Andreas Holzinger 185.A83 Machine Learning for Health Informatics 2018S, VU, 2.0 h, 3.0 ECTS

Lecture 09 - Module 07 - Week 23 - 05.06.2018



From Clinical Decision Support to explainable AI (ex-AI)

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Advance Organizer (2/2)

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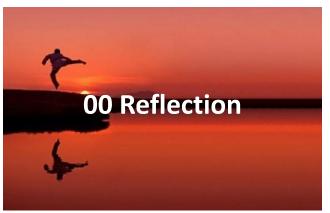
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- DXplain = a DSS from the Harvard Medical School, to assist making a diagnosis (clinical
  consultation), and also as an instructional instrument (education); provides a
  description of diseases, etiology, pathology, prognosis and up to 10 references for each
  disease;
- Etiology = in medicine (many) factors coming together to cause an illness (see causality)
- Explainable AI = Explainability = upcoming fundamental topic within recent AI; answering e.g. why a decision has been made
- Expert-System = emulates the decision making processes of a human expert to solve complex problems;
- GAMUTS in Radiology = Computer-Supported list of common/uncommon differential diagnoses;
- ILIAD = medical expert system, developed by the University of Utah, used as a teaching
  and testing tool for medical students in problem solving. Fields include Pediatrics,
  Internal Medicine, Oncology, Infectious Diseases, Gynecology, Pulmonology etc.
- Interpretability = there is no formal technical definition yet, but it is considered as a prerequisite for trust
- MYCIN = one of the early medical expert systems (Shortliffe (1970), Stanford) to identify bacteria causing severe infections, such as bacteremia and meningitis, and to recommend antibiotics, with the dosage adjusted for patient's body weight;
- Reasoning = cognitive (thought) processes involved in making medical decisions (clinical reasoning, medical problem solving, diagnostic reasoning;
- Transparency = opposite of opacity of black-box approaches, and connotes the ability
  to understand how a model works (that does not mean that it should always be
  understood, but that in the case of necessity it can be re-enacted

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**№ HCI-**KDD <del>%</del>



Keywords Keywords

- Decision support system (DSS)
- MYCIN Rule Based Expert System
- GAMUTS in Radiology
- Reasoning under uncertainty
- Example: Radiotherapy planning
- Example: Case-Based Reasoning
- Explainable Artificial intelligence
- Re-trace > Understand > Explain
- Transparency > Trust > Acceptance
- Fairness > Transparency > Accountability
- Methods of Explainable AI

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Learning Goals: At the end of this lecture you ...

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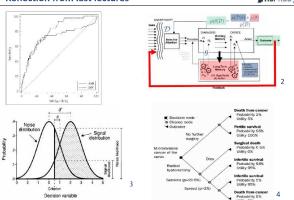
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 ... can apply your knowledge gained in the previous lectures to example systems of decision support;

- ... have an overview about the core principles and architecture of decision support systems;
- ... are familiar with the <u>certainty factors</u> as e.g. used in MYCIN;
- ... are aware of some design principles of DSS;
- ... have seen <u>similarities between DSS and KDD</u> on the example of computational methods in cancer detection;
- ... have seen basics of CBR systems;

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Reflection from last lectures



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Advance Organizer (1/2)

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- Case-based reasoning (CBR) = process of solving new problems based on the solutions
  of similar past problems:
- Certainty factor model (CF) = a method for managing uncertainty in rule-based systems;
- CLARION = Connectionist Learning with Adaptive Rule Induction ON-line (CLARION) is a cognitive architecture that incorporates the distinction between implicit and explicit processes and focuses on capturing the interaction between these two types of processes. By focusing on this distinction, CLARION has been used to simulate several tasks in cognitive psychology and social psychology. CLARION has also been used to implement intelligent systems in artificial intelligence applications.
- Clinical decision support (CDS) = process for enhancing health-related decisions and actions with pertinent, organized clinical knowledge and patient information to improve health delivery:
- Clinical Decision Support System (CDSS) = expert system that provides support to certain reasoning tasks, in the context of a clinical decision;
- Collective Intelligence = shared group (symbolic) intelligence, emerging from cooperation/competition of many individuals, e.g. for consensus decision making;
- Crowdsourcing = a combination of "crowd" and "outsourcing" coined by Jeff Howe
  (2006), and describes a distributed problem-solving model; example for crowdsourcing
  is a public software beta-test;
- Decision Making = central cognitive process in every medical activity, resulting in the selection of a final choice of action out of several alternatives;
- Decision Support System (DSS) = is an IS including knowledge based systems to interactively support decision-making activities, i.e. making data useful;

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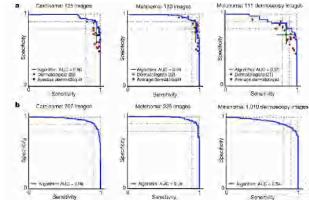
Agenda

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- 00 Reflection follow-up from last lecture
- 01 Decision Support Systems (DSS)
- 02 Computers help making better decisions?
- 03 History of DSS = History of AI
- 04 Example: Towards Personalized Medicine
- 05 Example: Case Based Reasoning (CBR)
- 06 Towards Explainable AI
- 07 Some methods of explainable AI

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How do you explain this ...



Sensitivity Sensitivity
Andre Esteva, Brett Kuprel, Roberto A. Novoa, Justin Ko, Susan M. Swetter, Helen M. Blau & Sebastian Thrun 2017

Dermatologist-level classification of skin cancer with deep neural networks. Nature, 542, (7639), 115-118

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- Remember: Medicine is an complex application domain dealing most of the time with probable information!
- Some challenges include:
- (a) defining hospital system architectures in terms of generic tasks such as diagnosis, therapy planning and monitoring to be executed for (b) medical reasoning in (a);
- (c) patient information management with (d) minimum uncertainty.
- Other challenges include: (e) knowledge acquisition and encoding, (f) human-computer interface and interaction; and (g) system integration into existing clinical legacy and proprietary environments, e.g. the enterprise hospital information system; to mention only a few.

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## **01 Decision Support Systems**

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### Decision Making is central in any (medical) work

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Medlock, S., Opondo, D.,

Wierenga, P., de Rooij, S. E. &

Abu-Hanna, A. (2011) LERM

Eslami, S., Askari, M.,

(Logical Elements Rule

Method): A method for

assessing and formalizing

clinical rules for decision

286-295

support. International Journal

of Medical Informatics, 80, 4,

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### Search in an arbitrarily high-dimensional space < 5 min.! SHCI-KDD Search in an arbitrarily high-dimensional space < 5 min.!



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### Digression: Clinical Guidelines as DSS & Quality Measure PHCI-KDD &

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- Clinical guidelines are systematically developed documents to assist doctors and patient decisions about appropriate care:
- In order to build DS, based on a guideline, it is formalized (transformed from natural language to a logical algorithm), and
- implemented (using the algorithm to program a DSS);
- To increase the quality of care, they must be linked to a process of care, for example:
  - "80% of diabetic patients should have an HbA1c below 7.0" could be linked to processes such as:
  - "All diabetic patients should have an annual HbA1c test" and
  - "Patients with values over 7.0 should be rechecked within 2 months."
- Condition-action rules specify one or a few conditions which are linked to a specific action, in contrast to narrative guidelines which describe a series of branching or iterative decisions unfolding over time.
- Narrative guidelines and clinical rules are two ends of a continuum of clinical care standards.



Remember Medical Action = **Decision Making** Search Task in  ${\mathcal H}$ **Problem: Time (t)** 

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### The Medical Domain and Decision Making

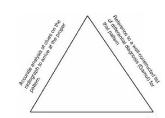
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- 400 BC Hippocrates (460-370 BC), father of western medicine:
  - A medical record should accurately reflect the course of
  - A medical record should indicate the probable cause of
- **1890** William Osler (1849-1919), father of modern western medicine
  - Medicine is a science of uncertainty and an art of probabilistic decision making
- Today
  - Prediction models are based on data features, patient health status is modelled as high-dimensional feature vectors ...

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### **Example: Triangulation to find diagnoses**

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Correlation of radiographic findings and Gamut with patients' clinica and lab findings to arrive at the most likely diagnosis

Reeder, M. M. & Felson, B. 2003. Reeder and Felson's aamuts in radiology: comprehensive lists of roentgen differential diagnosis, New York, Springer Verlag.

## PHRENIC NERVE PARALYSIS OR DYSFUNCTION

Gamut F-137

Tallogonic (eg. smg), al untry, cliest inte, therapeathe to utsion or infration, subclavium vein princetive)

Infection (eg. tubereniosis; fungus disease; abscess)

of tungs

### UNCOMMON

- Anctions a acrife or other Buttettauma (Erb's posy)
- 3. Harpes awter
- 4. Neurins, periphera (e.g. diabetic neuropadh);
- Neurologic disease, (es heminiona) encomititis, polio, Guillain-Barre S.)
- h Pacumonia
- 7 Trampa

Pressu S. Attrezz BH, Transe it controls of the places, nerve associated with best many, IAMA 1976;250:2532-2533.

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 Acute gaotritic (ag. albehal abcoe)
 Crahn's disease 3 Drugs leg, ashir n 🖽 U NSAID 🔟 sternes) 4 Helicopacter pylon maction 🖽

5 Idiopathic

( [Normal areas gastricae ] 7 Deptic alcer Fyperscidity

### ) Compsive gastribs 🖷

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- 3. [Lynphona] 4. Openumstic infection (eg. conditions (monitissis) IIII, helpes simplex, sylomegalourus)
- Postoperalive gasintis
- / Zollinger-Ellisch S. E. molliple endocrine modelasia (MaN) S.
- \* Superficial erosions or arinthold alcerations been especially with nouble contrast technique.
- [ | This condition does not actually cause the gamuted imaging finding that can produce maging changes that simulate it.

http://rfs.acr.org/gamuts/data/G-25.htm

Reeder, M. M. & Felson, B. (2003) Reeder

and Felson's gamuts in radiology:

comprehensive lists of roentgen differential diagnosis. New York, Springer

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**Example Prediction Models > Feature Generation** 

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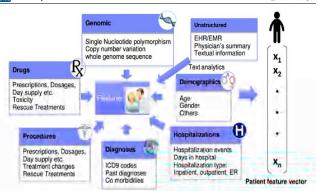


Image credit to Michal Rosen-Zvi

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100+ clinical and functional parameter per Patient



- 50+ Patients per day ~ 5000 data points per day ...
- Aggregated with specific scores (Disease Activity Score, DAS)
- Current patient status is related to previous data
- = convolution over time
- ⇒ time-series data

Simonic, K. M., Holzinger, A., Bloice, M. & Hermann, J. (2011). Optimizing Long-Term Treatment of Rheumatoid Arthritis with Systematic Documentation, Pervasive Health - 5th International Conference on Pervasive Computing Technologies for Healthcare, Dublin, IEEE, 550-554. Holzinger Group hci-kdd.org



of Rheumatoid Arthritis with Systematic Documentation. Pervasive Health - 5th International Conference on Pervasive Computing Technologies for Healthcare, Dublin, IEEE, 550-554.

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Iserson, K. V. & Moskop, J. C. 2007. Triage in Medicine, Part I: Concept, History, and Types Annals of Emergency Medicine, 49, (3), 275-281.

20 Image Source: http://store.gomed-tech.com08 Holzinger Group hci-kdd.org

Example: Rheumatology



Chao, J., Parker, B. A. & Zvaifler, N. J. (2009) Accelerated Cutaneous Nodulosis Associated with Aromatase Inhibitor Therapy in a Patient with Rheumatoid Arthritis. The Journal of Rheumatology, 36, 5, 1087-1088.

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Gaining out Knowledge of time-series data

Q2 Q3 Q4 2006 Q2 Q3 Q4 2007 Q2



Time [Quarters] Simonic, K. M., Holzinger, A., Bloice, M. & Hermann, J. (2011). Optimizing Long-Term Treatment

unction / Ability Reniedation Compensation HOAC =Hypothesis-Oriented Algorithm for Clinicians

Schenkman, M., Deutsch, J. E. & Gill-Body, K. M. (2006) An Integrated Framework for Decision Making in Neurologic Physical Therapist Practice. Physical Therapy, 86, 12, 1681-1702.

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Bone Changes ...

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Ikari, K. & Momohara, S. (2005) Bone Changes in Rheumatoid Arthritis. New England Journal of Medicine, 353, 15, e13.

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http://biomedicalcomputationreview.org/content/clinical-decision-support-providing-quality-healthcare-help-computer

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**Example:** Knee Surgery of a Soccer Player







- Example of a Decision Problem
- Soccer player considering knee surgery
- Uncertainties:
- Success: recovering full mobility
- Risks: infection in surgery (if so, needs another surgery and may loose more mobility)
- Survival chances of surgery

Harvard-MIT Division of Health Sciences and Technology HST.951J: Medical Decision Support, Fall 2005

Instructors: Professor Lucila Ohno-Machado and Professor Staal Vinterbo
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**Remember:** Expected Utility Theory E(U|d)

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For a single decision variable an agent can select D=d for any  $d\in dom(D)$ . The expected utility of decision D=d is



 $E(U \mid d) = \sum_{x_1,...,x_n} P(x_1,...,x_n \mid d) U(x_1,...,x_n,d)$ 

An optimal single decision is the decision D = dmax whose expected utility is maximal:

$$d_{\max} = \arg \max_{d \in \text{dom}(D)} E(U \mid d)$$

Von Neumann, J. & Morgenstern, O. 1947. Theory of games and economic behavior, Princeton university press.

Augmenting Human Capabilities ...



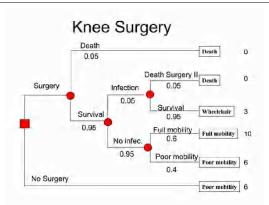
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Decision Tree (this is known since Hippocrates!)

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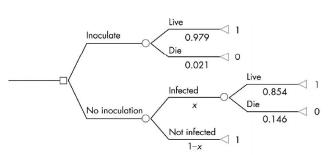
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Clinical Decision Tree (CDT) is still state-of-the-art



Ferrando, A., Pagano, E., Scaglione, L., Petrinco, M., Gregori, D. & Ciccone, G. (2009) A decisiontree model to estimate the impact on cost-effectiveness of a venous thromboembolism prophylaxis guideline. *Quality and Safety in Health Care*, 18, 4, 309-313. Two types of decisions (Diagnosis vs. Therapy)

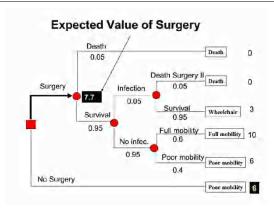
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- Type 1 Decisions: related to the diagnosis, i.e. computers are used to assist in diagnosing a disease on the basis of the individual patient data. Questions include:
- What is the probability that this patient has a myocardial infarction on the basis of given data (patient history, ECG, ...)?
- What is the probability that this patient has acute appendices, given the signs and symptoms concerning abdominal pain?
- Type 2 Decisions: related to therapy, i.e. computers are used to select the best therapy on the basis of clinical evidence, e.g.:
  - What is the best therapy for patients of age x and risks y, if an obstruction of more than z % is seen in the left coronary artery?
  - What amount of insulin should be prescribed for a patient during the next 5 days, given the blood sugar levels and the amount of insulin taken during the recent weeks?

Bemmel, J. H. V. & Musen, M. A. 1997. Handbook of Medical Informatics, Heidelberg, Springer.

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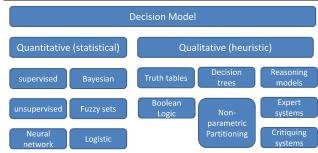
Helps to make rational decisions (risks vs. success)



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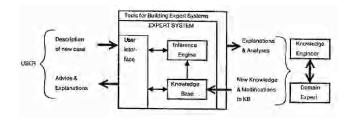
Extended by A. Holzinger after: Bemmel, J. H. v. & Musen, M. A. (1997) Handbook of Medical Informatics. Heidelberg, Springer.

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Early Knowledge Based System Architecture

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Shortliffe, T. & Davis, R. (1975) Some considerations for the implementation of knowledge-based expert systems ACM SIGART Bulletin, 55, 9-12.

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MYCIN – rule based system - certainty factors

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- MYCIN is a rule-based Expert System, which is used for therapy planning for patients with bacterial infections
- Goal oriented strategy ("Rückwärtsverkettung")
- To every rule and every entry a certainty factor (CF) is assigned, which is between 0 und 1
- Two measures are derived:
- MB: measure of belief
- MD: measure of disbelief
- Certainty factor CF of an element is calculated by: CF[h] = MB[h] - MD[h]
- CF is positive, if more evidence is given for a hypothesis, otherwise CF is negative
- CF[h] = +1 -> h is 100 % true
- CF[h] = -1 -> h is 100% false

doi:10.1007/BF02459570.

doi:10.1147/rd.33.0210.

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EXPLANATION

CAPABILITY

USER

Shortliffe & Buchanan (1984)

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■ 1943 McCulloch, W.S. & Pitts, W. A logical calculus of the ideas immanent in nervous activity. Bulletin

■ 1959 Samuel, A.L. Some studies in machine learning using the game of checkers. IBM Journal of research

of Mathematical Biology, 5, (4), 115-133,

intelligence, Mind, 59, (236), 433-460.

and development, 3, (3), 210-229,

■ **1950** Turing, A.M. Computing machinery and

1975 Shortliffe, E.H. & Buchanan, B.G. 1975, A

Mathematical biosciences, 23, (3-4), 351-379,

Judgmental Knowledg about domain

DATA BASE

Dynamic Knowledge

the problem

entered by user

made by system

model of inexact reasoning in medicine.

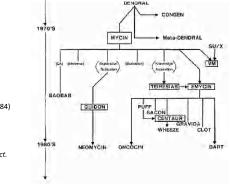
doi:10.1016/0025-5564(75)90047-4.

Static Knowledge versus dynamic knowledge

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RULE INTERPRETER

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Shortliffe, E. H. & Buchanan, B. G. (1984) Rule-based expert systems: the MYCIN experiments of the Stanford Heuristic Programmina Project. Addison-Wesley.

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Dealing with uncertainty in the real world HCI-KDD %

The information available to humans is often imperfect – imprecise - uncertain.

- This is especially in the medical domain the case.
- An human agent can cope with deficiencies.
- Classical logic permits only exact reasoning:
- IF A is true THEN A is non-false and IF B is false THEN B is non-true
- Most real-world problems do not provide this exact information, mostly it is inexact. incomplete, uncertain and/or un-measurable!

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**Original Example from MYCIN** 

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h<sub>1</sub> = The identity of ORGANISM-1 is streptococcus

h<sub>2</sub> = PATIENT-1 is febrile

h<sub>a</sub> = The name of PATIENT-1 is John Jones

There is strongly suggestive evidence (.8) that

the identity of ORGANISM-1 is streptococcus

 $CF[h_0, E] = -.3$ : There is weakly suggestive evidence (.3) that

PATIENT-1 is not febrile

 $CF[h_3, E] = +1$ ; It is definite (1) that the name of PATIENT-1 is

John Jones

Shortliffe, E. H. & Buchanan, B. G. (1984) Rule-based expert systems: the MYCIN experiments of the Stanford Heuristic Programming Project, Addison-Wesley,

MYCIN was no success in the clinical routine

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Image credit to Bernhard Schölkopf

Large Conference Attendance

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https://www.computer.org/csl/ mags/ex/2003/03/x3018.html

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Image credit to Bernhard Schölkop

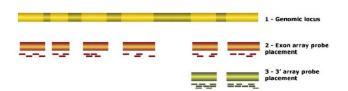
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## 04 Example: **P4-Medicine**

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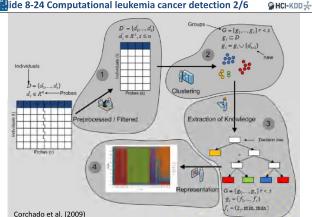
### ide 8-23 Computational leukemia cancer detection 1/6 HCI-KDD &

https://medium.com/machine-learning-in-practice/nips-accepted-papers-stats-26f124843aa0



Exon array structure. Probe design of exon arrays. (1) Exon—intron structure of a gene. Gray boxes represent introns, rest represent exons. Introns are not drawn to scale. (2) Probe design of exon arrays. Four probes target each putative exon. (3) Probe design of 30expression arrays. Probe target the 30end of mRNA sequence.

Corchado, J. M., De Paz, J. F., Rodriguez, S. & Bajo, J. (2009) Model of experts for decision support in the diagnosis of leukemia patients. Artificial Intelligence in Medicine, 46, 3, 179-200. ide 8-24 Computational leukemia cancer detection 2/6



https://blogs.dxc.technology/2017/04/25/are-we-heading-toward-an-ai-winter/

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### Slide 8-22 Example: Exon Arrays

(a) Genomic locus

(b) Exon array probe placemen

Kapur, K., Xing, Y., Ouyang, Z. & Wong, W. (2007) Exon arrays provide accurate assessments of gene expression. Genome Biology, 8, 5, R82.

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### ide 8-25 Computational leukemia cancer detection 3/6

A = acute, C = chronic,

L = lymphocytic, M = myeloid

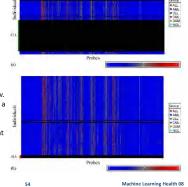
• ALL = cancer of the blood AND bone marrow caused by an abnormal proliferation of lymphocytes.

Probe type

Core

- · AML = cancer in the bone marrow characterized by the proliferation of myeloblasts, red blood cells or abnormal platelets.
- CLL = cancer characterized by a proliferation of lymphocytes in the bone marrow.
- · CML = caused by a proliferation of white blood cells in the bone marrow.
- MDS (Myelodysplastic Syndromes) = a group of diseases of the blood and bone marrow in which the bone marrow does not produce a sufficient amount of healthy cells.
- · NOL (Normal) = No leukemias Corchado et al. (2009)

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Corchado et al. (2009)

Aamodt & Plaza (1994)

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Further Reading: Breiman, Friedman, Olshen, & Stone (1984). Classification and Regression Trees. Wadsworth, Belmont, CA.

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# 05 Example: **Case Based Reasoning** (CBR)

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Slide 8-31 The task-method decomposition of CBR **MCI-KDD** ☆

Classification CLL—ALL. Representation of the probes of the decision tree which classify the CLL and ALL to 1555158\_at, 1553279\_at and 1552334\_at Scatterplot of 2 Corchado et al. (2009) Holzinger Group hci-kdd.org Machine Learning Health 08

Slide 8-29 Thinking - Reasoning - Deciding - Acting HCI-KDD % Critical **Thinking** Clinical Practice Critical Thinking, Clinical Reasoning, AND Clinical Judgment

Slide 8-32 CBR Example: Radiotherapy Planning 1/6 HCI-KDD &

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■ The model of Corchado et al. (2009) combines: • 1) methods to reduce the dimensionality of the

- original data set;
- 2) pre-processing and data filtering techniques;
- 3) a clustering method to classify patients; and
- 4) extraction of knowledge techniques
- The system reflects how human experts work in a
- 1) reduces the time for making predictions;
- 2) reduces the rate of human error; and
- 3) works with high-dimensional data from exon arrays

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Slide 8-30 Case Based Reasoning (CBR) Basic principle HCI-KDD %

> Confirmed Solution Solution

Aamodt, A. & Plaza, E. (1994) Case-based reasoning: Foundational issues, methodological variations, and system approaches. Al Communications, 7, 1, 39-59.

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Ilide 8-33 CBR Example: Radiotherapy Planning 2/6

HCI-KDD %



Source: Imaging Performance Assessment of CT Scanners Group, http://www.impactscan.org

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Weight learning

mechanism

New Patient

Retrieval

Similarity Degree

Case Base



Decision on

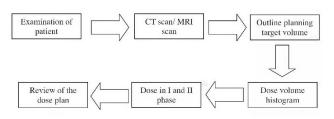
dose

Dnew

Treatment Plan for New

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HCI-KDD %



### Measures:

- 1) Clinical Stage = a labelling system
- 2) Gleason Score = grade of prostate cancer = integer between 1 to 10; and
- 3) Prostate Specific Antigen (PSA) value between 1 to 40
- Dose Volume Histogram (DVH) = pot. risk to the rectum (66, 50, 25, 10 %)

Petrovic, S., Mishra, N. & Sundar, S. (2011) A novel case based reasoning approach to radiotherapy planning. Expert Systems With Applications, 38, 9, 10759-10769.

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Petrovic, S., Mishra, N. & Sundar, S. (2011) A novel case based reasoning approach to

radiotherapy planning. Expert Systems With Applications, 38, 9, 10759-10769.

Most Similar

Modified Dempster Shafer Rule

### Slide 8-37 Case Based Reasoning 6/6

Petrovic et al. (2011)

HCI-KDD %

Dose plan suggested by Dempster-Shafer rule (62Gy+10Gy) Dose received by 10% of rectum is 56.02 Gy (maximum dose limit =55 Gy) Feasible dose plan Modification Yes Proposed dose plan

> Modification of dose plan: New dose plan: 62Gy +8 Gy Dose received by 10% of rectum is: 54.26 Gy (feasible dose plan)

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# 06 Towards **Explainable AI**

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David Silver, Aja Huang, Chris J. Maddison, Arthur Guez, Laurent Sifre, George Van Den Driessche, Julian Schrittwieser, Joannis Antonoglou. Veda Panneershelvam, Marc Lanctot, Sander Dieleman, Dominik Grewe, John Nham, Nal Kalchbrenner, Ilya Sutskever, Timothy Lillicrap, Madeleine Leach, Koray Kavukcuoglu, Thore Graepel & Demis Hassabis 2016. Mastering the game of Go with deep neural networks and tree search. Nature, 529, (7587), 484-489, doi:10.1038/nature16961

Deep Learning Context recognition state-of-the-art





an airplane is parked on the tarmac at an airport

a group of people standing on top of a beach

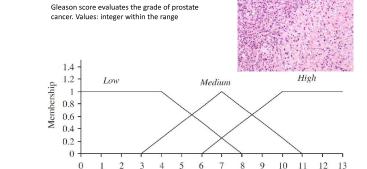
HCI-KDD &

Andrej Karpathy & Li Fei-Fei. Deep visual-semantic alignments for generating image descriptions. Proceedings of the IEEE conference on computer vision and pattern recognition, 2015, 3128-3137. Image Captions by deep learning: github.com/karpathy/neuraltalk2

Image Source: Gabriel Villena Fernandez; Agence France-Press, Dave Martin (left to right)

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Slide 8-36 Membership funct, of fuzzy sets Gleason score 5 HCI-KDD &



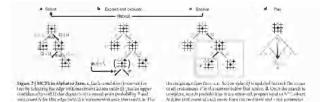
Petrovic, S., Mishra, N. & Sundar, S. (2011) A novel case based reasoning approach to radiotherapy planning. Expert Systems With Applications, 38, 9, 10759-10769.

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Gleason Score

HCI-KDD %

### Mastering the game of Go without human knowledge



neuval network  $(I(x, \cdot), V(x)) = f_{\theta}(x)$ , the vector of R-values are stored in Discourage and English Contact 1427.

$$(p, v) = f_{\theta}(s)$$
 and  $l = (z - v)^2 - \pi^T \log p + c \|\theta\|^2$ 

David Silver, Julian Schrittwieser, Karen Simonyan, Joannis Antonoglou, Ala 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 2017. Mastering the game of go without human knowledge. Nature, 550, (7676), 354-359, doi:doi:10.1038/nature24270.

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### Example: Discovery of causal relationships from data ... HICI-KDD &

Hans Holbein d.J., 1533. The Ambassadors, London: National Gallery

Lopez-Paz, D., Muandet, K., Schölkopf, B. & Tolstikhin, I. 2015. Towards a learning theory of cause-effect inference. Proceedings of the 32nd International Conference on Machine Learning, JMLR, Lille, France.



https://www.youtube.com/watch?v=9KiVNIUMmCc

Machine Learning Health 08 Holzinger Group hci-kdd.org Machine Learning Health 08 Joris M. Mooij, Jonas Peters, Dominik Janzing, Jakob Zscheischler & Bernhard Schölkopf 2016. Distinguishing cause from effect using observational data: methods and benchmarks. The Journal of Machine Learning Research, 17, (1), 1103-1204.









 $\mathbb{P}_Y = \mathbb{P}_{Y \mid \operatorname{do}(x)} \neq \mathbb{P}_{Y \mid x}$  $\mathbb{P}_X = \mathbb{P}_{X \mid \operatorname{do}(y)} \neq \mathbb{P}_{X \mid y}$ 

 $\mathbb{P}_Y = \mathbb{P}_{Y \mid \operatorname{do}(x)} \neq \mathbb{P}_{Y \mid x}$  $\mathbb{P}_X \neq \mathbb{P}_{X \mid \operatorname{do}(y)} = \mathbb{P}_{X \mid y}$ 



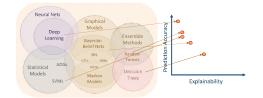




 $\mathbb{P}_{Y|s} \neq \mathbb{P}_{Y|\operatorname{do}(x),s} = \mathbb{P}_{Y|x,s}$  $\mathbb{P}_{X \mid s} \neq \mathbb{P}_{X \mid \text{do}(y), s} = \mathbb{P}_{X \mid y, s}$ Machine Learning Health 08

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HCI-KDD %



David Gunning 2016. Explainable artificial intelligence (XAI): Technical Report Defense Advanced Research Projects Agency DARPA-BAA-16-53, Arlington, USA, DARPA

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HCI-KDD % Neural Net Explainability ?? Interpretable Models Deep Explanation Model Induction Modified deep learning Techniques to learn more Techniques to infer an techniques to learn structured, interpretable, causal explainable features model as a black box

David Gunning 2016. Explainable artificial intelligence (XAI): Technical Report Defense Advanced Research Projects Agency DARPA-BAA-16-53, Arlington, USA, DARPA. Holzinger Group hci-kdd.org

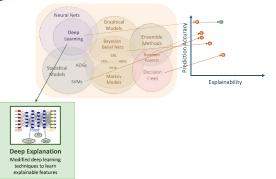
"How do humans generalize from few examples?"

- Learning relevant representations
- Disentangling the explanatory factors
- Finding the shared underlying explanatory factors, in particular between P(x) and P(Y|X), with a causal link between  $Y \rightarrow X$

Bengio, Y., Courville, A. & Vincent, P. 2013. Representation learning: A review and new perspectives. IEEE transactions on pattern analysis and machine intelligence, 35, (8), 1798-1828, doi:10.1109/TPAMI.2013.50. Tenenbaum, J. B., Kemp, C., Griffiths, T. L. & Goodman, N. D. 2011. How to grow a mind: Statistics, structure, and abstraction. Science, 331, (6022), 1279-1285, doi:10.1126/science.1192788

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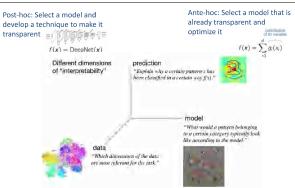
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David Gunning 2016. Explainable artificial intelligence (XAI): Technical Report Defense Advanced Research Projects Agency DARPA-BAA-16-53, Arlington, USA, DARPA. Holzinger Group hci-kdd.org Machine Learning Health 08

Post-hoc vs. Ante-hoc

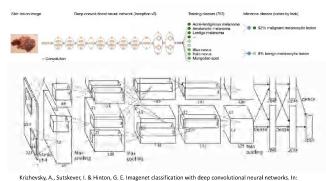
HCI-KDD &



Montavon, G., Samek, W. & Müller, K.-R. 2017. Methods for interpreting and understanding deep neural networks. arXiv:1706.07979.

Holzinger Group hci-kdd.org Machine Learning Health 08 Deep Convolutional Neural Network Pipeline

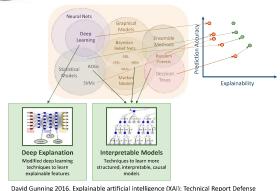
HCI-KDD 26



Pereira, F., Burges, C. J. C., Bottou, L. & Weinberger, K. Q., eds. Advances in neural information processing systems (NIPS 2012), 2012 Lake Tahoe. 1097-1105

Holzinger Group hci-kdd.org Machine Learning Health 08

HCI-KDD &



Advanced Research Projects Agency DARPA-BAA-16-53, Arlington, USA, DARPA.

Holzinger Group hci-kdd.org Machine Learning Health 08

Model/Data improvement: Reducing general errors

HCI-KDD &

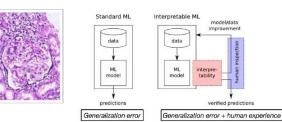


Image credit to: Samek, Montavon & Müller Tutorial at ICASSEP 2017

- Wrong decisions can be costly and dangerous!
- Verify that classifier works as expected
- Improve classifier continuously
- Human learning inspired by machine learning

- Interpretability as a novel kind for supporting teaching, learning and knowledge discovery,
- Particularly in abstract fields (informatics)
- Compliance to European Law "the right of explanation"
- Check for bias in machine learning results
- Fostering trust, acceptance, making clear the reliability

Andreas Holzinger 2018. Explainable AI (ex-AI). Informatik-Spektrum, 41, (2), 138-143, doi:10.1007/s00287-018-1102-5.

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Explainable AI is a huge challenge for visualization

HCI-KDD &



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HCI-KDD %

## 07 Methods of **Explainable AI**

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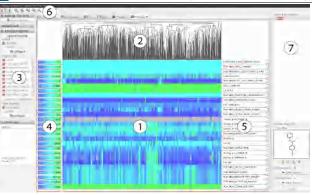
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Example for an Explanation Interface - open work @

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HCI-KDD %

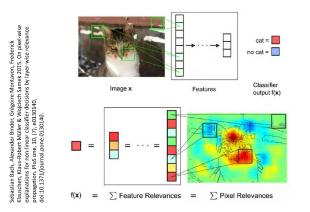
Machine Learning Health 08



Werner Sturm, Till Schaefer, Tobias Schreck, Andeas Holzinger & Torsten Ullrich. Extending the Scaffold Hunter Visualization Toolkit with Interactive Heatmaps In: Borgo, Rita & Turkay, Cagatay, eds. EG UK Computer Graphics & Visual Computing CGVC 2015, 2015 University College London (UCL). Euro Graphics (EG), 77-84, doi:10.2312/cgvc.20151247. Holzinger Group hci-kdd.org

LRP Layer-Wise Relevance Propagation

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https://www.vis.uni-konstanz.de/en/members/fuchs/

Holzinger Group hci-kdd.org Machine Learning Health 08

**Example for an Explanation Interface** 

HCI-KDD 26

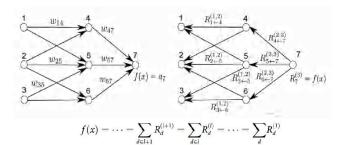


interactive machine learning. Proceedings of the 20th International Conference on Intelligent User Interfaces (IUI 2015), 2015 Atlanta. ACM, 126-137, doi:10.1145/2678025.2701399.

Holzinger Group hci-kdd.org Machine Learning Health 08

A NN-classifier during prediction time

HCI-KDD %



Sebastian Bach, Alexander Binder, Grégoire Montayon, Frederick Klauschen, Klaus-Robert Müller & Woiciech Samek 2015. On pixel-wise explanations for non-linear classifier decisions by layer-wise relevance propagation PloS one, 10, (7), e0130140, doi:10.1371/journal.pone.0130140

Marco Tulio Ribeiro, Sameer Singh & Carlos Guestrin, Why should i trust you?: Explaining the predictions of any classifier. 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, 2016. ACM, 1135-1144, doi:10.1145/2939672.2939778

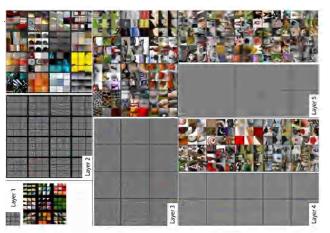
Holzinger Group hci-kdd.org Machine Learning Health 08

### Black Box Explanations through Transparent Approximations HCI-KDD Representations



Himabindu Lakkaraju. Ece Kamar, Rich Caruana & Jure Leskovec 2017. Interpretable and Explorable Approximations of Black Box Models, arXiv:1707.01154.

Holzinger Group hci-kdd.org Machine Learning Health 08

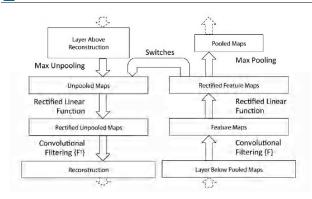




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### Example: Interpretable Deep Learning Model

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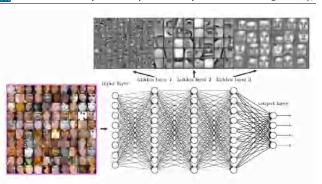


Matthew D. Zeiler & Rob Fergus 2013. Visualizing and Understanding Convolutional Networks. arXiv:1311.2901.

Holzinger Group hci-kdd.org Machine Learning Health 08

### The world is compositional (Yann LeCun)

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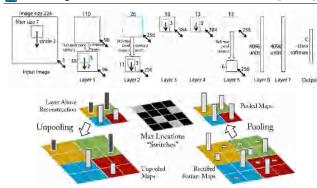
Matthew D. Zeiler & Rob Fergus 2013, Visualizing and Understanding Convolutional Networks, arXiv:1311.2901

Classifiers Statistical Structural Naïve Bayes Rule based Distance based Neural Networks Multi-Layer Production Rules Perceptron Functional Nearest Neighbor Spectral Vector

https://stats.stackexchange.com/questions/271247/machine-learning-statistical-vs-structural-classifiers

### Visualizing a Conv Net with a De-Conv Net

HCI-KDD %

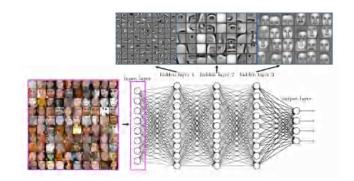


Matthew D. Zeiler & Rob Fergus 2014. Visualizing and understanding convolutional networks. In: D., Fleet, T., Pajdla, B., Schiele & T., Tuytelaars (eds.) ECCV, Lecture Notes in Computer Science LNCS 8689. Cham: Springer, pp. 818-833, doi:10.1007/978-3-319-10590-1\_53.

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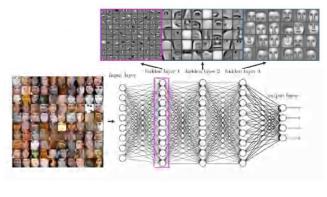
### The world is compositional (Yann LeCun)

HCI-KDD %

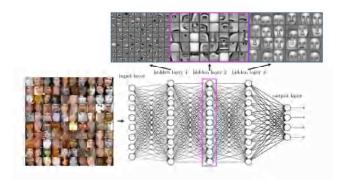


Matthew D. Zeiler & Rob Fergus 2013. Visualizing and Understanding Convolutional Networks. arXiv:1311.2901. Machine Learning Health 08 Holzinger Group hci-kdd.org Holzinger Group hci-kdd.org

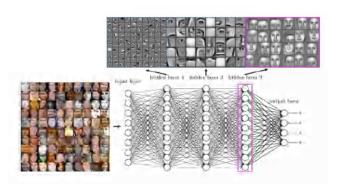




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Holzinger Group hci-kdd.org 101 Machine Learning Health 08



Holzinger Group hci-kdd.org 102 Machine Learning Health 08

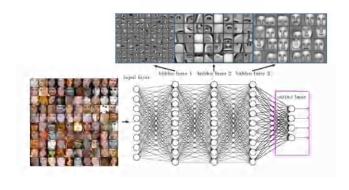
**₩** HCI-KDD ☆

)%

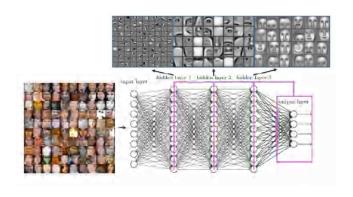
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Stochastic AND-OR Templates for visual objects

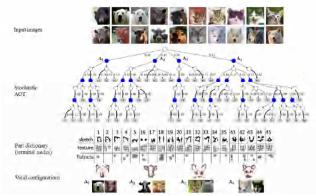
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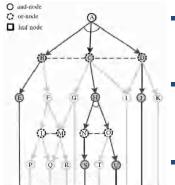
Zhangzhang Si & Song-Chun Zhu 2013. Learning and-or templates for object recognition and detection. IEEE transactions on pattern analysis and machine intelligence, 35, (9), 2189-2205, doi:10.1109/TPAMI.2013.35.

Holzinger Group hci-kdd.org 105 Machine Learning Health 08

Stochastic Model on AND-OR graph: Zhaoyin Jia (2009)

### Framework for vision: AND-OR Graphs

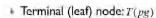
AHCI-KDD 🍰



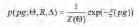
- Algorithm for this framework
  - Top-down/bottom-up computation
- Generalization of small sample
- Use Monte Carlos simulation to synthesis more configurations
- Fill semantic gap

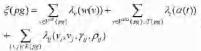
Images credit to Zhaoyin Jia (2009)

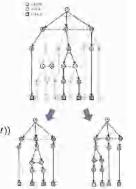
### Stochastic Model on AND-OR graph: Zhaoyin Jia (2009)

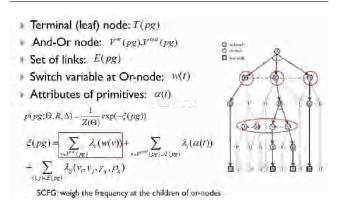


- And-Or node: Vor (pg), Vond (pg)
- Set of links: E(pg)
- Switch variable at Or-node: w(t)
- # Attributes of primitives:  $\alpha(t)$

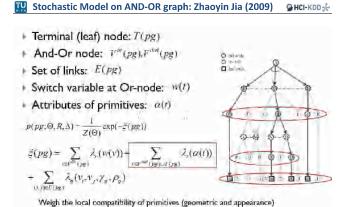




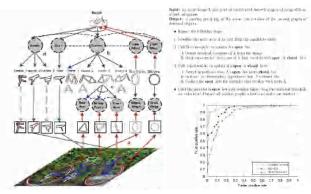




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Liang Lin, Tianfu Wu, Jake Porway & Zijian Xu 2009. A stochastic graph grammar for compositional object representation and recognition. Pattern Recognition, 42, (7), 1297-1307, doi:10.1016/j.patcog.2008.10.033.

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Seemingly trivial questions ... ?

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- What is a good explanation?
- (obviously if the other did understand it)
- Experiments needed!
- What is explainable/understandable/intelligible?
- When is it enough (Sättigungsgrad you don't need more explanations – enough is enough)
- But how much is it ...

🔣 Stochastic Model on AND-OR graph: Zhaoyin Jia (2009) 🛛 😭 HCI-KDD 🧩

O country

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▶ Terminal (leaf) node: T(pg)

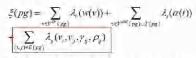
And-Or node: V<sup>er</sup>(pg),V<sup>aud</sup>(pg)

Set of links: E(pg)

Switch variable at Or-node: w(I)

Attributes of primitives: α(t)

 $p(pg, \Theta, R, \Delta) = \frac{1}{Z(\Theta)} \exp(-\xi(pg))$ 



Spatial and appearance between primitives (parts or objects)

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## **Future Work**

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Explanations in Artificial Intelligence will be necessary



https://www.newyorker.com/cartoon/a19697

🔣 Stochastic Model on AND-OR graph: Zhaoyin Jia (2009) 🥒 😭 НСІ-КОД 🧩

Terminal (leaf) node: T(pg)
 And-Or node: V<sup>or</sup>(pg), V<sup>oud</sup>(pg)

Set of links: E(pg)

► Switch variable at Or-node: w(t)

• Attributes of primitives:  $\alpha(t)$ 

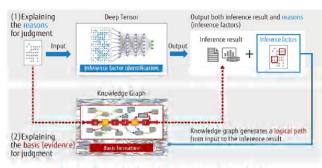
$$p(pg;\Theta,R,\Delta) = \frac{1}{Z(\Theta)} \exp(-\xi(pg))$$

$$\begin{split} \xi(pg) &= \sum_{v \in V^{(g)}(pg)} \lambda_v(w(v)) + \sum_{v \in P^{2kg}(pg) \cup T(pg)} \lambda_v(\alpha(t)) \\ &+ \sum_{(v,j) \in F(pg)} \lambda_{ij}(v_{i,s}v_{j}, \gamma_{ij}, \rho_{ij}) \end{split}$$

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Combination of Deep Learning with Ontologies

HCI-KDD 🖟



Explainable AI with Deep Tensor and Knowledge Graph

http://www.fujitsu.com/jp/Images/artificial-intelligence-en\_tcm102-3781779.png

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IBM is doing it now: teaching meaningful explanations

nations 🏻 🔓 HCI-KDD 🦟



Noel C. F. Codella, "Michael Hind." Karthikeyan Natesan Ramamurthy,"
Murray Campbell, Amit Dharandhur, Kush R. Varchoey, Demis Wei,
Aleksandra Majdenker
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Abstract

The distription of madium learning is our job-sides, applications, so who is besidence and he has larged in pure because registricture are not accounted by equilibrations conceptionable out of constituents, show these hadden interest conceptionable out of constituents, show the large and the production of the constituents of the constituents of the constituents was explanations which considers do be interested to distribute the Kanters and shortly explanations of them discounted to the proof former, if the state transmits is market to be likely and explanations from the proof former. This wastername is recorded to the constituent of the constituent of

1 Introduction

Noel C.F. Codella, Michael Hind, Karthikeyan Natesan Ramanurthy, Murray Campolel, Amit Dhurandhar, Kush R. Varshey, Dennis Wei, & Aleksandra Mojsilovic 2018. Teaching Meaningful Explanations, arXiv:1805.11648.

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- Engineers create a set of logical rules to represent knowledge (Rule based Expert Systems)
- Advantage: works well in narrowly defined problems of well-defined domains
- Disadvantage: No adaptive learning behaviour and poor handling of p(x)

Image credit to John Launchbury

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Myth 1a: Superintelligence by 2100 is inevitable!

Myth 1b: Superintelligence by 2100 is impossible!

it needs no body - only an Internet connection

123

Myth 3: Al can never control us humans

Fact: Intelligence is an enabler for control:

We control tigers by being smarter ...

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Three (selected) dangers and myths about AI generally

Myth 2: Robots are our main concern Fact: Cyberthreats are the main concern:

■ Fact: We simply don't know it!

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The second wave of AI (1975 – ): Statistical Learning

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- Engineers create learning models for specific tasks and train them with "big data" (e.g. Deep Learning)
- Advantage: works well for standard classification tasks and has prediction capabilities
- Disadvantage: No contextual capabilities and minimal reasoning abilities

Image credit to John Launchbury Machine Learning Health 08 Holzinger Group hci-kdd.org 121

Our goal: Contextual adaptations can explain decisions

understand why

understand why not know when you'll succeed I know when you'll fail

know when to trust you know why you made tha

Image credit to John Launchbury

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- HCI-KDD &
- and stupid,
- and brilliant.

https://www.benshoemate.com/2008/11/30/einstein-never-said-that

Das Dumme an Zitaten s dem Internet ist. ass man nie weiß. ob sie echt sind' hert Finstein

•Computational approaches can find in  $\mathbb{R}^n$ what no human is able to see

- ■However, still there are many hard problems where a human expert in  $\mathbb{R}^2$  can understand the context and bring in experience, expertise, knowledge, intuition, ...
- ■Black box approaches can not explain WHY a decision has been made ...

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The third wave of AI (?): Adaptive Context Understanding HCI-KDD &

Perceiving Learning Abstracting Reasoning

- A contextual model can perceive, learn and understand and abstract and reason
- Advantage: can use transfer learning for adaptation on unknown unknowns
- Disadvantage: Superintelligence ...

Image credit to John Launchbury

A final citation attributed to Albert Einstein ...

- Computers are incredibly fast, accurate
- humans are incredibly slow, inaccurate
- together they are powerful beyond imagination

(Einstein never said that)

Thank you!

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