

CHAPTER THIRTEEN

Scientific Discovery and Inventive Engineering Design

Cognitive and Computational Similarities

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INTRODUCTION

Michael Faraday was a scientist and an inventor. It was the same piece of work, the discovery that a magnetic field could generate electricity, and the resultant invention of the electric generator, that entitled him to both of these appellations. The goal of this chapter is to explain how a single piece of work could qualify him for both titles, and more importantly how these seemingly disparate activities are surprising similar. To do this we will attempt to delineate the domains of invention and discovery, showing how they are structured and how the underlying cognitive processes that generate both activities are broadly equivalent, even though their goals may differ. It is our contention that the activities that are commonly included in design creation and scientific discovery are often heavily intertwined, have similarly structured domains, are accomplished by very similar cognitive activities, can be simulated or emulated by similar computational models, and, many times, even yield similar artifacts, processes, or knowledge. In these latter cases, not only do they have similarly structured domains and equivalent mechanisms, but their outputs can be viewed both as invention and as discovery. With regard to Faraday, it was the invention of the electric generator (motor) and discovery of magnetism – electricity equivalency that entitles him to his dual status as inventor and scientist.

This book focuses on formal methods for design synthesis, with “formal” implying approaches that are driven by specified goals and computationally realized. In the scientific domain, the attempt to understand how people have made discoveries has similarly led to formal models of discovery. These formal models have been instantiated as computer programs that have proven able to rediscover many fundamental scientific findings. If many activities used in the discovery process are equivalent to many activities in the design process, then many techniques found in automated discovery will be useful in automated design and vice versa. We show in this chapter that at the process level this is quite accurate, that approaches used in automated discovery programs are quite similar to approaches used in automated design programs. Note that we include invention in design; just as paradigm-shifting breakthroughs

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are at the creative end of the continuum of scientific discovery, so too is invention at the creative end of the design continuum.

This chapter compares historical, cognitive, and algorithmic aspects of discovery and design. We will survey what is known about the theory of invention, by which we mean innovative engineering design, and the theory of discovery, by which we mean innovative science, with a particular interest in seeing in what ways they are the same, and in what ways different. We begin with a brief look at three historically important examples in order to demonstrate the intertwining of science and design in both domains: first, Michael Faraday's research on the magnetic induction of electricity, a piece of scientific discovery that also produced an invention – the electric generator; second, Hans Krebs' research that rested on a new experimental technique (the tissue-slice method invented by Warburg for studying metabolic processes in vivo) and led to Krebs' discovery of the reaction path for the synthesis of urea in mammals; third, the Wright Brothers' invention of the airplane, which, in addition to being a major invention, led them to discover significant aerodynamic principles. We next explore cognitive models of discovery and design. We follow with computational models in the discovery programs BACON and KEKADA and the design program A-Design. Throughout, we look across these human and computer efforts to understand cognitive and algorithmic similarities and differences across the two domains.

CASE STUDIES OF HUMAN INVENTION AND DISCOVERY

MICHAEL FARADAY

Because his complete laboratory notebooks have been published, Michael Faraday's work provides us with excellent insights into the processes of scientific discovery: not only the finished work, but the experimental and conceptual steps along the way. His discovery, in the autumn of 1831, of the magnetic induction of electrical currents illustrates what we can learn from this kind of step-by-step account of experimentation. It is especially interesting because Faraday's discovery, a basic scientific advance that provided one of the two components in Maxwell's equations, also constituted the essential step in the invention of the electric generator.

From the time of H. C. Oersted's discovery in 1821 that an electric current generates a surrounding magnetic field, a number of leading scientists, the young Faraday among them, entertained the idea that, by symmetry, perhaps a magnet could generate an electric current in a nearby wire. During the succeeding decade, Faraday conducted a number of experiments that produced significant electrical phenomena, but not the desired magnet-generated electricity. After a lapse of several years, he resumed his search in 1831. Stimulated by news of the powerful electromagnets that Joseph Henry was designing in America, Faraday had an iron ring constructed, and he began investigating whether, by winding a battery-connected wire around one side of it to magnetize it and a circuit containing an ammeter around the other side, closing the battery connection would create a current in the latter circuit.

To Faraday's surprise, he obtained no steady current, but he observed a momentary transient electrical pulse just when the battery connection was made, and

another, in the reverse direction, when the connection was broken again. He then undertook dozens of experiments to see how the transient would be strengthened or weakened (and implicitly, whether it could be converted into a continuous current) if he changed his apparatus in any of a large number of ways (the number of windings, the material of the wires, the distances between parts of the apparatus, and so on). He made a number of attempts to design an apparatus that would yield the desired results, experimenting with electromagnets activated by a Voltaic pile, natural iron magnets, and the Earth's magnetism. He was testing no specific hypothesis, but looking for electrical phenomena.

After several months of effort and over 400 experiments, in which the only effects were stronger or weaker electrical transients, and noticing that the transient was of a little longer duration when a natural magnet was pushed rapidly into a circuit in the form of a hollow coil of wire, he was reminded of an experiment of Arago, in which the rotation of a magnet above a copper disk caused rotation of the disk, an effect that the existing theory of magnetism could not explain (copper is not magnetic). Faraday began to wonder if, just as plunging a magnet into a coil produced a transient electric pulse, the rotation of the magnet in Arago's experiment might have caused electrical effects in the copper disk. He was quickly led to the design of analogous experiments (inverting the roles of magnet and disk) rotating a disk between the closely spaced poles of a powerful magnet, and was rewarded, when the rotation was continuous, with the production of a continuous current. He also recognized and commented that this arrangement could be the basis for a generator, leading to our conclusion that his was an act of invention as well as an act of discovery.

The records that Faraday left behind in his notebooks demonstrate several important characteristics of his methods of discovery that were quite different from those we find in standard discussions of scientific method (e.g., Popper, 1959). Such discussions typically assume that an experiment begins with a clearly formulated hypothesis, which is to be validated or rejected by the experimental data. They ignore the question of where hypotheses come from, and consequently do not focus on discovery at all, but only upon validation of what has already been discovered.

Faraday began his research with only a very vague hypothesis: that, by symmetry with Oersted's Phenomenon, it should be possible to use magnetism to generate an electrical current. Bringing circuits into the proximity of magnetic forces should produce the desired effect or some other phenomenon of interest. It produced the latter, a surprising effect: an electrical transient. Faraday reacted to the surprise as other innovative scientists have done to their surprises. He asked how, by changing the experimental arrangement, he could magnify the effect, define its boundaries, and if possible, convert it into the quite different effect he had hoped for: a steady current.

Faraday's experimental strategy (not only in this case, but throughout his career) was not to take given hypotheses and test them, but, guided by general and often rather vague concepts, to construct conceivably relevant situations in which to look for interesting phenomena, that, if found, could be modified and enhanced. He behaved like a miner searching for an ore body rather than the same miner extending a mine in a previously discovered lode. He had a goal, in the form of a desired kind of effect, but no strong theory providing a plan for reaching that goal. In all of these respects, he resembled an inventor who has in mind a function to be

performed, and searches through a large space of possible devices to contrive one that will perform it.

Faraday was not antagonistic to theory. For example, when he observed the unexpected transient in his first experiment, he spent some time formulating a hypothetical mechanism (which he called the “electrotonic state”) to explain the phenomenon as produced by a change of state in the electrical circuit. In best textbook fashion, he carried out, unsuccessfully, a number of experiments to obtain empirical evidence of the wire’s change in state.

Much later, after he had found ways to produce steady current, and in order to clarify some ambiguities about the direction of the current, he used iron filings (a technique that had been known for several centuries) to examine the shape of the magnetic field in which the phenomena were being produced. He observed (again without prehypothessizing it) that currents occurred in a closed circuit whenever the wire moved across the lines of magnetic force marked by the filings, regardless of whether it was the electrical wire or the magnet that moved. Now he formulated a new (and essentially correct) theory: that current was produced when lines of force were cut, the theory that ultimately made its way into Maxwell’s Equations. Finally, he explained the transient that had appeared in his first experiments by the further assumption that when the battery circuit was closed, the magnetic lines around the magnet ring expanded; when the circuit was opened, they collapsed, thus cutting the ammeter circuit in both cases, but in opposite directions.

Having satisfied himself that the theory accorded with the phenomena he had observed (verification), he put aside the earlier speculative and unverified notion of the “electrotonic state.” In this research episode, the principal task was not to test given theory but to produce phenomena that were interesting or desired. A very general goal led to the observation of the initial electrical transients; this led to further exploratory experimentation that evoked a memory of Arago’s experiment and discovery of an experimental procedure that produced steady current. Confusion about the directions of the currents under different conditions led to experiments using iron filings to visualize the magnetic field, calling attention to a circuit’s cutting magnetic lines as the condition for the induction of current and the determinant of its direction, and immediately to a theory of electromagnet induction that later became a component of Maxwell’s Equations and the progenitor of the electric generator. Important aspects of design are evident in a number of ways in this work. These include the actual design of various magnetic artifacts with which to produce electricity, the iterative process (cycling between synthesis of attempted designs and analysis of obtained results), and the final results consisting of both an important discovery (the interactive equivalence of electricity and magnetism) and an important invention (the electric generator).

HANS KREBS

The lab notebooks of Hans Krebs, who discovered the Krebs Cycle of Organismic Metabolism, and earlier, the reaction path for the synthesis of urea in the liver, are also available to us. In the case of urea synthesis, they reveal events very similar to those in the previous example. This time, as in Faraday’s case, the experiments took

place over a period of a few months. The process begins with a problem: to discover the reaction path that synthesizes urea in the liver. Biochemists already knew that the likely sources of the nitrogen in the urea were ammonia (from the decomposition of amino acids) or amino acids (from the deamination of proteins) as well as purines from DNA and RNA.

Experimenters had already searched unsuccessfully for the reaction path, but they used cumbersome methods involving entire organs. Krebs took up the task because he had acquired his new "secret weapon" as a postdoc in Otto Warburg's lab – a method had been designed that used thin tissue slices, which enabled him to carry out experiments many times faster than could be done by using perfused whole organs.

Krebs had a straightforward strategy: using this newly designed tissue-slice testbed, he applied ammonia and various amino acids and purines to the tissue slices and measured the yield of urea. Obtaining no interesting results, he began (for no reason that has been clearly established) to use combinations of ammonia and an amino acid. One day, when testing ammonia and ornithine (an amino acid that appeared mainly in the liver, and at the time of Krebs' experiment had no known function), he obtained a large yield of urea. With the aid of the chemical literature, he was fairly soon able to find a plausible reaction path that combined the ammonia and ornithine; then, after several further steps, used the nitrogen derived from the ammonia to form urea, recreating and releasing the ornithine for repeated use. Thus, although the experiment was probably run to test whether ornithine might be a source of urea nitrogen, the nitrogen was found to come, in fact, entirely from the ammonia. The ornithine, retaining its nitrogen, served as a powerful catalyst to speed up the reaction by a large factor.

Here we see another example of the generation of an important phenomenon "for the wrong reason." Recognized with surprise, the phenomenon leads to the desired outcome and provides evidence that leads rather directly to the correct theoretical explanation. The catalytic action of ornithine was discovered by experiment, not verified by testing after it had been hypothesized on other grounds. As in the case of Faraday, we see the scientist seeking "interesting" phenomena related to some broad goal (e.g., exploiting the supposed symmetry of electricity and magnetism), finding a law that describes the observed phenomena, and then searching for theoretical explanations of the law. At a general level of description, this rapid convergence on a new solution (explanation or theory) once a surprising discovery is made can be viewed as a sudden move to a new area of the problem space, or even to searching a new or different problem space. In design, as we will see below, a similar phenomenon arises when a genuinely new design is generated: it rapidly leads to the exploration of a new portion of the design space or even a new space in cases in which, for example, the search shifts from seeking a component that performs a certain function to searching for an entirely new design approach, producing a new set of solutions to the design problem.

THE WRIGHT BROTHERS

In turning to an examination of design, we will consider the Wright Brothers' invention of the airplane as a classic case of inventive design. We base our analysis of the Wright Brothers' contributions as inventors-scientists on the extensive treatment afforded their work in Voland's *Engineering by Design* (Voland, 1999), where

he presents their work as his example of "methodical design," and in *The Wright Flyer, an Engineering Perspective*, edited by Howard S. Wolko (1987). The Wright Brothers' historic feat provides a useful view of the design process.

Contrary to the popular view that the Wright Brothers' accomplishment was primarily an experimental, empirical enterprise that relied on trial-and-error attempts to fly in windswept Kitty Hawk, North Carolina, in reality their efforts were strongly rooted in the science of fluid mechanics and in addition, made substantive contributions to that science. As Volland puts it,

In contrast, the Wright Brothers more closely followed the structured problem-solving procedure that we now call the engineering design process to develop and refine their glider and airplane concepts. As a result, Wilbur and Orville Wright behaved more like today's engineers than yesteryear's inventors: They were not only creative but truly methodical and analytical in their work, adding the steps of synthesis and analysis that were missing in the earlier efforts of others (p. 23).

G. Volland, *Engineering by Design* (1999)

With regard to their scientific contributions, the following quotations are typical evaluative comments: "The Wrights' understanding of the true aerodynamic function of a propeller, and their subsequent development of a propeller theory are important firsts in the history of aeronautical engineering" (Anderson, 1983, p. 16)², and "probably the best-known scientific work by the Wrights is their program to obtain data for airfoils and wings" (Culick and Jex, 1987, p. 20). In addition to their contributions to many aspects of aircraft design, one lasting contribution they made to the science of aeronautics was their deduction of a correct value for Smeaton's coefficient for drag (discussed below), which had been overestimated by a third for the previous 150 years (Culick and Jex, 1987).

The basic relations between drag and lift and its implication for power had been worked out prior to the time of the Wright Brothers' achievement, and they formed the basis for the design of their airplane. In particular, lift (the upward component of force) $L = kV^2AC_l$, where V is the velocity, k is a constant, A is the area of the lifting surface (the wing), and C_l is a lift coefficient that depends on both the wing camber (height to cross-sectional length ratio) and angle of attack (angle with respect to the horizontal line of travel). For drag (the force resisting forward travel) there are two components, induced drag (D_i) and parasitic drag (D_p). The relations are $D_i = kV^2AC_d$ and $D_p = kV^2A_fC_d$, where k is a constant, C_d is the coefficient of drag, A is the wing area, and A_f is the frontal surface area. (They achieved a reduction in frontal surface area by having the exposed pilot lie flat rather than being seated.) They calculated the power necessary to propel their vehicle in a very straightforward manner as $P = D \times V$, where D is the total drag or force needed to overcome drag and V is the desired velocity. As discussed below, the coefficient k above, known as Smeaton's coefficient, formed the basis for one important scientific discovery of the Wright Brothers. According to Volland, they designed with these relations in mind and iterated between experimentation and redesign. As he puts it,

With these rather rudimentary mathematical models of flight behavior, the Wrights were able to develop their aircraft designs. Whenever failure struck (as it did

² Others (Lanchester, Drzewiecki, and Prandtl in Germany) had started to evolve a propeller theory independently of the Wrights, but according to Lippincott, "— the Wright Brothers evolved this theory independently without knowledge of the work of the earlier scientists" (Lippincott, 1987, p. 79).

repeatedly), they returned to careful experimentation and observation in order to correctly adjust the values of constants and variables appearing in the above equations. This methodical and iterative transition between scientific theory and its practical application – through which both the theory itself and its application are successively developed and refined – is the essence of good engineering practice (p. 32).

G. Voland (1999)

It is also, as we have seen above, the core of much scientific practice!

As they moved to the issue of control, there was a similar alternation between theory and design, especially in regard to the issue of sideslipping in the control of yaw. Over subsequent summers from 1900 to 1902, they tested a number of gliders, working out control systems for each of the three major axes of turning. They adopted a horizontal elevator in the front of the glider for pitch control and twistable wings for roll axis control. In 1901, they embarked on a sizable research project to find ways of combating some problems arising from inadequate lift. They constructed a wind tunnel to experiment with the variables that determine lift and, through testing of over 200 wing designs, found that the values in the equations for lift (reported earlier by Lilienthal) were generally accurate, with the quite surprising exception of the Smeaton's coefficient, k , which they had to significantly revise downward by a little more than a third (from 0.0049 to within a few percent of the correct value of 0.003; see Culick and Jex, 1987; Jakab, 1990).

With the use of this revised value, they modified their wing to yield more lift. They then confronted the issue of sideslipping that occurred when the airplane banked in a turn. The raised wing (as a result of changes in the attack angle) had increased drag, resulting in a turning around the yaw axis, and a decrease in lift, leading to downward sideslipping, a dangerous condition in low-flying airplanes or gliders. In 1902, they at first experimented with a pair of fixed vertical rudders to prevent sideslipping, but they soon replaced them by a single vertical rudder that could be controlled so as to both prevent sideslipping and allow control around the yaw axis. This solved a major problem in their design and allowed them to go on to successful flight. The final stage in the design of the initial airplane was the propulsion unit. Orville Wright determined specifications for the engine from an analysis of the power required and the allowable weight. This was based on a number of variables, including all of those that contribute to lift, drag, weight of the airplane and pilot, and desired velocity. His calculations yielded a value of 8.4 hp with a maximum weight of 200 lb, and his mechanic, Charles Taylor, delivered an engine that could generate 12 hp and weighed 180 lb, thus enabling the successful manned flight in December of 1903.

Through the progression of the design process by the Wright Brothers, we repeatedly observe goal-directed problem solving, both in the main goal of obtaining flight, but also in subgoals toward the main goal such as solution of the sideslip problem. We also observe an iterative process between configuration synthesis and evaluation (both analytical and experimental). Finally, although the focus is on the design of a complex device, the experimental observations led to fundamental scientific findings in fluid dynamics (Smeaton's coefficient), propeller design, and sideslip and its control. Note that although the Wright Brothers may not have made any major discoveries, they clearly made scientific advances as well as used scientific

results in their invention. Their scientific impact was from the cumulative effect of their both using science and advancing our understanding of the science of aerodynamics. However, as we have noted, in both design and science there is a continuum from the routine to the creative. The important lesson is that, in order to move to the creative end of one continuum, aspects of the other continuum frequently must be addressed; that is, some level of science is usually needed to effectively invent things, and some level of design is usually needed to support scientific exploration.

SUMMARY

Krebs was considered a scientist who made a great discovery. To do so he invented new methods to perform his experiments. The Wright Brothers are known as inventors or designers who invented an important machine. However, it is clear that along the way they discovered new scientific principles. Faraday is considered both an inventor and discoverer, having needed to be both to accomplish his goals. In many ways the classification of these people comes from knowledge of the domain in which they operated. However, Krebs could be considered an inventor and the Wright brothers could be considered scientists. At the process level, in all three cases there is an iteration between a synthesis phase (of an artifact or scientific experiment, explanation, or theory) and an evaluation phase, until a desired goal is achieved, the sought-after invention or discovery. We now move on to a comparison of cognitive models of discovery and design.

COGNITIVE MODELS

THE PROCESSES OF DISCOVERY

We turn now from these historic examples to a more general discussion of what is involved in scientific discovery. There is a large literature of research on scientific discovery, produced by historians and philosophers of science, cognitive psychologists, and scientists (some of it autobiographical), and a gradual convergence is taking place toward a common picture of the discovery process. Some recent examples of, and guides to, this literature are Finke, Ward, and Smith (1992), Giere (1988), Holland et al. (1986), Holmes (1991), Langley et al. (1987), Nickles (1978), Weisberg (1993), and Dunbar (1993).

As noted above, scientific discovery can range from the breakthrough major discovery, as in the examples cited above, to the more mundane or routine small extensions of previous work that are often referred to as *paradigmatic science* (such as determining the dose-response curve for some newly discovered medication or whether an experimental result obtained with one species also holds in another). By examining a large range of examples of major discoveries, we learn that "discovery" is not limited to a single kind of scientific activity. Scientists do many things, although individual scientists may specialize in just one or two of them (Langley et al., 1987). Among the important kinds of discoveries that result from

scientific activity are the following.

1. Discovery of ways of describing and thinking about some domain of phenomena; that is to say, forming representations of the domain: the problem spaces.
2. Discovery of an interesting puzzle or problem in the domain (e.g., the problem of describing and explaining the orbits of the planets around the Sun).
3. Discovery (or design) of instruments and experimental strategies for attacking empirical or theoretical problems (e.g., the thermometer, recombinant DNA, the calculus).
4. Discovery of new, often surprising and puzzling, phenomena. (We have already provided several examples.)
5. Discovery of laws or creation of models that explain the described phenomena (e.g., Newton's Law of Gravitation, which explains Kepler's descriptive Laws of Planetary Motion; Bohr's model of the hydrogen atom, which explains Balmer's Law, a description of the hydrogen spectrum).
6. Discovery of laws that describe bodies of phenomena (e.g., Hooke's Law, Ohm's Law, Mendel's Laws).

The list is undoubtedly incomplete, but it covers the main categories of discovery. Historical research has revealed a great deal about how discoveries of each of these kinds are achieved, and our understanding of the processes has been augmented and sharpened by a number of computer-simulation models that constitute testable and tested theories of these processes: see Grasshoff and May (1995), Langley et al. (1987), Shrager and Langley (1990), Shen (1993), and Valdes-Perez (1995). In the fourth section, we will briefly describe two examples of such models: one, called BACON, works solely from data to construct descriptive laws that fit them (Category 4, above); another, called KEKADA, plans sequences of experiments in order to produce observations that can be used to formulate descriptive and explanatory theories of problematic phenomena (Categories 3–6, above, especially 4 and 5).

From historical analyses and computer simulations of the kinds we illustrate below, an empirically based and rather comprehensive theory of discovery has emerged. Perhaps the most important feature of the theory is that it is built around the same two processes that have proved central to the general theory of expert human problem solving: the process of recognizing familiar patterns in the situations that are presented, and the process of selective (heuristic) search of a problem space. Basic to these are the processes of formulating a problem space and of representing available information about the problem, as well as new information acquired through observation and experimentation, in that problem space.

Put in simplest terms, human experts solve difficult problems (including problems of discovery) by selective searches through problem spaces that are sometimes very large, but they greatly abridge their searches by recognizing familiar patterns, associated in memory with information about how to proceed when a particular pattern is present. To do this, they have to represent the problem in a form that will reveal the familiar patterns and access the memory already stored for dealing with them (Simon and Kotovsky, 1963; Newell and Simon, 1972).

Efficient problem solving may require both general knowledge and a large body of knowledge that is peculiar to particular problem domains. This is true both of

knowledge required for selective search (the heuristics that guide selection) and knowledge required for recognizing patterns and exploiting that recognition. Hence, expertise, including expertise in scientific discovery, is transferable from one domain to another only to a very limited degree. However, knowledge about the calculus and differential equations, and knowledge about computer programming, are examples of knowledge that has potential for broad transfer.

In summary, everything that has been learned about making discoveries suggests that discovery is just a special case of expert problem solving. The faculties we call "intuition," or "insight," or "creativity" are simply applications of capabilities for pattern recognition or skillful search to problems of discovery, albeit in very large and ill-defined problem spaces.

THE PROCESSES OF DESIGN

Design, as illustrated by the Wright Brothers, is an activity whose goal is the creation of a new or improved artifact or process. It is characterized by deliberate planned activity directed toward a goal or set of goals and is subject to constraints and often-conflicting evaluative criteria. In addition to deliberate stepwise progress, design can and often does involve flashes of insight, evidence of incubation (off-line work) and what has broadly been termed "intuitive" behavior. As argued above, such behavior, although sometimes seemingly mysterious, is amenable to a cognitive analysis. The domain of activities that constitute design can range from the fairly mundane (selection of gear ratios in a transmission or substitution of different materials to make a lighter-weight knife handle) to the highly creative (design of the first cellular device for communicating or, in the case of the airplane, creation of the magic of flight).

The latter design activities are often labeled *invention*, a term that designates one subset (the creative or "new artifact" extreme) of the design continuum. One of our claims is that invention is not essentially different from other types of design activities, but rather represents this more creative or innovative end of the design continuum. In addition, as the Wright Brothers' example demonstrates, the activity of invention or design often involves operating in a number of different modes. Artifact synthesis by means of design and construction, scientific analysis and evaluation, and empirical experimentation, all conducted in an iterative manner that (when successful) converges on a good design, are three of the major activity modes that comprise the overall activity of design.

When humans engage in a creative endeavor such as designing a new artifact, they are assumed to operate under the guidance of a goal or purpose, that is, a conception of what is to be created (Ullman, Dietterich, and Stauffer, 1988). The process has been likened to that of human problem solving, whereby people search a "problem space" that consists of possible configurations of elements, applying move operators that take them from state to state until they find a solution (Newell and Simon, 1972; Anderson, 1983). Attempts have been made to analyze the cognitive problem-solving processes (primarily search and analogizing – see Gentner, 1983; Falkenhainer, Forbus, and Gentner, 1989; Forbus, Gentner, and Law, 1994) that operate within the design process (Adelson et al., 1988; Ullman et al., 1988; Adelson, 1989). One finding is that search often goes on in multiple problem spaces. For example, in science, people often alternate between searching a space of

experiments with searching a space of hypotheses (Klahr and Dunbar, 1988; Dunbar, 1993). Similarly, in design, the search may move between a space of components to instantiate or realize a given design idea (e.g., the search for an appropriate airfoil shape for a fixed wing) and a space of design conceptions or new approaches to a design problem (whether to have flapping, birdlike wings or a fixed airfoil, for example). The general cognitive architecture, *Soar* (Laird, Newell, and Rosenbloom, 1987), uses this multiple problem space search as a basic, almost universal, method for search that is practicable in a wide variety of problem domains.

Representational issues along with problem space size are also important in problem solving in diverse problem domains. Cagan and Kotovsky (1997) have modeled the problem-solving process based on data from human problem-solving performance through a learning algorithm in conjunction with a simulated annealing search strategy. Although the problem space might be vast, consisting of all possible legal configurations of the elements that make up the problem, nonetheless, the designer does not always know the whole space or have to search it in its entirety, given adequate heuristics for selecting propitious portions of the space to search. In fact, the size of the problem space has been shown to be but one of a number of factors that determine problem difficulty. Representational issues have also been shown to be a major determinant of problem difficulty in humans (Hayes and Simon, 1977; Kotovsky, Hayes, and Simon, 1985; Kotovsky and Simon, 1990). As we have seen, choice of an appropriate representation of the problem is a central issue in scientific discovery as well.

The processes underlying design include a broad array of cognitive activities, including search through a space or spaces of possibilities (often conducted in a stepwise or piecemeal fashion as the design is progressively instantiated with a set of components), the use of analogical reasoning to import useful ideas or substructures from previous designs, other ways of accessing memory for relevant general or domain-specific knowledge, and an evaluative phase or set of tests for whether a satisfactory end state has been reached. They include both analysis and synthesis, often (as we have seen) operating iteratively in the creation of a new design. Once a successful design is created, it is often progressively generalized or otherwise extended to create a range of possible options or extensions. In our example of a truly creative design, there is a loop between analysis and synthesis as a design concept evolves. It is our claim that this is not only true of design, but that the processes that yield new artifacts are similar to those found in a related enterprise – scientific discovery.

COMPARISON

Similarities

We have, to this point, seen similarities between discovery and invention or design in:

- the intertwining of the two (invention depending on and yielding scientific discoveries and scientific discoveries depending on and yielding inventions),
- the iterative synthesis–analysis cycle,

- the underlying cognitive activities based on problem solving, pattern recognition, analogical reasoning, and other cognitive knowledge retrieval mechanisms; and
- heuristically guided search in large ill-defined problem spaces.

In both design and scientific discovery, the respective domain of activities can range from the fairly routine or mundane to the highly creative, in which major scientific advances or designed inventions create new paradigms or change our way of interacting with or understanding the world. In both design and scientific discovery, each is generally an intrinsic part of the other process (design is needed to make discoveries, and science is needed to succeed in invention). However, the real similarity between the activities that fall under the rubric of design invention and those that are labeled scientific discovery is not only that the process of doing science is comingled with that of design, but that the underlying cognitive processes are essentially the same.

Design is a planned activity, directed toward a goal or set of goals, and subject to an evolving set of constraints. The processes underlying design include a broad array of cognitive activities, including search through a space or spaces of possibilities or components, reliance on general and domain-specific knowledge including the use of analogical reasoning to import useful ideas or substructures recognized as familiar and relevant from previous designs, and an evaluative phase or set of tests for whether a satisfactory end state has been reached. It operates iteratively between analysis and synthesis in creating new designs. Design is thus accomplished through knowledge-based pattern recognition and problem-solving search processes. Such pattern recognition activities are an important part of human cognition and are fairly central to scientific reasoning as well (Simon and Kotovsky, 1963).

The processes underlying scientific discovery also include a broad range of cognitive activities including search through a space of hypotheses and activities designed to test those hypotheses (often conducted in a stepwise fashion as the space is progressively searched.) This is often accomplished by use of analogical reasoning (from similar scientific findings) and testing of possible "solutions" (scientific results or conclusions) to determine whether an adequate understanding or conclusion about a hypothesis or theory has been attained. There is frequently an additional attempt to broaden the finding to an extended range of situations or circumstances. Finally, the process is iterative, moving between experiment generation and theory refinement. As with design, scientific discovery is characterized by deliberate planned activity directed toward a goal or set of goals and is also subject to constraints and multiple evaluative criteria (e.g., accuracy of prediction vs. parsimony of free parameters). It too involves stepwise search through a space (or multiple spaces) of possible hypotheses, experiments, and theories, as well as flashes of insight, incubation, and intuition, all of which can be described as pattern recognition, memory retrieval, and problem-solving activities operating to generate and search within an appropriate representation or problem space.

This broad-stroked description of the cognition of scientific discovery matches in surprising detail the description of the design process; they are both problem-solving activities that to date have occurred primarily in the human mind, and thus reflect its operating characteristics. Thus, when considered from a fairly broad perspective,

the structure of the domains and the underlying cognitive activities exhibit a high degree of unity.

Differences

Of course there are obvious differences between discovery and invention. These differences focus on the purpose or goal of the endeavor, the knowledge used to generate the problem space being searched, and the training of engineers and scientists in today's educational environment. The fundamental difference that differentiates the two domains is the *goal* of the process: scientific explanation versus creation of a new artifact. Scientists wish to discover new knowledge about how the existing world works, whereas designers invent new devices that function within that world. Design starts with a desired function and tries to synthesize a device that produces that function. Science starts with an existing function and tries to synthesize a mechanism that can plausibly accomplish or account for that function; the mechanism already exists but it is unknown, so the scientist must still create or synthesize a model or theory that replicates or explains it.

The second significant difference between scientific discovery and invention is the knowledge base, that is, the knowledge of facts and bounds on the physical world, and the experience one has in an area. Note that knowledge is a part of cognition in that it forms the knowledge base that cognitive processes operate on, but it should not be confused with the cognitive processes themselves that are our focus. The knowledge base for engineering designers includes an understanding of the behavior of components, materials or fluids, an understanding of the applicable science of the domain, and an understanding of heuristics about the bounds on the feasible space. Designers also have developed intuition through experience and stored that knowledge in memory. Similarly, scientific discovery requires knowledge about what is known in say chemistry, biology, or physics, and also heuristics about the bounds on the feasible space. Scientists also have intuition and experience in a domain. But we might also point out that differences in the knowledge base occur not only between the two areas (invention and discovery) but within each as well; a chemist and a physicist or geologist have very different knowledge bases even though they are all scientists, and an automobile designer and the designer of chemical processing plants similarly have quite different knowledge bases.

This knowledge defines the problem space in which designers and scientists search. We differentiate between two spaces: First is the potential problem space that includes all combinations of parts or articulations of, say, geometries, whether feasible or infeasible, efficient or inefficient. The other space is the heuristic space generated by an efficient or heuristic search process. The generation of the space is dependent on the domain knowledge base; however, once the space is generated, or the method of generating the heuristic space articulated, then the cognitive process of search of that space is the same.

The third difference between scientific discovery and engineering invention is only one of perception. Scientists are perceived as those that discover and engineers as those that design. It is surprising, however, that beyond the differences in their respective knowledge base, their education is not that different! Although engineers

are perceived as designers, in reality very little of their training focuses on design or synthesis methods. Most courses in an engineering curriculum focus on understanding analytical models of how the world behaves, that is, science, whereas few courses focus on synthesis methods. We recognize, and have argued strongly above, that scientific knowledge is critical to engineering design; however, we also argue that synthesis is what enables engineers to practice the design process. We argue that engineering curricula should be broadened for more inclusion of synthesis methodology and the means to apply science in the synthesis process.

In a similar vein, much training of science students, at least at the undergraduate level, focuses on teaching the findings or knowledge base of science, that is, models of how the world behaves in various scientific domains. The inclusion of more teaching of the methods of science, the tools for discovering new knowledge or synthesizing scientific experiments and theories, is often relegated to advanced graduate training. In this fashion, the training of engineering and of science students exhibits a somewhat nonpropitious parallel. Our focus on the interplay of analysis and synthesis raises the issue of the optimal pedagogical approach to allow students to acquire and use both types of tools or approaches. Perhaps individuals with the breadth and perspective of Faraday, the Wright Brothers, and Krebs would be less rare.

So again, although education and training between scientific discoverers and design inventors is quite different as a result of the knowledge taught, their cognitive models of search, once the problems are defined, are the same. Under this view, an engineer given a knowledge base of biology and the experience and insight of an experienced biologist could discover new theories, and a biologist given the knowledge base, experience, and insight of a mechanical design engineer could use his or her problem-solving processes to invent new artifacts.

COMPUTER MODELS

We turn now to observation of computer models of discovery and design. The discovery programs were created to capture cognitive models of human discovery directly. The design program was developed with the intention of automating the process of invention by using the generation and search capabilities of the computer along with insights gained from human design activities where beneficial.

DISCOVERY

BACON

BACON is a computer program that simulates (by actually doing it) the process of discovering laws that describe the data provided to it (Langley et al., 1987). Basically, BACON works by generating mathematical functions, then fitting them, by adjustment of parameters, to the data. It requires no knowledge of the meanings of the data points, but operates wholly by searching for invariant patterns of data (e.g., a pattern such as $y = ax^2$, for fixed a , that holds for all y 's and their corresponding x 's in the

data set). It does not generate functions at random, but determines what function to generate next by examining the ways in which those previously generated have failed to fit the data.

For example, if y/x decreases as x increases, and y/x^2 increases as only x not y increases, BACON considers their product: y^2/x^3 , finding, in this case, that it is constant (within a given allowance for measurement error). BACON then concludes that $y = ax^{3/2}$, where a is a constant. When y is identified as the period of revolution of a planet around the Sun and x as the distance of the planet from the Sun, this can be recognized as Kepler's Third Law.

The core of BACON is a small set of productions (if \rightarrow then rules) that generate a sequence of hypotheses $z = f(x)$, where x is the observed independent variable, and z is a prediction of the observed dependent variable, y . As we have seen in the example, if the hypothesis doesn't fit the data (as it usually doesn't), BACON then examines y and one of the new variables already computed, say y/x , to see if the former increases or decreases monotonically with the latter. In the first case it introduces their ratio as a new variable and tests for its constancy; in the second case it introduces their product and tests for constancy. If the test is satisfied in either case, the new variable, say w , is a law, for $y = w = f(x)$. Thus, in the example, having found that y/x^2 and y/x are not constant but vary with x in opposite directions, it tests their product, finding the constant law.

Because BACON requires no knowledge about the meanings of the variables, it is a completely general data-driven discovery engine, which is, of course, not guaranteed to find a pattern in any given application. Nevertheless, without any changes in the heuristics or other features of the program, or any prior knowledge of the nature of the variables, it has (re)discovered Kepler's Third Law, Coulomb's Law of Static Electricity, Ohm's law of electrical resistance, Archimede's Law of displacement, Snell's Law of Light Refraction, Black's Law of Specific Heat, the law of conservation of momentum, the law of gravitation, and formulas for simple chemical compounds. In all of these cases it has to generate only a small number of functions (seldom as many as a score) in order to find one that fits the data.

Not only does BACON (re)discover these and other important scientific laws, but it also introduces new theoretical concepts into its functions, assigning them as properties to various parameters. For example, in the Snell experiment, it introduces the coefficient of refraction as a property of each of the substances that the light traverses; in the Black experiment, it introduces and determines the value of a specific heat for each substance; in the experiments in mechanics, it introduces gravitational and inertial mass (and distinguishes them); in the chemical experiments, it introduces atomic and molecular weights (and distinguishes them). Hence BACON discovers theoretical terms as well as laws.

BACON introduces new concepts when it discovers that a given law holds only when a discrete experimental variable (say, whether the liquid being tested is water or alcohol) is held constant, but, with a change in parameter, also holds for other values of the variable. It then assigns that parameter as the value of a new property of the variable. Thus, in Black's Experiment it finds that it can assign a specific parameter value (which we know as "specific heat") to each distinct liquid and thereby generalize the law to apply to mixtures of liquids as well as to a single liquid.

BACON's searches can often be substantially shortened if it need not work in total "blindness," but is provided with some prior theoretical constraints: for example, conservation of mass and heat in Black's experiments on temperature equilibrium; or conservation of atoms in the chemical experiments. So, although designed as a data-driven discovery system, it can also operate in a combined data-and-theory-driven mode.

KEKADA

In BACON, empirical data are the required inputs. KEKADA (Kulkarni and Simon, 1990) is a computational model that simulates experimental strategies for acquiring and interpreting data. It has to be provided with substantive knowledge about some domain of science, with knowledge of feasible experimental manipulations and with a scientific problem to be solved. Its task is to plan successive experiments aimed at solving the problem. After it plans an experiment, it is provided with knowledge of the data obtained by carrying it out (provided to the program by the user), and it then uses this new information, together with the knowledge it already had, to plan a new experiment. Both knowledge and experimental strategies are represented as productions, that is, if \rightarrow then rules.

KEKADA's knowledge takes the form, then, of a system of productions, but, in contrast to BACON, there are a large number of these, for they must represent not only general heuristics of search and experiment construction, but also domain knowledge. As an example of a general heuristic, from the outcomes of experiments it forms estimates of the yields of certain substances that are to be expected when the next experiment is performed. If a quite different yield is observed, KEKADA reacts with "surprise." It then designs new experiments to test the scope of the surprising phenomenon, and subsequently experiments to search for causal factors.

Here is an example of domain-specific knowledge: in the search for the mechanism of urea synthesis in the mammalian liver, Krebs' problem discussed earlier, KEKADA is provided, at the outset, with the relevant chemical knowledge and knowledge of experimental methods that Krebs possessed. It plans a series of experiments using the tissue-slice method of Warburg with ammonia and/or amino acids (already known, with near certainty, to be the sources of the nitrogen in urea). It eventually comes to try an experiment with ammonia and ornithine, as Krebs did, and it then goes on to find the reaction path and the role of ornithine as a catalyst. It is interesting that the reason why KEKADA (and Krebs) experimented with ornithine (because it was a likely source of nitrogen) was unrelated to its actual function (as a catalyst of the reaction that incorporated ammonia in urea). The discovery, in both cases, was an "accident" that happened, in the words of Pasteur, "to a prepared mind."

KEKADA makes important use of a surprise heuristic in focusing its attention on ornithine after obtaining the first evidence of that amino acid's large effect on urea production. To be surprised, one must have expectations, which KEKADA forms on the basis of the results of experiments. Having formed an expectation of a small yield of urea in similar experiments, it is surprised when ammonia with ornithine gives a very much larger yield. The surprise heuristic then causes it to plan experiments that will seek to amplify the effect and to determine the range of conditions under which

it will be observed: for example, what substances similar to ornithine will produce the effect (in this case, none); how will it (volume of urea produced) vary with the inputs of ammonia and ornithine (experimentally derived answer: directly with the ammonia, very little with the ornithine); and so on.

KEKADA has also been exercised, although with somewhat less attention to detail, on Faraday's experiments seeking to obtain magnetic induction of electrical currents. As in the case of the simulation of Krebs' work, the surprise heuristic played a large role in the simulation of Faraday. The initial experiment was motivated by the goal of obtaining electricity from magnetism; the observed transient was treated as a surprising phenomenon, leading to a series of experiments, similar to Faraday's, aimed at exploring the range of the phenomenon and intensifying it. Knowledge of Arago's experiment could be used to motivate experiments with disks. The simulation was in good agreement with the actual history. Of greater importance in the case of Faraday than in the case of Krebs was the former's great skill in designing and building laboratory equipment and using it to devise new experimental arrangements.

There is a growing number of other computational models of discovery systems, a number of which have been cited above.

DESIGN

We now turn to a brief discussion of a computational model of design that incorporates the same kinds of cognitive mechanisms as those seen to be central to scientific discovery; specifically, the knowledge-based recognition of patterns, the formation of a propitious representation of the design problem space, within which the design problem is formulated, and heuristically based search through that constructed problem space for an adequate solution. Lessons learned from work in cognition forms a basis for the development of the agent-based structure of A-Design and, in particular, the actions of the management agents in guiding what we refer to as top-down search.

A-Design

A-Design (Campbell, Cagan, and Kotovsky, 1999 and 2000) is a program that automates the invention of electromechanical artifacts. The theoretical basis for the program is derived from a model of the design process, namely a mapping from conceptualization to instantiation, the bridge between synthesis and analysis, and iterative refinement. These aspects of the program are true for all good design. Other aspects may or may not connect to human design but nevertheless assist the computer in invention. The approach taken in A-design is to use design agents to act on a representation of the problem domain to create design configurations, instantiations, and modifications. The program also compresses the design process by exploring multiple solutions in parallel and uses computer iteration to evolve new designs.

A-Design's search for optimal designs is accomplished through intelligent modification of alternatives by a collection of agents. The agents interact with designs and

other agents based on their perception of the design problem, the relative preferences of the design goals presented by the user, and an agent's individual preferences. Agents affect their environment by adding or subtracting elements to designs, or by altering other agents. At a high level the A-Design program is a model of (human) group activity.

The program creates designs by working on different levels of abstraction. The agents are able to place components into a configuration based on their knowledge of how components behave. This knowledge is modeled in a functional representation for describing components and designs. The representation developed for this work is based strongly on qualitative physics (Forbus, 1988), bond graphs (Paynter, 1961; and Ulrich and Seering, 1989), and function block diagrams (Pahl and Beitz, 1988), and more specifically on work done by Welch and Dixon (1994), and Schmidt and Cagan (1995, 1998).

The fundamental issue in creating a representation for describing a design configuration is developing a formal method to infer how individual components behave and, further, how the connected sum of components behaves. In this representation, components are described by their ports, or points of connectivity with other components, called *functional parameters*. Information about how components are constrained at their ports, how energy and signals are transformed between ports, and how energy variables within the system relate to others throughout the design is found in the component descriptions. These descriptions, known as *embodiments*, also contain information about the kinds of parameters that describe the component such as length, spring constant, resistance, and cost or efficiency. The use of an appropriate representation defines the problem space and is thus a major contributor to A-Design's being able to solve the problem of creating successful designs. See Chapter 6 for further discussion of this representation.

Once a configuration is created, it is instantiated. Here actual components are selected from a catalog of components indexed by their functionality and ability to instantiate an embodiment. It is here that real values of the variables in the design's embodiments are set.

The need to link between synthesis and analysis is critical in all levels of A-Design. At the embodiment level, the program uses analytical models of components to set up physical constraints on the system. Though not necessarily at the level of the Wright brothers' wind tunnel experiments, the rough analysis still uses science to help direct the design process. The program also calls on analysis simulators to evaluate complete designs after instantiation, enabling a robust representation of physics in the process.

Iteration is an important part of the process. The agents initially create functionally feasible but inefficient designs. In a genetic algorithm-like fashion the process iterates by pruning out ineffective designs and mutating others to create a new population of designs. The process evolves designs toward the optimal arrangement of components that best meet user preferences across multiple design goals. Just as in scientific discovery where there is an iteration between experiment and theory or hypothesis refinement, so too in A-Design there is an iteration between the creation of new abstract designs and the instantiated realization of those designs. This iterative search in dual or multiple domains or problem spaces is a characteristic of human scientific and inventive activity (Klahr and Dunbar, 1988; Dunbar, 1993).

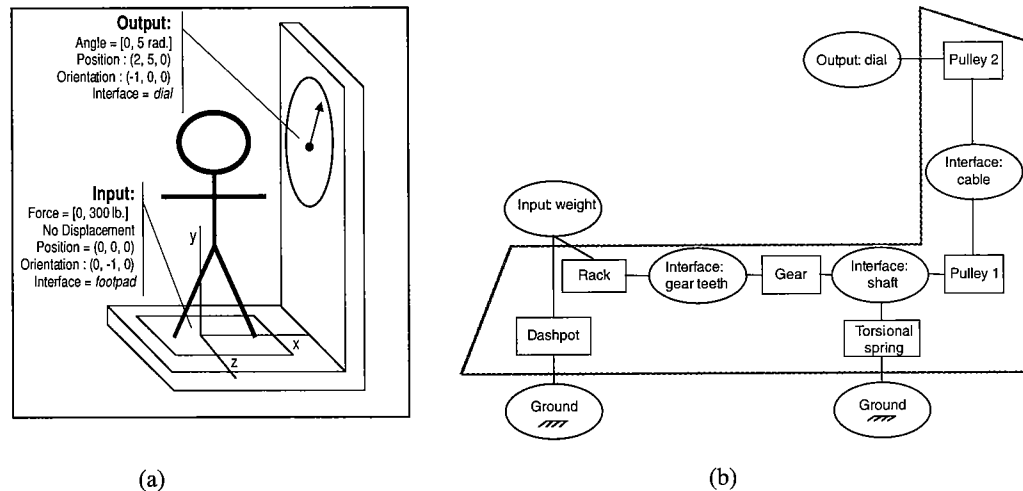
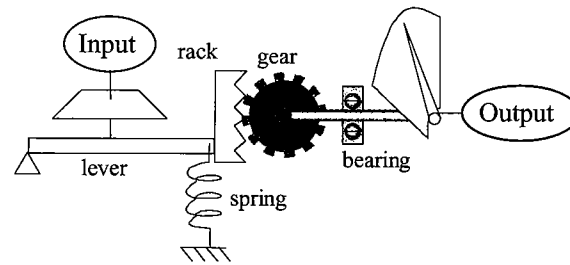


Figure 13.1. Weighing Machine: (a) user-defined functional specifications, (b) possible configuration of embodiments that meet the weighing machine specifications.

There have been several applications using A-Design. One application found in Campbell et al. (1999) shows the design of weighing machines; in another (Campbell, 2000), MEMS accelerometers were created. The weighing machine problem is outlined in Figure 13.1, where the problem description consists of an input-output specification. The input is a person's weight at a certain location, and the output is a dial reading that reflects the input weight. In this example, four objectives were chosen for optimization: minimize cost, minimize mass, minimize dial error, and minimize input displacement. Note that whereas the first two objectives are calculated by summing data provided within the catalog on each of the components used in the design, the latter two are results of the interaction of the components in the completed design and depend on the values of the components used as well as the behavior predicted by the behavioral equations (a.k.a., physics). The catalog consists of 32 embodiments and their instantiations, including motors, pistons, potentiometers, worm gears, and levers. For each of the embodiments, there exist actual components drawn from several catalogs totaling just over 300 components available for constructing designs. In Figure 13.1 is an example configuration of embodiments created by the program. Figure 13.2 shows two weighing machines created by the process for different user utilities or preference weightings for the objectives with rendering of the compound.

The A-Design program is one approach to automating the design process. Other programs with similar goals follow similar strategies, namely iteration toward improved solution, looping between synthesis and evaluation, and at least a reference to cognitive models. Included in this group are the FFREADA/GGREADA programs by Schmidt and Cagan (1995, 1998), which apply simulated annealing to a top-down functional hierarchy. Also included is the structural shape annealing program of Shea and Cagan (1997, 1999), which models structural topologies by means of shape grammars and uses simulated annealing to search the space generated by the grammar; the program has created a wide variety of structural trusses and domes, addressing a variety of design goals. The structural shape annealing work



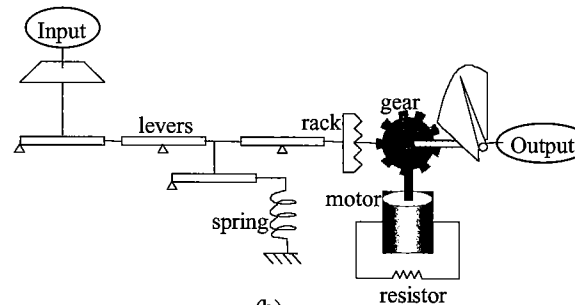
(a)

Components:

lever: 5 cm bar stock $w=1.0"$, $t=0.25"$
spring: ERS-A1-36 \$0.93, $K=16.0\text{lb/in}$
rack: KHS-F2-142 \$26.75, pitch=64
gear: LAS-F7-28 \$5.75, 28 teeth
shaft: AAS-A8-20
bearing: ABS-A2-19

Design objectives:

cost = \$46.82, **mass** = 0.2kg,
input dx = 4.1mm, **accuracy** = 0.4rad.



(b)

Components:

lever-1: 4 cm bar stock $w=1.0"$, $t=0.25"$
lever-2: 4 cm bar stock $w=1.0"$, $t=0.25"$
lever-3: 13 cm bar stock $w=1.0"$, $t=0.25"$
lever-4: 7 cm bar stock $w=1.0"$, $t=0.25"$
spring: ERS-A1-7 \$0.78, $K=14.6\text{lb/in}$
rack: KHS-F2-142 \$26.75, pitch=64
gear: LAS-F7-128 \$12.03, 128 teeth
motor: 542-0130 \$34.19, 300rpm
resistor: 297-7751 \$0.01, 180K?

Design objectives:

cost = \$90.20, **mass** = 0.5kg,
input dx = 0.7mm, **accuracy** = 0.2 rad.

Figure 13.2. Two different alternatives created by the A-Design process. Design (a) is found by an equal preference for four design objectives: minimize cost, minimize mass, minimize dial error, and minimize input displacement; design (b) is found by placing more importance on minimizing the input displacement.

calls a finite-element analysis code in each iteration to evaluate the effectiveness of the evolving design solutions (See Chapter 4 for a further discussion of this technique). In these works, simulated annealing is used as the search strategy based on a high-level analogy to human creative design, where random directions are chosen and pursued if seemingly beneficial or else reversed if seemingly inferior; Cagan and Kotovsky (1997) demonstrated the effectiveness of simulated annealing in models of human problem solving as applied to tavern problems that had been empirically explored by Kotovsky and Simon (1990).

MAPPING ACROSS PROGRAMS

As discussed throughout the presentation of this work, the five similarities across programs of design and discovery are (1) the definition of the problem through input and output states, (2) the iterative synthesis-analysis cycle, (3) the progressive evolution of solutions through iterations, (4) the large problem spaces upon which the programs search, and (5) the direct or indirect mapping of underlying cognitive activities based on problem solving and pattern recognition within the search strategies. In each of these programs the problem representation defines the domain structure. In A-Design this representation is the functional abstract description and specific embodiment and instantiation details; in the KEKADA solution of Krebs' problem the representation is the existing knowledge of chemistry and experimental

techniques of the domain at the time of Krebs. From the domain structure, the search space is defined and in each case is quite large.

Next the initial and final state in each domain is defined. In the weighing machine problem, the initial state is the size and location of the input force and the final state is the location and performance of the dial indicator (with the goal being to determine a connection of devices that connect initial to final state). For KEKADA solving Krebs' problem, the initial state is the set of known chemical constituents contained within the bodies' cells and the final state is the urea that those cells produce (with the goal being to ascertain the sequence of reactions that connect the input state to the final state). The solution sequence is the chain of events that lead from initial to final state. In the KEKADA solution of the Krebs problem, this chain is the sequence of reactions and the relative proportions of chemicals added to and removed from the process as it links the initial to final states; in A-Design the chain is the sequence of component embodiments and their specific parameter values that convert the input to output specification.

The processes are all iterative. They loop between analysis and synthesis. This iteration is consistent with what we understand about both human invention and discovery. For example, Krebs performed over 400 experiments to test his reaction sequences as he progressed toward his discovery. The Wright brothers iterated between physical prototypes and experimentation and analysis. For example, they tested over 200 airfoil and wing shapes in a wind tunnel to determine the best airfoil shape.

The programs each use goal-directed heuristic strategies to work toward improved solutions. KEKADA uses heuristics to focus on improved solution concepts. A-Design uses heuristic strategies through agents and keeps alive several disparate alternatives based on a Pareto analysis (Campbell et al., 1999). Along the way the programs each "recognize" surprises in the solutions, altering their search patterns as a result; in KEKADA the recognition of ornithine's catalytic effect on urea production led to a new line of search, whereas in A-Design the use of a motor and resistor in parallel similarly led to a decidedly new solution to the subproblem of providing damping to the system; see Figure 13.2(b).

In addition to the use of KEKADA to discover the solution of Krebs' problem, it was also shown to recreate Faraday's invention of the generator. In this high-level application there appear many similarities to the approach taken by A-Design. Here experimental setups were configured to eventually discover the reason and means for magnet-generated electricity. A catalog of apparatus components was given to the program. The program chose the configuration of the experiments and instantiated parameter values, basing each decision on the outcome of previous experiments, until the right reaction sequence (or configuration) was found.

BACON, too, demonstrated the evolution of solutions through iterations, the iterative synthesis-analysis cycle, and the direct mapping of underlying cognitive activities based on problem solving and pattern recognition. Here the initial state is the data, for example Kepler's data, and the final state is the goal of determining a function that matches that data. The configuration sequence adds new multiplicative or divisor components to the function resulting in a final function that models the data; BACON's catalog consists of functional terms.

In examining the basics of the design synthesis (A-Design) versus scientific discovery (KEKADA and BACON) programs, we find that, although they were developed

for very different purposes, they have strong similarities at the process level. Both types of programs search a large space in a goal-directed fashion, both use an initial and final state to define the overall characteristics of the problem, both use an appropriate representation of the problem to define the problem space, both define a catalog of components to be assembled into a chain representing the solution state, and both use a synthesize-evaluate loop to verify performance characteristics of the solution state and direct future decisions on changes to the current configuration.

CONCLUSIONS

Four conclusions emerge about the processes of discovery and design: The first is that both science and design are often intermingled with each other, and both require analysis and synthesis. So, invention often involves science and scientific discovery often involves design. This is true of both the processes (where in science experiments and their apparatus have to be designed, and in design scientific principles have to be developed to support designs or design choices).

The second is that both consist of a broad array of activities that range from routine to the creative and revolutionary. Thus, science can range from routine paradigmatic science ("Does the speed of mental rotation decrease with age similarly to the decrease in the speed of memory search?") to the revolutionary discovery ("Does the constancy of the speed of light have implications for length, weight, and time as objects increase their velocity?"). Similarly, design can range from the routine ("Given the usefulness or popularity of the "GoodGrips" potato peeler and can opener, can a similar bottle opener be designed?") to the creative and revolutionary invention ("Can a germ-free environment be created in which to store food by heating and then sealing containers?")

The third and major conclusion we reach is that at a deep level, the cognitive and computational processes that accomplish both activities are virtually identical, namely pattern learning and recognition, processes of constructing adequate representations of some part of the world, and processes of intelligently searching through a vast and often ill-defined problem space that incorporates that representation.

The fourth conclusion is that the processes of design and discovery are structurally similar but differ in their goals and their knowledge bases. Both start from function and move to device or mechanism, but in design the goal is the creation of a device that accomplishes a desired function whereas in science the goal is the creation of a model of a mechanism that accomplishes an existing function. The implication of this and the previous conclusion is that computational models of the two domains operate with similar search and recognition strategies but act on different problem representations, thus allowing for fortuitous cross-fertilization of the algorithms.

Many ideas, methods, and findings from the field of scientific discovery have implications for or are involved in design, design automation, and design education, and vice versa. The similarities between the processes underlying these two superficially different areas of human (and more recently, machine) endeavor may exist for a very simple reason. They are both the product of human minds' trying to solve challenging and complex problems: The problem of discovering the nature of the world we inhabit and the problem of designing processes and artifacts that "improve" that

world and, when operating correctly, make it even more inhabitable. Faraday was both a scientist and an inventor, and our conclusion is that what Faraday really was was a brilliant problem solver.

REFERENCES

- Adelson, B. (1989). "Cognitive research: uncovering how designers design; cognitive modelling: explaining and predicting how designers design," *Research in Engineering Design*, **1**(1):35-42.
- Adelson, B., Gentner, D., Thagard, P., Holyoak, K., Burstein M., and Hammond, K. (1988). "The role of analogy in a theory of problem-solving." In *Proceedings of the Eleventh Annual Meeting of the Cognitive Science Society*, Erlbaum.
- Anderson, J. R. (1983). *The Architecture of Cognition*, Harvard University Press, Cambridge.
- Cagan, J. and Kotovsky, K. (1997). "Simulated annealing and the generation of the objective function: a model of learning during problem solving," *Computational Intelligence*, **13**(4):534-581.
- Campbell, M. (2000). "The A-Design invention machine: a means of automating and investigating conceptual design," Ph.D. Dissertation, Carnegie Mellon University, Pittsburgh, PA.
- Campbell, M., Cagan, J., and Kotovsky, K. (1999). "A-Design: an agent-based approach to conceptual design in a dynamic environment," *Research in Engineering Design*, **11**: 172-192.
- Campbell, M., Cagan, J., and Kotovsky, K. (2000). "Agent-based synthesis of electromechanical design configurations," *ASME Journal of Mechanical Design*, **122**(1): 61-69.
- Culick, F. E. C., and Jex, H. R. (1987). "Aerodynamics, stability, and control of the 1903 Wright Flyer." In *The Wright Flyer, An Engineering Perspective*, H. S. Wolko (ed.), Smithsonian Institution, Press, Washington, DC.
- Dunbar, K. (1993). "Concept discovery in a scientific domain," *Cognitive Science*, **17**:397-434.
- Falkenhainer, B., Forbus, K., and Gentner, D. (1989). "The structure-mapping engine: algorithm and examples," *Artificial Intelligence*, **41**:1-63.
- Finke, R. A., Ward, T. B., and Smith, S. M. (1992). *Creative Cognition*. MIT Press, Cambridge, MA.
- Forbus, K. D. (1988). "Qualitative physics: past, present, and future." In *Exploring Artificial Intelligence*, H. Shrobe (ed.), Morgan Kaufmann, San Mateo, CA, pp. 239-296.
- Forbus, K. D., Gentner, D., and Law, K. (1994). "Mac/Fac: a model of similarity-based retrieval," *Cognitive Science*, **19**:141-205.
- Gentner, D. (1983). "Structure mapping: a theoretical framework for analogy," *Cognitive Science*, **7**:155-170.
- Giere, R. N. (1988). *Explaining Science: A Cognitive Approach*. University of Chicago Press, Chicago.
- Grasshoff, G. and May, M. (1995). "Methodische analyse wissenschaftlichen entdeckens," *Kognitionswissenschaft*, **5**:51-67.
- Hayes J. R. and Simon, H. A. (1977). "Psychological differences among problem isomorphs." In *Cognitive Theory*, W. J. Castellan, N. B. Pisoni, and G. R. Potts (eds.), Erlbaum, Englewood Cliffs, N. J., Vol. 2, pp. 21-41.
- Holland, J. H., Holyoak, K. J., Nisbett, R. E., and Thagard, P. R. (1986). *Induction: Processes of Inference, Learning, and Discovery*. MIT Press, Cambridge, MA.
- Holmes, F. L. (1991). *Hans Krebs: The formation of a scientific life, 1900-1933*. Oxford University Press, New York.
- Jakab, P. L. (1990). *Visions of a Flying Machine, The Wright Brothers and the Process of Invention*. Smithsonian Institution Press, Washington, DC.
- Klahr, D. and Dunbar, K. (1988). "Dual space search during scientific reasoning," *Cognitive Science*, **12**:1-55.
- Kotovsky, K., Hayes, J. R., and Simon, H. A. (1985). "Why are some problems hard: evidence from Tower of Hanoi," *Cognitive Psychology*, **17**:248-294.

- Kotovskiy, K. and Simon, H. A. (1990). "What makes some problems really hard: explorations in the problem space of difficulty," *Cognitive Psychology*, **22**:143–183. Reprinted in Simon, H.A. (1989). *Models of Thought, Volume Two*. Yale University Press, New Haven, CT.
- Kulkarni, D. and Simon, H. A. (1990). "Experimentation in machine discovery." In *Computational Models of Scientific Discovery and Theory Formation*, J. Shrager and P. Langley (eds.), Morgan Kaufmann, San Mateo, CA.
- Laird, J. E., Newell, A., and Rosenbloom, P. S. (1987). "Soar: an architecture for general intelligence," *Artificial Intelligence*, **33**:1–64.
- Langley, P., Simon, H. A., Bradshaw, G. L., and Zytkow, J. M. (1987). *Scientific Discovery*, MIT Press, Cambridge, MA.
- Lippincott, H. H. (1987). "Propulsion systems of the Wright Brothers." In *The Wright Flyer, An Engineering Perspective*, H. S. Wolko (ed.), Smithsonian Institution Press, Washington, DC.
- Newell, A. and Simon, H. A. (1972). *Human Problem Solving*. Prentice-Hall, Englewood Cliffs, NJ.
- Nickles, T., Ed. (1978). *Scientific Discovery, Logic and Rationality*. Reidel, Boston, MA.
- Pahl, G. and Beitz, W. (1988). *Engineering Design – A Systematic Approach*, Springer-Verlag, New York.
- Paynter, H. M. (1961). *Analysis and Design of Engineering Systems*. MIT Press, Cambridge, MA.
- Popper, K. R. (1959). *The Logic of Scientific Discovery*. Kitchin, London.
- Schmidt, L. C. and Cagan, J. (1995). "Recursive annealing: a computational model for machine design," *Research in Engineering Design*, **7**:102–125.
- Schmidt, L. C. and Cagan, J. (1998). "Optimal configuration design: an integrated approach using grammars," *Journal of Mechanical Design*, **120**:2–9.
- Shea, K. and Cagan, J. (1997). "Innovative dome design: applying geodesic patterns with shape annealing," *Artificial Intelligence in Engineering Design, Analysis, and Manufacturing*, **11**:379–394.
- Shea, K. and Cagan, J. (1999). "The design of novel roof trusses with shape annealing: assessing the ability of a computational method in aiding structural designers with varying design intent," *Design Studies*, **20**:3–23.
- Shen, W. M. (1993). "Discovery as autonomous learning from the environment," *Machine Learning*, **12**:143–165.
- Shrager, J. and Langley, P., Eds. (1990). *Computational Models of Scientific Discovery and Theory Formation*. Morgan Kaufmann, San Mateo, CA.
- Simon, H. A. (1993). "A very early expert system," *Annals of the History of Computing*, **15**(3):63–68.
- Simon, H. A. and Kotovsky, K. (1963). "Human acquisition of concepts for sequential patterns," *Psychological Review*, **70**:534–546; reprinted in Simon, H. A. (1979). *Models of Thought*. Yale University Press, New Haven.
- Ullman, D. G., Dietterich, T. G., and Stauffer, L. A. (1988). "A model of the mechanical design process based on empirical data," *Artificial Intelligence in Engineering Design, Analysis, and Manufacturing*, **2**(1):33–52.
- Ulrich, K. and Seering, W. (1989). "Synthesis of schematic descriptions in mechanical design," *Research in Engineering Design*, **1**:3–18.
- Valdes-Perez, R. E. (1995). "Some recent human/computer discoveries in science and what accounts for them," *Artificial Intelligence*, **16**(3):37–44.
- Voland, G. (1999). *Engineering by Design*. Addison-Wesley, Reading, MA.
- Weisberg, R. W. (1993). *Creativity: Beyond the Myth of Genius*. Freeman, New York.
- Welch, R. V. and Dixon, J. (1994). "Guiding conceptual design through behavioral reasoning," *Research in Engineering Design*, **6**:169–188.
- Wolko, H. S., Ed. (1987). *The Wright Flyer, An Engineering Perspective*. Smithsonian Institution Press, Washington, DC.

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