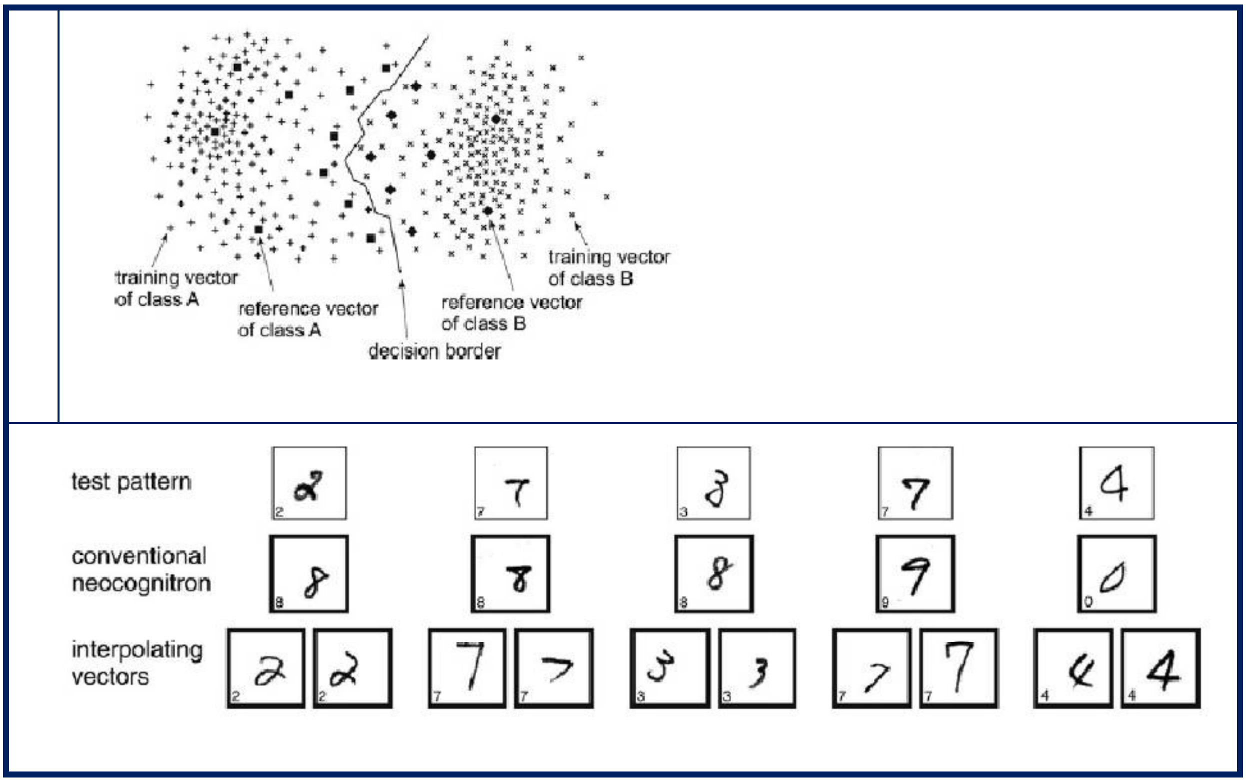



| NN | Neocognitron | |
|---|---|---|
| Architecture | Multi-layered convolutionalnetwork | |
| | Intermediate layers | Local featuresextracted from input patterns |
| | Highest (or deepest) Layers | Interpolating-Vector method used for classifying patterns based on the features extracted byintermediate layers |
| Application | robust recognition of visual patterns | |

| Deep Convolutional Network Neocognitron: Improved Interpolating-Vector | IEEE, 2015, xxx |
|---|---|
| KunihikoFukushima, HayaruShouno | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI--**

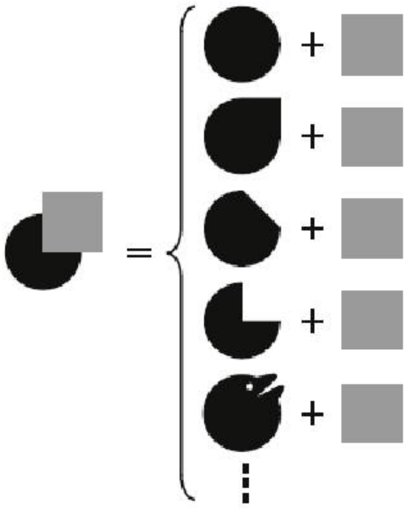
| NN | Neocognitron |
|---|---|
| Learning rule | Competitive learning<br>o Interpolating vectors for classifying patterns.<br>o Labeled reference vectors in a multi-dimensional feature space |
| Application task | Digit recognition |
| Data | o Blind test set of 5000 handwritten digits<br>+ Error rate educed from 1.52% to 1.02% |



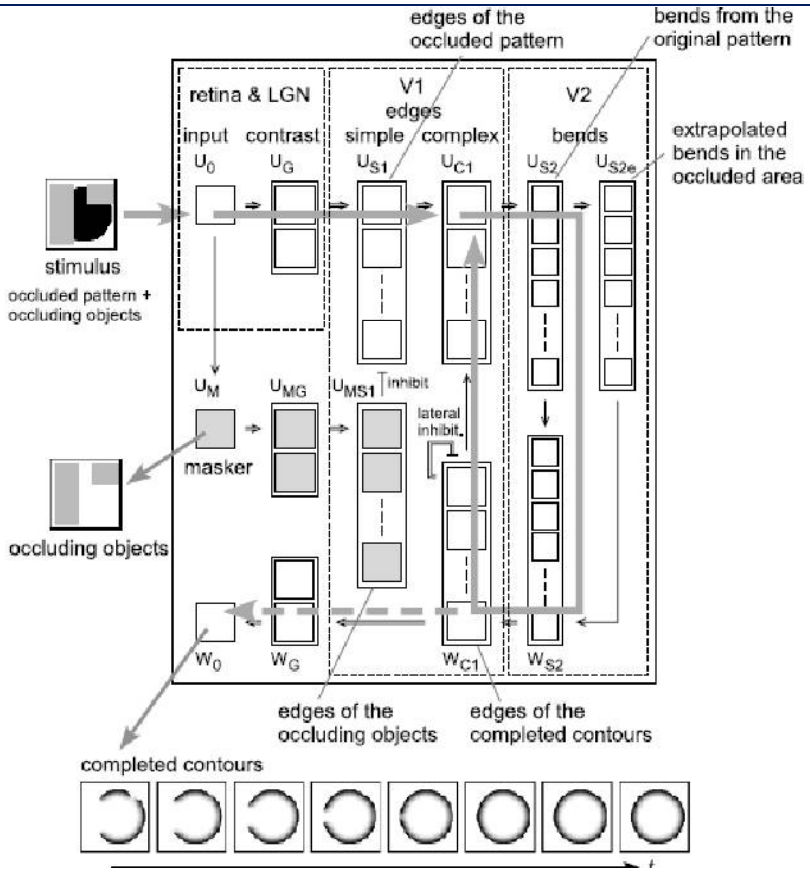

| | |
|---|---|
| Interpolating vectors for robust pattern recognition | Neural Networks 20 (2007) 904–916, doi:10.1016/j.neunet.2007.06.003 |
| KunihikoFukushima | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI--**

| NN | Neocognitron + Amodal completion | |
|---|---|---|
| Architecture | o Hierarchical multilayered Network<br>▪ bottom-up and top-down signal paths. | |
| | Cells of area V1 | Respond selectively to edges of a particular orientation, |
| | Cells of area V2 | Respond selectively toa particular angle of bend. |
| | Responses of bend-extracting cells | Model predicts<br>o Curvature<br>o Location of occluded contours<br>o Missing contours gradually extrapolated/interpolated from the visible contours |
| Application | Estimation of shape of occluded contours from visible parts of the contoursby.amodal completion | |



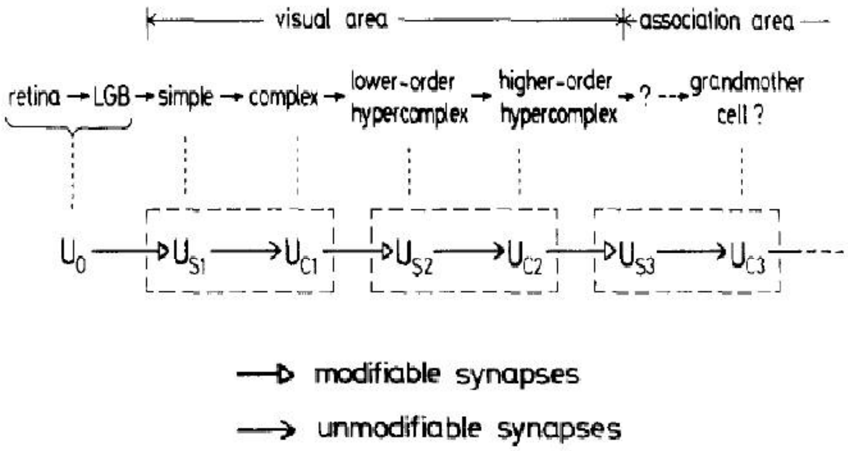
Architecture of the model for amodal completion




| Neural network model for completing occluded contours | Neural Networks 23 (2010) 528540, doi:10.1016/j.neunet.2009.10.002 |
| --- | --- |
| KunihikoFukushima | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI--**

| NN | Neocognitron |
| --- | --- |

| Architecture |  |
|---|---|

| Neocognitron: A Self-organizing Neural Network Model for a Mechanism of Pattern Recognition Unaffected by Shift in Position | Biol. Cybernetics 36, 193 202 (1980) |
|---|---|
| KunihikoFukushima | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI—**

| NN | Neocognitron |
|---|---|
| Method | IntVec (interpolating-vector) |
| Learning rule | Margined Winner-Take-All (mWTA) for training the deepest layer |
| Algorithm | Learning<br>For each training pattern<br>If result of recognition by WTA (Winner-Take-All) is in error<br>a new cell is generated in the deepest layer.<br>End if<br>End for<br>▶ Margin introducing to the WTA<br>▶ A compact set of cells can generated with high recognition rate |

| A Deep Neural Network Architecture Using Dimensionality Reduction with Sparse Matrices | A. Hirose et al. (Eds.): ICONIP 2016, Part IV, LNCS 9950, pp. 397–404, 2016, DOI: 10.1007/978-3-319-46681-1_48 |
|---|---|
| Wataru Matsumoto, Manabu Hagiwara, Petros T. Boufounos, KunihikoFukushima, ToshisadaMariyama, and Zhao Xiongxin | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI—**

| Automatic Design of Neural Network Structures Using AiS | ICONIP 2016, Part II, LNCS 9948, pp. 280–287, 2016. DOI: 10.1007/978-3-319-46672-9_32 |
|---|---|
| ToshisadaMariyama, KunihikoFukushima and Wataru Matsumoto1 | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI—**

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| A Probabilistic WKL Rule for Incremental Feature Learning and Pattern Recognition | J. Advanced Computational Intelligence and Intelligent Informatics,.18 (4) 2014,672-681 |
| Jasmin Leveille, Isao Hayasi, and KunihikoFukushima | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI--**

| | |
|---|---|
| Margined winner-take-all: New learning rule for pattern recognition | Neural Networks 97 (2018) 152–161, https://doi.org/10.1016/j.neunet.2017.10.005 |
| KunihikoFukushima | |

**AI -- Neocognitron — NN — Fukushima — Neocognitron — NN — Fukushima — AI--**

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| Rectier Nonlinearities Improve Neural Network Acoustic Models | Proceedings of the 30 th International Conference on Ma-chine Learning, Atlanta, Georgia, USA, 2013. JMLR |
| Andrew L. Maas, Awni Y. Hannun, Andrew Y. Ng | |

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| Digital selection and analogue amplification coexist in a cortex-inspired silicon circuit | Nature, 405, 2000, 947-951 |
| Richard H. R. Hahnloser, Rahul Sarpeshkar, Misha A. Mahowald, Rodney J. Douglas & H. Sebastian Seung | |

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| Gradient-Based Learning Applied to Document Recognition | Proceedings of the IEEE, 86, 11,1998 |
| YANN LECUN, MEMBER, IEEE, L´EON BOTTOU, YOSHUA BENGIO, AND PATRICK HAFFNER | |

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| Deep Sparse Rectier Neural Networks | Proceedings of the 14th International Con-ference on Articial Intelligence and Statistics(AISTATS) 2011, Fort Lauderdale, FL, USA. Volume 15 of JMLR |
| Xavier Glorot Antoine BordesYoshuaBengio | |

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| PHONE RECOGNITION WITH DEEP SPARSE RECTIFIER NEURAL NETWORKS | IEEE ICASSP 2013, 6985-6989 |
| LaszloToth | |

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