

Prominence of Expert System and Case Study- DENDRAL

Namita Mirjankar, Shruti Ghatnatti
Karnataka, India

namitamir@gmail.com, shru.312@gmail.com

Abstract—Among many applications of Artificial Intelligence, Expert System is the one that exploits human knowledge to solve problems which ordinarily would require human insight. Expert systems are designed to carry the insight and knowledge found in the experts in a particular field and take decisions based on the accumulated knowledge of the knowledge base along with an arrangement of standards and principles of inference engine, and at the same time, justify those decisions with the help of explanation facility. Inference engine is continuously updated as new conclusions are drawn from each new certainty in the knowledge base which triggers extra guidelines, heuristics and rules in the inference engine. This paper explains the basic architecture of Expert System, its first ever success DENDRAL which became a stepping stone in the Artificial Intelligence field, as well as the difficulties faced by the Expert Systems

Keywords—Artificial Intelligence; Expert System architecture; knowledge base; inference engine; DENDRAL

I INTRODUCTION

For more than two thousand years, rationalists all over the world have been striving to comprehend and resolve two unavoidable issues of the universe: how does a human mind work, and can non-people have minds? In any case, these inquiries are still unanswered. As humans, we all are blessed with the ability to learn and comprehend, to think about different issues and to decide; but can we design machines to do all these things?

Some philosophers are open to the idea that machines will perform all the tasks a human can do. But also there are some, who openly ridicule this idea and they believe that humans are very sophisticated creatures created by nature and no machine can be equal to it.

This quest to create machines which think and behave like humans has led us to the invention of Artificial Intelligence (AI). ENIAC was the first digital computer and from the time of its invention, engineers as well as other professionals have continuously tried to automate some or the other tasks in their fields. This has led us to the advancement in the field of AI that we see today. All these advancements in the field of AI and related topics can be classified into different specialized branches like robotics, expert systems, genetic algorithms, neural networks and so on.

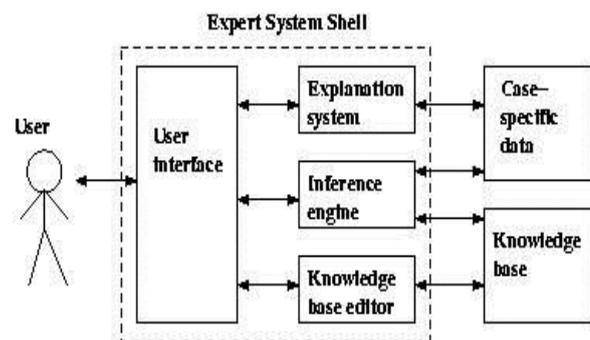
[2] Expert system (ES) is the primary genuine business application of the innovative work completed in the AI field. As we very well know, an expert in any field is a person, who has deep knowledge, practical as well as theoretical, and also, has the proficiency in making correct judgments in taking decisions in that particular field.

An expert system is called a system, not a program, since it incorporates a few distinct parts, like, knowledge base, inference engine and user interface. All these diverse segments collaborate together in reenacting the critical thinking procedure by a recognized expert in that field. In this paper, we will study some architecture of Expert System, basic important experiments conducted, future potential and pros-cons of Expert System.

II ARCHITECTURE OF EXPERT SYSTEMS

Different architectures of Expert Systems have been proposed by different scholars and computer scientists. But

the main components that remain same are: User Interface, Knowledge Base and Inference Engine.



a. Knowledge Base:

[2]The knowledge base contains the knowledge essentials for comprehension, planning and for understanding the problems arranged as schemas. Knowledge engineer is the one who creates the knowledge base by conducting a series of interviews with the experts in the specific domain. Also, he organizes the captured knowledge in a form that can be directly useful by the proposed ES. It is vital for the knowledge engineer to have the basic knowledge of terminologies and ideologies used in the proposed system.

We can categorize the knowledge captured by the knowledge engineer into three types: assembled knowledge, subjective knowledge and quantitative knowledge. The assembled knowledge is the knowledge that is captured from the advices of experts, standard experiments, previous journals, textbooks, research materials, handbooks, etc. Subjective knowledge comprises of general guidelines, estimated speculations, causal models of procedures and sound judgment. Quantitative knowledge manages systems in light of scientific speculations, numerical procedures, mathematical solutions and so forth.

Thus, knowledge base is a stockroom of the domain specific knowledge collected from different means in accordance with the information obtaining module called expert acquisition module. For the knowledge representation purpose, different rules, outlines, rationale, semantic net and so on are utilized in the knowledge base.

b. Inference Engine:

[2] Inference Engine is the most vital part of the design of any ES framework. Inference mechanisms are control systems or search strategies, which look through the knowledge base to come up with the decisions. In simple terms, we can say that, inference engine is the search module of ES.

For effective processing of ES, the inference engine works on different symbols with the help of different rules and facts; deriving the knowledge from the knowledge base. This process is recursively executed until a predetermined objective is not reached. In achieving the implementation of inference engine, many approaches are used and in them, the two most popular ones are: backward chaining and forward chaining. The main focus of backward chaining is on the final goal, whereas in the forward chaining, it is data. These two can even be combined to get a hybrid approach.

Thus, the work of the inference engine is to carry out the reasoning whereas that of the expert system is to reach to a solution

c. Explanation system:

The explanation module is the one that enables the user to ask the expert system how a particular conclusion is reached. An ES must be able to explain its actions and justify why it has concluded to a particular decision.

[4] The methods of explanations used can be classified in three categories: (a) explanation of inference on a specific input data set, (b) explanation of the knowledge base itself, and (c) explanation of the control strategy.

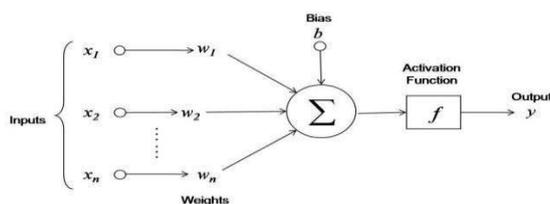
The explanation module basically answers the questions with the words: with why, how and what. Why will answer the reason, how will answer how the conclusion is reached.

d. User Interface:

It is a means through which the user communicates with the user. It makes use of different menus, graphical interface, displays etc. to make the communication easier. Obligation of the user interface is to change over the guidelines from its non-comprehensible representation to the comprehensible structure.

III ARTIFICIAL NEURAL NETWORK (ANN)

[10] A neural network is an interconnected assembly of simple processing elements, units or nodes, whose functionality is loosely based on the animal neuron. The processing ability of the network is stored in the inter unit connection strengths, or weights, obtained by a process of adaptation to, or learning from, a set of training patterns. It can be viewed in a simple way as shown in Fig.2



[12] An Artificial Neural Network consists of main four parts:

i. Inputs:

Let $X = (x_1, x_2, \dots, x_n)$, where the x_i are real numbers, represent the set of inputs presented to the network

model.

ii. Weights:

Each input has an associated weight that represents the strength of that particular connection. Let $W = (w_1, w_2, \dots, w_n)$, with w_i real, represent the weight vector corresponding to the input vector X .

iii. Summation:

Applied to Σ , these weighted inputs along with the bias value, produce a net sum given by

$$-b + \sum_{i=1}^n x_i w_i$$

iv. Activation Function:

The value of this will be then be passed onto the activation, or *threshold* function. The threshold function might be best viewed as a single-step function, where say once the input α reaches a certain value, it will output a certain value. Next, once the threshold is activated or not, we will get an output from this neuron. We can string many neurons together and in different patterns with different layers to create a network.

Artificial Neural Network is a very vital concept for the developments in Artificial Intelligence as it resembles the human brain.

IV CASE STUDY - DENDRAL

The DENDRAL project is a good example of the rising innovation. DENDRAL was created at Stanford University to investigate chemicals. The venture was bolstered by NASA, in light of the fact that an unmanned shuttle was to be dispatched to Mars and a project was required to decide the sub-atomic structure of Martian soil, in light of the mass unearthy information gave by a mass spectrometer. The project started in 1965. Edward Feigenbaum, Bruce Buchanan and Joshua Lederberg framed a group to take care of this testing issue.

Domain	Organic chemistry- mass spectrometry
Task	To identify molecular structure of unknown compounds from mass spectra data
Input	Histogram giving mass number
Output	Description of structure of the compound
Architecture	plan-generate-test with constrained heuristic search

Table 1

Feigenbaum had been looking for an environment in which to examine procedures of empirical induction, had arranged his reasoning toward finding such an errand situation among the exercises that researchers do. Lederberg was a geneticist. He had worked in 1965 on exobiology included the mass spectra of ammunition acids, proposed the assignment of breaking down mass spectra. Later, Buchanan also joined the team and he introduced the theory of science mixed with AI, and his interest leaned towards the scientific discoveries and their related information processes. This project was largely an experimental one. But, it became a landmark for the Expert System field.

DENDRAL stands for DENDRitic Algorithm. It is a procedure for thoroughly and non-repetitively specifying all the topologically distinct arrangements of any given set of atoms, as per the rules of chemical valence.

The central issue of diagnostic chemistry is to decide the compound structure of molecules. The general issue to

which the DENDRAL programs apply is a critical, substantive issue in the chemistry and that is structure elucidation. Structure elucidation is defined as the process of determination of the structure of a compound. The issue is critical in light of the fact that the physical as well as chemical properties of the compounds are resolved not simply by numbers of the atoms, however by their topological and geometric arrangements also. A few observational means are accessible for acquiring data about the structure of a compound. Noticeable among these is mass spectrometry and DENDRAL initially tended to the issues related just with this technique, in spite of the fact that it developed to manage the issues of structure elucidation on more broad terms.

Originally the main focus of DENDRAL was on the topologies or data of molecules, in light of the fact that the connection of its advancement was mass spectrometry. In this way to DENDRAL, diverse geometric types of the same topology were completely proportionate. In the later versions also, the basic structure of the system remained the same.

The recognizable proof of a molecule implies at any rate that its topological association is referred to; it is typically referred to as a diagram with atoms represented as nodes and bonds represented as edges between these atoms.

At first, because specified calculation and algorithms were not yet developed for some cyclic compounds, DENDRAL was connected to aliphatic compounds only. The compounds concentrated on were amino acids, ethers, alcohols, amines etc. After developments of the algorithms, the features to DENDRAL were added consolidating the cyclic structure generator, and they worked on steroids, specifically estrogens, marine sterols, and other compounds related to it.

Roughly speaking, 100 atoms is the limit on size of molecules amiable to the DENDRAL and customary mass spectrometry investigation techniques. As of late, mass spectrometry has been effectively connected to the estimation of mass quantities of proteins with a large number of atoms. On the off chance that mass phantom investigation of pieces of proteins had been accessible, DENDRAL may have been connected to that examination (and without a doubt will be later on), utilizing super atoms to speak to individual amino acids of twenty sorts masterminded in straight successions, or to speak to DNA groupings. As it might have been, the applications were chosen to some degree for their quality in adding to the DENDRAL ideas and to a limited extent since they were of enthusiasm for their significance to contemporary chemistry.

The basic method of Heuristic DENDRAL makes use of the important concept of the generate-and-test paradigm in which a generator enumerates potential solutions, and creates all conceivable atomic structures predictable with the mass spectrum. After that, the mass spectrum is resolved or anticipated for every structure and tried against the real range spectrum. In any case, this strategy fizzled in light of the fact that a large number of conceivable structures could be created – the issue quickly got to be unmanageable notwithstanding for good estimated molecules

In addition to this, at that time, logical calculation for mapping the mass spectrum to its molecular structure was still not developed. Be that as it may, expository scientists, for example, Lederberg, could take care of this issue by

utilizing their aptitudes, experience and skills. They could hugely decrease the quantity of conceivable structures by searching for surely understood examples of crests in the spectrum, and in this manner give only a couple of plausible answers for further examination. In this way, Feigenbaum's job got to be to join the aptitude of Lederberg into a software program to make it perform at a human level. Such frameworks were later named as expert systems. To comprehend and embrace Lederberg's information and work with his phrasing, Feigenbaum needed to learn essential basics in chemistry and spectral analysis. In any case, it got to be evident that Feigenbaum utilized basic rules of science as well as his own heuristics, or dependable guidelines, his own experience, and even some guessing on his part. Before long Feigenbaum recognized one of the significant troubles in the task, which he called the 'knowledge acquisition bottleneck'. He understood how difficult it is to transform information collected from human experts to apply to the computers. For this purpose, Lederberg even expected to study fundamentals in processing. In this way, Feigenbaum, Buchanan and Lederberg worked as a team and created DENDRAL, the first fruitful ES.

The main three parts of DENDRAL are: generator, planning programs and testing-ranking programs.

e. The Generator:

[7]The generator can be said as the heart of the program. The generator in the Heuristic DENDRAL is based on the DENDRAL algorithm developed by Lederberg. This algorithm determines a methodical list of molecular structures. It regards molecules as planar graphs and produces progressively bigger diagram structures until every single synthetic atom are incorporated into the graphs in every single conceivable course of arrangement. Since diagrams with cycles displayed uncommon issues,' introductory work was constrained to chemical structures without rings.

f. The planning programs:

[7]The DENDRAL Planner utilizes a lot of information of mass spectrometry to induce requirements. In the generator's lists, planning data of good and bad basic structure is put. Arranging has been restricted altogether to mass spectrometry, however the same procedures can be utilized with other information sources also.

The planning programs in DENDRAL take into consideration helpful (man-machine) critical thinking in the translation of mass spectra. It utilizes the knowledge of mass spectrometry acquired from scientists and applies it efficiently to the spectrum of an unknown molecule. That is, utilizing the scientist's meanings of the basic arrangements of the molecules and the related applicable rules, the planning programs do the accounting of fragment peaks with sections and the combinatorics of discovering predictable methods for setting substituent around them.

The output of this planning program is a structure description lists with as much detail filled in as the information and characterized fragmentations will permit.

g. *The testing and ranking programs:*

[7] These programs utilize a large amount of information of mass spectrometry to make testable forecasts from each conceivable applicant molecule. The predicted information is contrasted with the information from the unknown compound. These programs utilize a genuinely basic theory of mass spectrometry to predict commonly expected fragmentations for every applicant structure. Expectations which stray incredibly from the observed range are viewed as at first sight proof of error; the comparing structures are removed from the lists. Then they use more subtle rules of mass spectrometry for ranking the remaining structures.

Thus, we can summarize the Organization of the heuristic DENDRAL programs as below:

Operation	Components	Input	Output
Planning	MOLION Planning rule generator PLANNER	Mass Spectrum Planning rules Planning rules	Molecular ion constraints Constraints Superatoms GOODLIST BADLIST
Generating	Acyclic generator CONGEN GENOA STEREO	Constraints	Candidate molecular structures
Testing	PREDICTOR MSPRUNE REACT	Candidate molecular structures Mass spectrometry rules Reaction chemistry rules	Most plausible structures Structures consistent with spectrum Structures consistent with known reactions

[8] Table 2

[8] The secret to the success of DENDRAL- however not special to it- is that it attempted a very narrow, but very much characterized domain for which there was a reasonable measure of progress. The real lesson DENDRAL has for Artificial Intelligence, and for those who are intrigued by the utilization of Artificial Intelligence strategies, is that it is conceivable to select a domain of modest complexity and to decrease the issues of that domain to help the human insight. By bringing down one's sights from explaining expansive, general issues to taking care of a specific issue, by applying as much particular information to that issue as can be earned from the experts, and by systematizing and mechanizing the utilization of this information, a valuable Expert Systems can be delivered. This lesson underlies the achievement of today's Expert Systems.

V DIFFICULTIES FACED BY EXPERT SYSTEMS

Expert systems are confined to a very narrow domain. Because of this, they are not as vigorous, robust and adaptable as a user may need. Besides, ES can experience issues perceiving the boundaries of the domains. Moreover, Expert Systems have restricted explanation capabilities. They can demonstrate the rule sequence they applied to achieve an answer, however cannot relate the acquired knowledge to any more profound comprehension of the problem domain.

Verifying and validating an expert system is a very difficult job. No broad procedure has yet been created for examining their completeness and consistency. This results in difficulty in identifying incorrect, incomplete or inconsistent data.

The first generation Expert Systems had practically no capacity to gain from their experience. In addition to that, Expert Systems are assembled exclusively and can't be created quickly. It may take from five to ten man years to fabricate an Expert System framework. After so much effort, however, if the system performance and improvement depends on continuous attention from its developers then the success of the system cannot be justified.

—A good way to think about where AI fits in the entire spectrum of IT and CS is what I call the *'what-to-how'* spectrum. We all know about the *'how'* and AI sits at the very far end of the spectrum at the other side- the what end of the spectrum- the end of the spectrum where you would as a user tell the machine what it is you want it to do and it would have the knowledge and the reasoning power and the heuristics to employ to do it for you, so you didn't have to be a programmer, you didn't have to know any *'how'*. One other things that we don't know how to do very well yet is to accumulate immense amounts of, what Doug Lenat calls- commonsense knowledge.

One of the great inventions of all times was writing. To write it down, to pass it on to the next generation, we move our culture to the next generation mostly by reading text, the knowledge of ordinary things, not the knowledge of specific like how you build a computer or how had the car run or something like that and we'll get that from reading text. So that's AI's number one problem today. There will be in coming up in the next ten, twenty years some really sensational computer-human interfaces in which computers can do vastly better things than they are currently doing in the service of human work. And people can do whatever residual there is that people do best and these interfaces will allow that mixture of human-computer interaction, not just where the machine is serving the person, but where the human and the computer are cooperating on a task and to profoundly greater consequences than we now think!

VI CONCLUSION

In this paper, we have identified and discussed the Expert Systems with its architecture and case study of its first success- DENDRAL. Expert System can be an extremely valuable extension of Artificial Intelligence. It can provide tremendous commercial applications in the field of medicine, agriculture, education, business accounting, legal systems, nuclear industry, and weather prediction and so on. They can be used in as simple application as offering salespersons some assistance with selling constructed homes to the complex applications like offering NASA some assistance with planning the support of a space transport in readiness for its next flight. Designing and developing an Expert System is not an easy task. It requires tremendous efforts in data acquisition, knowledge representation, application of rules etc. In spite of the fact that their utilization is far reaching, there are some professionals who are skeptic about it. As a first success, DENDRAL became the stepping stone in the field of Expert System. In the future, scientists all over the world are expecting advanced

developments in the field of Expert System in commercial as well as personal territories, which is the need of the hour.

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