

Molecules and Thoughts

Pattern Complexity and Evolution in Chemical Systems and the Mind

Yuri Tarnopolsky

January, 2003

SUMMARY

Pattern Theory is representation of complexity in terms of atom-like blocks and bonds between them, similar to chemical structures. The paper attempts to look at chemistry from pattern perspective, “patternize” some general ideas of chemical kinetics, and import them into the pattern representation of the mind. In particular, it is intended to complement the recent *Patterns of Thought* by Ulf Grenander [1], which is the main frame of reference for this paper. The chemical concepts in question are: chemical complexity, transition state, catalysis, non-equilibrium systems, competition and selection of chemical species, and molecular evolution. Distinction is made between Ar-complexity (Aristotelian), which displays in the fixed generator space, and He-complexity (Heraclitean), which displays in the expanding generator space. The mind is regarded as an expanding configuration space, with the topology of a subset of the scale of sets (Bourbaki), where configurations compete for presence in consciousness. The concept is illustrated with computer simulations of building a He-system and spontaneous activity on some connectors.

Abbreviations:

LMS: Life, Mind, Society; **AI:** Artificial Intelligence; **NI:** Natural Intelligence; **Alife:** Artificial Life; **PT:** Pattern Theory; **Ar-System:** A system in a fixed generator space (Aristotelian); **He-System:** A system in a changing generator space (Heraclitean).

CONTENTS

Introduction	3	9. Competition and selection of	
1. Chemical complexity	7	configurations	57
2. Molecular patterns	14	10. The competitive mind	67
3. Regularity and probability		10.1. BIRDS	70
in chemistry	20	10.2. PROTO	76
4. Thoughts and molecules	27	10.3. Discussion	86
5. Stability in LMS	31	11. SCALE	89
6. Patterns of transformation.	36	Conclusion	99
7. Chemical kinetics and		References	104
transition state	39		
8. Catalysis	50		

Introduction

A lecturer tells some students to learn the phone-book by heart.

The mathematicians are baffled: `By heart? You kidding?'

The physics-students ask: `Why?'

The engineers sigh: `Do we have to?'

The chemistry-students ask: `Till next Monday?'

source: <http://www.talisman.org/~erlkonig/humour/science-jokes>

Pattern Theory (PT) is a mathematical representation of objects with large and incompressible complexity [2, 3, 4]. Some of complex objects are static, as for example, telephone directory, others are natural and artificial dynamical systems, among them, life, mind, and society, for which the abbreviation LMS will be further used without distinction between natural and artificial.

There is an obvious conceptual isomorphism between PT and chemistry. Both share the same principles of atomism, bonding, and transformation. Molecules, forms of life, thoughts, and social structures are typical and frequent illustrations of pattern analysis and synthesis in Ulf Grenander's works on Pattern Theory [2, 3, 4]. The parallel with chemistry is widely used in [1], for example:

Note the resemblance to chemistry: generators correspond to atoms, configurations (ideas) to molecules, and bonds to bonds ([1], 2.4: *Regularity of Mind States: Conformation of Ideas*).

A chemist can easily recognize in PT a kind of meta-chemistry. Molecules look and behave like configurations and they are configurations in the eye of a chemist at least superficially familiar with PT.

The similarity between the mind in *Patterns of Thoughts* [1] and a chemical system is especially conspicuous because of dynamic aspects. To an imaginative chemist, Ulf Grenander's representation of the mind may look like a Faustian apparatus, where the content is brewing in a blend of order and spontaneity, out of which Golem, instead of Homunculus, is about to jump out. To decide whether the parallel with chemistry is just a metaphor, we need to look at chemistry from the point of view of pattern meta-chemistry.

The science of chemistry is about 150 years old, but only during the last 70 years, which is comparable with the 50 years of Artificial Intelligence (AI), chemistry has developed a series of concepts, approaches, and subjects that give it the modern shape. A set of abstract ideas of chemical origin, known as Artificial Life [5], a mathematical discipline of significant generality, is among the developments of the last few decades.

Thinking about why Roomba [6], the recent "intelligent sweeper vac", the descendant of turtle CORA (Conditioned Reflex Analog) built by W. Grey Walter [7] in Great Britain in the 40's, still has a too limited intelligence for such a simple job as sweeping a floor, one may suggest that a little bit of life, however artificial, would not harm intelligence.

In this preliminary paper, written from the meta-chemical (i.e., pattern) perspective, the relevance of Artificial Life (Alife) for AI and NI is in the focus of attention. Some possible applications of generalized and hybridized pattern-chemical ideas to social sciences are also briefly considered.

While it may appear questionable what kind of input AI can have from chemistry, Ising model is an excellent example of importing a general idea from "hard science" to AI.

Ernst Ising, following ideas of Wilhelm Lenz, worked in the narrow area of ferromagnetism. Thinking on the reasons why his idea has spread over such vast areas, including

AI and Alife, a chemist could note that the model came from the area of condensed matter, i.e., structured systems, far removed from the traditional chaotic gas-like ensembles of independent particles. Condensed matter is an elementary “natural” case of probabilities on structures where interaction is defined on a meaningful topology. Ising’s initial object, a linear spin model, was, actually, a stochastic cellular automaton long before the birth of this term.

Life, mind, and society (LMS), apparently, belong to the same large class of condensed systems as ferromagnetics: the statistical ensemble is constrained by a structure, and this is what Pattern Theory is about. A cardinal difference between the condensed matter of physics and that of LMS is the non-equilibrium thermodynamics of the latter, combined with a quasi-solid medium for information storage (Erwin Schrödinger: “life is aperiodic crystal”). Besides, the variety of connectors in chemistry and LMS is exceptionally wide. From this point of view, some new areas of chemical experience, natural and artificial life in particular, can present a case for importing them, in a generalized pattern form, into pattern theory. As a sample of this import, genetic algorithms in pattern recognition can be mentioned [8]. The current trend is to map dynamical systems of AI and Alife onto the area of science of complexity as foundation.

Modern chemistry consists of a large number of separate fields and means different things for different people. In this paper, chemistry is meant to deal with molecular structure, addressing the following three problems:

- 1. Analysis:** Reconstruct an unknown configuration from a set of its transformations into known configurations.
- 2. Synthesis:** Given the initial and final configurations, design the shortest sequence of transformations from one to the other.
- 3. Reactivity:** Given an initial configuration C_1 at time t_1 , predict the most probable configuration C_2 at time t_2 .

Organic chemistry is in charge of all three problems, as well as of configurations of highest known complexity. It looks like a kind of a theater where some chapters of PT are played live.

The following Table lists parallels between chemistry and PT. In pattern symbolism, the concepts of transition state, catalysis, replication, and competitive selection would not be tied to

any specifically chemical substrate. It is an intent of this paper to fill, in a very general form, the empty blanks in the right column.

Table: Comparison of chemistry and PT

	Chemistry	Pattern Theory
1	Atoms	Generators
2	Bonds	Bond couples
3	Molecules	Configurations
4	Types and classes	Patterns
5	Reaction	Transformation
6	Concentration	Probability of configuration
7	Energy $E \sim \sum_i E_i$	Energy $E \sim \sum_i \log P_i$
8	Transition state	
9	Catalysis	
10	Replication	
11	Molecular Evolution	

It is important to forewarn that the description of chemistry in this paper, addressed to non-chemists, is very simplistic. Although this paper is a work of a chemist with life long interests in AI and NI, for whom comparison of molecules with thoughts has been quite natural, author's knowledge of mathematics, AI, and A-life is superficial and fragmentary. The paper is an invitation to a more professional bridge-building from the other bank.

1. Chemical complexity

Judging by the volume of publications, chemistry is the largest separate body of scientific knowledge. The combinatorial complexity of molecules is enormous. Chemistry studies transformations of configurations of unlimited size on the set of about one hundred basic generators of the Periodic Table. The most common generators have arity from 1 to 4. There is a cornucopia of connector graphs, among them cycles and bridged cycles that play the role of stable atom-like subconfigurations. There are also an infinite variety of text-like linear sequences.

The *Chemical Abstracts Registry* (CAS Registry) counts practically each known substance and chemical transformation. Their numbers are constantly growing. Figure 1.1 presents a typical report, constantly updated at [9]. On January 2, 2003, there were 20,809,353 organic and inorganic substances, 24,206,720 sequences, and 6,559,626 single- and multi-step reactions.

Each substance or transformation can be described in numerous publications and some of them are subjects of thousands of papers. The number of recorded chemical species, however, is but a small subspace of the entire chemical configuration space.

For comparison, all human thoughts, in the form of sequences of symbols, form yet uncounted but, probably, an equally staggering sequence space. Some mental configurations, for example, Ising model and Shakespeare's *Hamlet*, are subjects of countless publications in sciences and humanities respectively.

Chemical information is as incompressible and devoid of generality as a telephone directory. In addition, chemistry has a limitless craving for intimate details. Chemistry consists mostly of painstakingly described facts observed at certain conditions. The facts belong to two types: unitary structures and binary transformations. A novice in chemistry is often overwhelmed by the apparent absence of any rigorous theory of a mathematical nature, but this can be stated about works of Shakespeare, too.

**CAS is the leading provider of organic, inorganic,
and biosequence substance information.**

The Latest CAS Registry Number® and Substance Count

Date	Mon Mar 4 10:08:41 EST 2002
Count	19,417,310 organic and inorganic substances
	17,601,341 sequences
Total	37,018,651 chemical substance registrations
CAS RN	397841-96-2 is the most recent CAS Registry Number

Figure 1.1 Example of the CAS Registry count

Chemistry provides a good illustration to the distinction between configuration and image in PT, see [2], p. 52 and [3], p. 91. Chemical configuration is an abstraction. Its images are *conformations* with similarity transformation: **rotation around single bond**, Figure 1.2 A, wherever this rotation is possible. Chemists usually ignore conformations, unless they are relatively stable, and in biochemistry they often are.

Conformations, in turn, are abstractions, too. The images of a conformation have similarity transformation: **stretching and/or bending** (changing the distance and angle between bonds), Figures 1.2 C and B. The deformations are observable in molecular spectra. Mostly, but not exclusively, protein folding is a process of going through a sequence of conformations, complicated by various interactions.

At the level of configuration, chemistry can be as much reduced to statistical averages as *Hamlet* to the statistics of its word usage. This circumstance is often another source of distress for a student of chemistry with an analytical frame of mind, but a source of delight for dedicated chemists with a more romantic attitude to the world where it is individuality that matters.

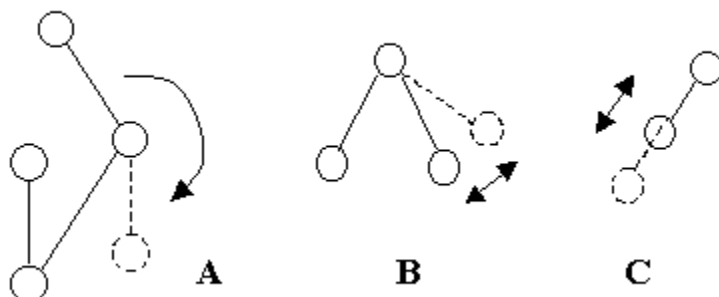


Figure 1.2 Bond deformations: A: Rotation, B: bending, C: stretching.

The type of combinatorial complexity that chemistry displays deserves a closer look.

There are two different ways toward a combinatorial explosion. The obvious way is expanding the base set. Another way was pointed to by Bourbaki in *Theory of Sets* [10, p. 259] and called *the scale of sets*.

In the following excerpt, \mathcal{P} , substituted for the original Gothic letter \mathbf{P} , denotes a set of subsets.

1. Given, for example, three *distinct* sets E, F, G, we may form other sets from them by taking their sets of subsets, or by forming the product of one of them by itself, or again by forming the product of two of them taken in a certain order. In this way we obtain *twelve* new sets. If we add these to the three original sets E, F, G, we may repeat the same operations on these fifteen sets, omitting those which give us sets already obtained; and so on. In general, any one of the sets obtained by this procedure (according to an explicit scheme) is said to belong to the *scale of sets on E, F, G as base*.

For example, let M, N, P be three sets of this scale, and let $R \{x, y, z\}$ be a relation between generic elements x, y, z of M, N, P , respectively. Then R defines a subset of $M \times N \times P$, hence (via a canonical correspondence) a subset of $(M \times N) \times P$, i.e., an element of $\mathcal{P}((M \times N) \times P)$.

Thus to give a *relation* between elements of several sets in the same scale is the same as to give an *element* of another set in the scale. Likewise, to give a mapping of M into N , for example, amounts (by considering the graph of this mapping) to giving a subset of $M \times N$, i.e., an element of $\mathcal{P}(M \times N)$, which is again a set in the scale. Finally, to give two elements (for example) of M amounts to giving a single element in the product set $M \times M$.

Thus being given a certain number of elements of sets in a scale, relations between generic elements of these sets, and mappings of subsets of certain of these sets into others, all comes down in the final analysis to being given a *single element* of one of the sets in the scale, [10], p. 259.

Here the combinatorial base set is constantly expanding because each new combination enters the set as a new element. Therefore, the number of initial elements can be quite small, as the following sequence, built of two symbols, but potentially infinite, illustrates:

$$\{(AB) (AB) [(AB) (AB)](BA)\} \{(AB) (AB) [(AB) (BA)](BA)\} \dots$$

The treatise by Bourbaki starts with describing mathematics as combinations (called *assemblies*) of *letters* and *signs* and fits prophetically well the structure of both chemical space and space of ideas. The letters correspond to generators and signs, including brackets, to bonds. Thus, not only mathematical formulas, but also sentences like “every finite division is a field” [10, p. 1] are listed as assemblies.

From the point of view of a chemist, the static chemical structures are no less *assemblies* than formulas and phrases because linearity of connector is not among Bourbaki's conditions and any connector graph is a *sign*.

It is a chemist's impression that both chemistry and PT go further by introducing measures on "assemblies" space, which leads to a thermodynamics of a kind.

The difference between the two ways of complexification, which could be referred to as conservative and progressive, is that in the conservative combinatorial space the elements do not have copies, while in the progressive one the elements have multiple entries into the combinations, which is the case with chemistry and ideas. New clusters of ideas get a new name or a new meaning of the old name and thus expand the base set recorded in dictionaries. This process is examined in detail in *Patterns of Thoughts* ([1], 3.3), where generalization creates macrogenerators and encapsulation adds a new idea to the envelope of the mind:

ENCAPSULATION : $idea \rightarrow env (MIND)$

Note, that specialization can create new generators, too, when a new species of a taxonomic unit is discovered.

The process of generation of new ideas leads to progressive combinatorial explosion, unless there is a counteracting factor, which will be considered later. Without dissipating or depleting the envelope, combinatorial explosion might take over and paralyze the mind, with zero probability of retrieving any idea into content, which happens with Web sites during a massive "denial of service" attack, sometimes, spontaneously. While conservative combinatorial space is fully defined by the base set and the combinatorial operation, the progressive space must be generated in the process of evolution consisting of a series of choices. This is just a way to say that a progressive space has a *history*.

Whether we consider chemistry or AI, knowledge at any given moment has nothing to do with the history of the area. Nevertheless, the work of the collective mind has a historical dimension reflected in CAS registry, citation indexes, and in plain references to previous works that allow for reconstruction of history. In social structures, as well as in any individual human mind, however, history can have an enormous bearing on both popular mindset and individual character with its prejudices and motivations, Freud or no Freud.

The chemical configuration space is oppressively cumulative: each new structure remains on record. Against all odds, however, modern chemistry can successfully navigate its own real, not virtual, complexity with a modest number of tools of high power. This is why chemical experience might be relevant for handling other natural systems of towering complexity.

Whether it is fortunate or not that we still do not have the same power of simplification in LMS, is a matter of personal philosophy.

Since terms *conservative* and *progressive* are overloaded with connotations, to distinguish between two kinds of combinatorial complexity, terms Ar-complexity (Aristotelian) and He-complexity (Heraclitean) are suggested. The first one is defined by the fixed base set or, in terms of PT, fixed generator space, while the second one builds up as a mapping onto the scale of sets. In terms of PT, it would sound as expanding generator space.

It has always been among major scientific goals to work on well-defined structures, which is, probably, the main reason for the rift between sciences and humanities. He-complexity could be a way to mathematically accommodate history of individual life, biological species, ideas, and nations by reflecting the distinction between old and new.

According to Bourbaki's terminology, any scale of sets built according to explicit instructions, *belongs* to the scale of sets on a particular basis. Taking some liberties, we will use term *scale of sets* for this kind of a partial scale, too.

Chemistry serves as an example of He-complexity because almost every chemical structure can be combined with another and given a new name and a new CAS number, which would allow for tracing the evolution of chemical space. A similar kind of complexity can be found in the development of algorithms by combining subroutines into new standard blocks. Any block is always *younger* than its constituents and thus the evolutionary axis is established without the physically explicit variable of time.

Remarkably, Pattern Theory in its current state does not need any modification to accommodate both Ar- and He-systems. It is inherently fit to describe patterns of history, to which physical sciences have been traditionally blind.

A different example is the scientific citation space, where a point refers down to previous points and is referred down to in subsequent citations, which is similar to the *levels* along Ulf Grenander [1]. Notably, the citation space, is not a hierarchy in the sense any taxonomic space is: all citations are equal and refer to real works. The citation network is partially ordered and it establishes a direction of natural historical time.

One may wonder whether the gigantic molecules of DNA are also organized as the scale of sets, coding the phylogenesis of the species as well as the basics of ontogenesis.

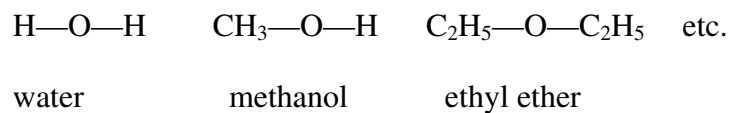
We return to this idea later because it seems to be of utmost importance for the structure of working mind.

2. Molecular patterns

It may look on the surface that chemistry lacks an explicit concept of pattern. Nevertheless, the concept of pattern is deeply ingrained into chemical thinking and is one of the most efficient ways to manage the unbearable burden of chemical complexity.

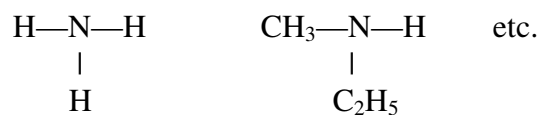
The initial ideas of chemistry about structure had a lot of pattern spirit. According to *theory of types* of Auguste Laurent (1807-1853), molecules were supposed to fall into certain structural patterns, called *types*, for example, of water and ammonia.

The type of water is $A-O-B$, where O is oxygen and A and B can be any combinations of atoms, among them:



Here the similarity transformation is substitution of other atomic subconfigurations for H in water. In this sense, chemical patterns are simply taxonomic units of classification of molecules and their transformations. Certain chemical subconfigurations (called *functional groups*) usually display a common behavior and are only partially influenced by their structural environment.

The type of ammonia $\begin{array}{c} \text{A—N—B} \\ | \\ \text{C} \end{array}$ comprises amines:



Theory of types gave a strong impetus to chemical theory and already by 1865 the modern concept of chemical connector, in PT terms, was ready to hatch.

Up to present, the basic organic chemistry has been taught to students by types of structure: alcohols, amines, sugars, proteins, etc. The starting chapters are typically entitled as:

Alkanes and Cycloalkanes

Alkenes

Alkynes

Alcohols, Diols, and Ethers

etc., i.e., by patterns of chemical structure, without too much overlapping .

Looking at a big and complex chemical formula, a novice in chemistry is immediately lost, while a more experienced chemist perceives them in terms of known types of subconfigurations. Later, some connector graphs were added to the intuitively defined types, such as the alternating single and double bonds



as well as more complicated ones.

For example, trying to understand formulas in Figure 2.1, a chemist first suspects the pattern of steroids in the connector and then looks at the neighborhoods of atoms.

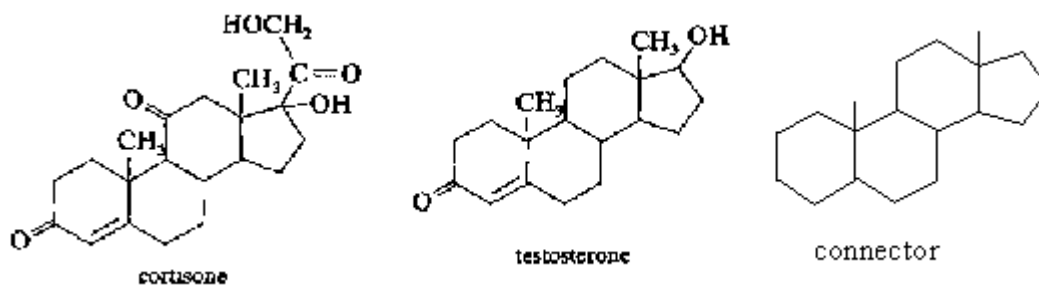


Figure 2.1 Steroids and their connector

Similarly, the connector of porphin defines a pattern to which such important substances as heme and chlorophyll belong, Figure 2.2.

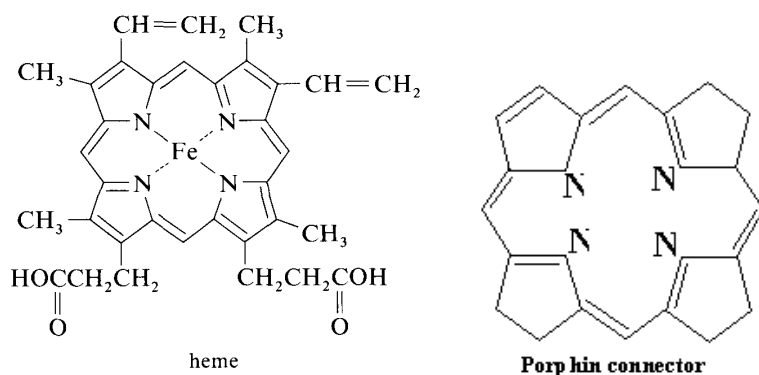


Figure 2.2 Heme and its porphin connector

The chemist perceives an unfamiliar structure in terms of standard superatomic blocks and their connectors. Similarly, the formula of an unknown substance is reconstructed block by block, according to their patterns of behavior and topology. Two blocks are, possibly, neighbors if they belong to a larger block and can be found in the products of its decomposition.

Most practically important molecules belong to several patterns at the same time. Taking to account the interaction between different groups within the same molecule, the concept of pattern in chemistry, clearly visible from a distance, is significantly blurred at a close range. No doubt, however, that a student of chemistry learns to perceive the immense complexity of the molecular world in terms of patterns that look like mathematical formulas where symbols stand for types of structure and transformation. Not accidentally, various shortcuts for large blocs are popular. Thus, R in R—O—H can stand for 61 atoms ($C_{20}H_{41}$) with a very intricate connector.

In the chemical formula of aspirin, Figure 2.3, we find at least three stable subconfigurations from countless other structures: *ortho*-substituted benzene nucleus (*ortho* means side-by-side), carboxyl, and acetoxy-group. Aspirin, therefore, displays at least four patterns:

1. Aromatic compounds, i.e., derivatives of benzene;
2. carboxylic acids;
3. esters;
4. *ortho*-substituted aromatic compounds, i.e., derivatives of benzene with two substituents side by side.

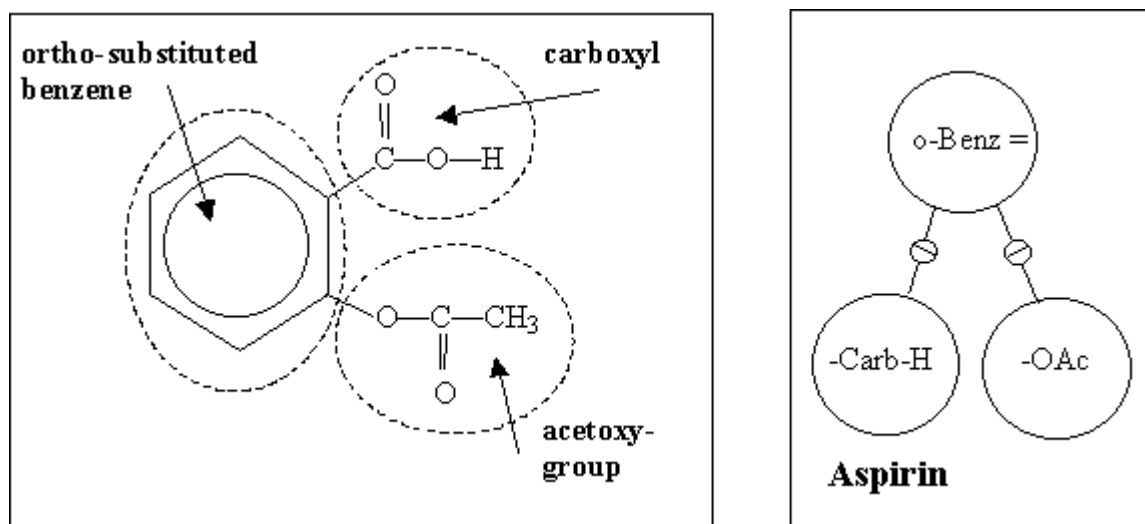


Figure 2.3 Overlapping patterns of aspirin

Any molecular structure can be converted, by standardized international rules, into a string of letters from which the structure can be drawn. Thus, aspirin is 2-(acetyloxy)-benzoic acid, which would look differently in Russian, but have the same meaning. This correspondence resembles, in inverse order, the relation between the text of *Hamlet* and its stage production.

Information contained in a chemical formula can be coded by a matrix of bonding, as the example of formaldehyde in Figure 2.4 shows. Aspirin, $C_9H_8O_4$, requires a 21x21 matrix. Matrices for all large molecules are sparse.

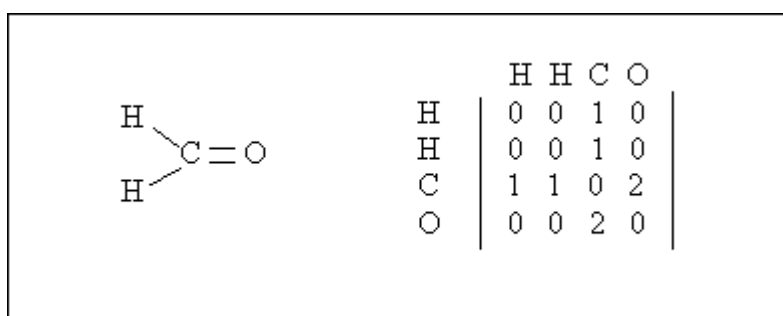


Figure 2.4 Two representations of the structure of formaldehyde

In dynamic representations of configurations, the connectivity matrix can contain probabilities or affinities instead of just Boolean incidence. Moreover, a multidimensional array can comprise all essential aspects of the configuration, including its history, if the configuration is a scale of sets. Thus, the diagonal can store the data for generators and other elements can specify types of bonds: single, double, etc. This method is actually used in computer coding of chemicals.

Chemistry as a testing ground for pattern ideas is interesting also from another angle: perception and understanding of images.

The chemist deals with very complex and large chemical formulas that must be understood. The process of understanding of a chemical formula consists of compiling (partly, subconsciously) a list of all its patterns, as in Figure 2.3. The verbal description and writing the exact chemical name of the substance is the final proof of understanding because **it can be**

shared with another chemist, in accordance with the old saying that the best way to understand something is to explain it to somebody else.

Similarly, the understanding of a picture consists of listing the object in the picture in such a way that it can be shared with another person who cannot see the picture itself. For example: “I see two birch trees on a grassy foreground against the background of a conifer forest.” This renders not the picture but its pattern.

Human understanding, in a way, is a social phenomenon. As soon as the components of an image and their spatial relation are identified in such a form that can be shared, the image, whether a picture or a chemical formula, is understood. Unlike the natural objects that must be subjected to pattern analysis before they can be processed further, for example, in computer vision and recognition, chemical formulas are “turnkey ready” because they are already naked patterns.

3. Regularity and probability in chemistry

Chemistry is a very liberal science in the sense that it has few, if any, strict rules without exceptions. It constantly discovers something that was unthinkable before and is always on the prowl for monsters and chimeras.

To give an example, it had been an axiom that noble gases were unable to form compounds, until in the 1960's the axiom was shattered. This puts a teacher of chemistry on a shaky ground because whatever the students say may be true.

When the authors of this book were undergraduates we were taught that the noble gases did not form chemical compounds. Then several noble gas compounds were discovered in the *early 1960s* [11].

This is why chemistry does not have much to say about regularity. It is part of the chemical credo, rarely expressed publicly, that anything we can imagine is possible. The hidden foundation of this belief is, probably, the isomorphism of thoughts and things in chemistry.

Chemical chimeras can be inspired by some very distant reality. For example, the chemical structures in Figure 3.1—two interlocked rings and a ring on a dumbbell—were synthesized just because of the challenge of the shape. They are, so to say, materialized ideas. By doing that, a chemist becomes an architect.

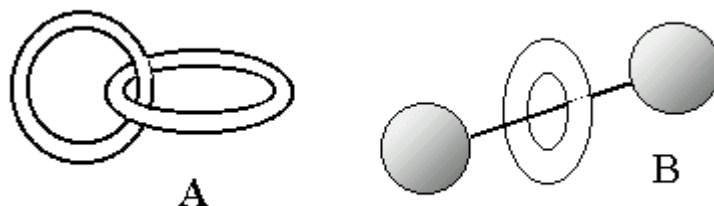


Figure 3.1 Topology of catenanes (A) and rotaxanes (B)

If atoms can combine and form various configurations in our imagination, they most probably can do it in a flask. This kind of philosophical idealism would not survive for long if it were not confirmed by experiment.

“Yes, everything thinkable is possible in fact, but how stable is it?” The chemist asks this kind of question in the situation where the mathematician would ask, “Yes, but how probable is it?” Here lies an apparent difference between PT and chemistry. Where the mathematician thinks in terms of **probability**, the chemist (and, probably, architect) thinks in terms of **stability**. There must be some serious reasons for that, and the main reason is that the configuration space in chemistry is a scale of sets, while a mathematician would probably prefer to deal with individual sets, however fuzzy. It does not mean that the chemist has an aversion to probabilities, but they are expressed as concentrations, i.e., probabilities to find a molecule of certain kind in a unit volume. The law of large numbers works over the entire “real world” chemistry, with the exception of special cases when a single molecule is the object of investigation, as in protein folding.

An important set of rules of regularity comes from quantum chemistry. Quantum-chemical regularity means preserving a certain arrangement of the external (valent) electrons

between atoms. A single line portrays the covalent chemical bond, typical for complex organic molecules. A double or triple line between two atoms (example: $\text{H}-\text{C}\equiv\text{C}-\text{H}$) does not mean two or three identical bonds: the second and third bonds are very much different from the first, and the chemist always keeps that in mind.

Without going into quantum-theoretical specifics, **chemical stability** requires the configuration to have certain regular neighborhoods of atoms. The regular neighborhoods have a certain number of outbonds at the central atom, each of them portrayed by a single bond corresponding to a pair of shared valent electrons. The sum of valencies is eight (octet rule), **for some of the most wide spread atoms**, two for hydrogen, and usually up to twelve for other atoms. It seems like a lack of regularity, but each particular case is explainable by quantum chemistry.

Figure 3.2 illustrates the use of octet rule.

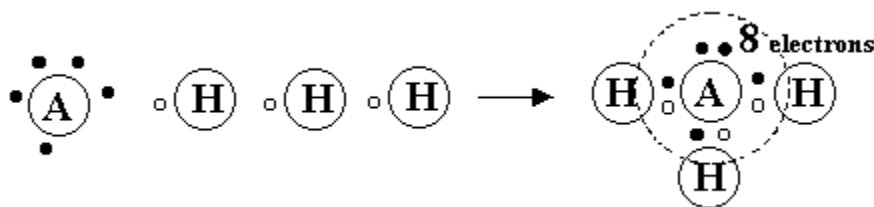


Figure 3.2 An illustration of octet rule

Atom **A** forms a stable compound AH_3 because the neighborhoods of **H** (hydrogen) have regular pairs of shared electrons, and the neighborhood of **A** has the regular eight shared electrons. The different fill of the little circles symbolizes different contributors to the shared pair. The structure is regular and, therefore, expected to be stable, which is always better to check experimentally.

However, even the octet rule is ridden with exceptions. Thus, there are simple molecules where the number of electrons at an atom is seven, as it is at atom **A** in Figure 3.2, where **B** means just another atom, not boron. Nitrogen dioxide, a brownish gas present in the engine exhaust, belongs to this type. The transition between the two forms, monomer and dimer, the latter being quite regular, happens to fall in the interval of temperatures commensurate with

human existence. At the room temperature, the monomer prevails, while at the temperature of melting ice, the dimer dominates, so that the brown color of the monomer disappears. Regularity in chemistry is relative: it is more or less defined for a certain temperature interval.

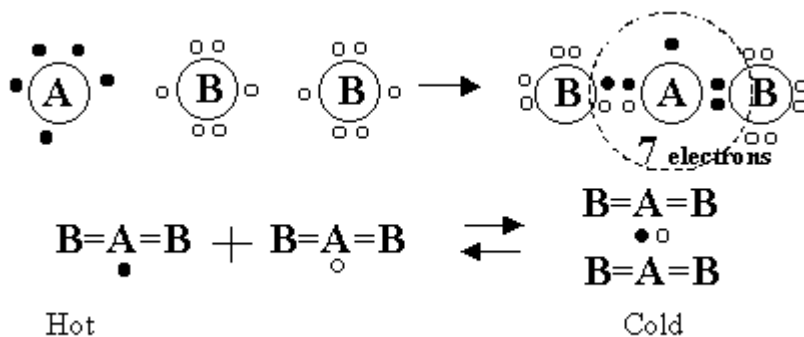


Figure 3.3 Example of a formally irregular but stable structure (B=A=B)

For most other chemical bonds, the interval of reversible dissociation and association is much higher, somewhere near the red heat. At any temperature, the two forms are in equilibrium:



Or, in a more typical for chemistry notation,



The position of the equilibrium between these two forms can be exactly calculated because equation (3.2) describes a canonical Gibbs ensemble with complete list of entries, leaving nothing to imagination. In chemical notation, concentration, i.e., **the probability to find** a molecule of a certain type in a volume of the mixture, is symbolized by square brackets and defined by:

$$\frac{[A_2B_4]^2}{[AB_2]} = K \quad ; \quad [A_2B_4] + [AB_2] = \text{const} \quad (3.3)$$

Since the total concentration of molecular species, $[A_2B_4] + [AB_2]$ is known, the concentrations of each species can be calculated.

Naturally the temperature dependence of equilibrium constant K is expressed by

$$RT \ln K = G_{A_2B_4} - G_{AB_2}, \quad (3.4)$$

where T is temperature, R is constant, and G stands for (no surprise!) Gibbs energy, which in chemistry is misleadingly called *free energy*, the term that will be avoided here. We shall return to it later.

Equation (3.1) is not the only possible transformation. For example, we can imagine a decomposition of two **BAB** into perfectly stable two **BB** and one **AA**. And in fact, this is what happens in the catalytic converter of an automobile where the poisonous nitrogen oxide NO_2 is decomposed into harmless nitrogen N_2 and oxygen O_2 . Moreover, the position of chemical equilibrium favors this decomposition! However, it practically never happens if the oxides are left at normal conditions.

If unexplained, the chemical liberalism could take a good bite off our faith in chemistry. Of course, a chemist can eliminate the spontaneous decomposition simply because it has never been observed at normal temperatures (it will definitely happen at high temperatures). But there must be some scientific reason for that if chemistry should not be taken for a kind of soot-saying.

Certain imaginary things happen in fact, since the times of Jules Verne, but others are impossible or need sophisticated tricks to make them real. It seems important to find the constraints of realism to be applied to such areas of thought as mathematical systems, statistical mechanics, and Gibbs ensembles, too beautiful for the challenges of real life.

The reasons for the irrational stability of NO_2 and the persuasive power of catalytic converters will be considered in Part 8.

Theoretically, any combination of atoms is possible, but most of them have such a high energy that they could not exist at normal conditions. The idea of regularity in chemistry, therefore, is tied to conditions. What is regular at one set of conditions becomes irregular at another. Irregularity appears only if we define regularity.

Thus, if we trust the Bible or the Koran to define a set of regular ideas, any other idea becomes irregular.

Chemical regularity, therefore, forms a continuum. Nevertheless, there is a common understanding of what is practically regular. **Regular is what is stable.** Regular molecules are, approximately, those that that can be kept in a jar, at least overnight. This probably can be said also about thoughts: a regular idea is the one that can survive in the mind, say, five minutes, all the more, overnight. Probably, scores of vague and irregular ideas fly through our mind every minute, some of them even beyond verbal expression, and most subconscious. Certainly, what is formulated in words has at least a look of regularity.

The chemists operate with energies instead of probabilities because energy is measurable while probability is not. Energy is linked in a chemist's mind with stability: low energy means stability and high energy means instability. Of course, as with everything in chemistry, the borderlines are diffuse.

The chemists do not use probability as a measure of stability, and for a good reason: the complete list of combinations of atoms has a complexity of the scale of sets. Chemical systems do not have a list of all configurations in the configuration space. There is no set of exhaustive and mutually exclusive alternatives or events. This is why chemists rarely use absolute energies, either, focusing instead on differences.

It looks like the chemists are intuitively Bayesian in their approach. The typical question is: we know for sure that the system is in the state **A**. What is the probability of the state **B** at the next observation, **on the condition that it really happens** and nothing else does? To ask such questions, we need to imagine **B** first. Suppose, there is **A** and derived from it **B**. How probable are both if there is nothing else? On such conditions, we arrive at the classical statistical mechanics that ignores what cannot be imagined.

For a chemist, the question what is going to happen the next moment is rhetoric, especially when dealing with evolving systems. The chemist must know the options beforehand. The “Bayesian” form of question, however, allows the chemist to operate not with absolute energies but with differences, i.e., ratios of probabilities, deliberately idealizing the system.

If regularity in chemistry is closely tied to stability, i.e., to energy, it is no different from the situation in any Gibbs ensemble, but **over time**, not over space. If we consider a disjoint chemical configuration in a single copy, the expected result is also a statistical ensemble over a long observation time, provided the system is isolated. Naturally, if the temperature goes up, the regularity will relax.

Chemical synthesis consists of mixing stable compounds, letting the reaction take its course under certain conditions, and, finally, isolating stable products.

To compare, thinking consists of acquiring reliable data, letting the process in the mind take its course, and, finally, formulating the results. In creative thinking, the timing of the process is hardly predictable, which is an oblique evidence that thinking deals with a single mental configuration.

This implies that a chemical transformation runs through a series of **intermediate irregular configurations** that do not last for too long. Otherwise, the result will always be the Gibbs equilibrium. It should be noted that some reactions come to equilibrium pretty fast, but so do competing undesirable reactions.

Unlike mathematics, chemistry not only refuses to deal with infinity but is also hardly ever interested in chemical reactions that take a long time, except in winemaking. The chemical system is dramatically different from a Gibbs ensemble, which is devoid of the time axis. Chemistry is as much controlled by kinetics as by thermodynamics.

A realistic model of the mind, therefore, must accommodate not only for an expanding configuration space, or, in terms of PT, an expanding envelope, but also for the kinetics that distinguishes between theoretically and practically possible events.

4. Thoughts and molecules

Can thoughts have a “chemistry” in more than metaphorical sense? The formal treatment of *assemblies* in set theory and configurations in PT brings the chemical formulas and ideas into the class of formal constructs. If so, **do thoughts about molecules behave like molecules?** This question invokes the spirit of Gödel: are the Gödel numbers of statements about numbers in fact statements? Coming back to the Bourbaki’s theory of structures, in which a mathematical theory contains rules that assign to assemblies the status of terms, signs, or theorems, while the rules themselves do not belong to the formal mathematics, we find that the above question can be answered positive at least as a hypothesis. To add more weight to the answer, we first need to know how the molecules really behave.

Although texts look like polymers of words, there is a notable difference between texts and molecules. The number of atoms is limited by the Periodic Table but the variety of ways they are connected is enormous. The number of linguistic terminal generators, i.e., words, is extremely large, but the variety of their connectors is practically exhausted by a grammar that is much thinner than a telephone book of a small city.

To name its countless objects of study, chemistry uses its own language with a very special relation between the sign and the signified. Regarded as configurations, **the sign is isomorphic to the signified**. In the terminology of linguistics, it is a pictograph, i.e., the most primitive method to code objects by their pictures and to paint a beer mug as the sign for a tavern.

All ancient symbols for small numbers were pictographs: the symbol contained as many elements as the number it symbolized, and it is still true about small numbers in Arabic and Chinese, and, of course, Roman numerals: I, II, III, V, and X. The three first initial Chinese numerals are the same as the Roman ones, only horizontal.

In most languages, a distinction exists between letters and words. The words are combinations of letters, but not separate letters. Chinese characters, used also in the Japanese language, in some aspects, level out the field for letters and words. Various characters, when combined, acquire a new meaning and become a new character, see Figure 4.1. If so, where does this end? Characteristically, in the Chinese and Japanese languages the space between either characters or words does not exist (there are some means of quasi-spacing in the Japanese language). There is no formal difference between characters and words.



Figure 4.1 Examples of compound Chinese characters. Components *great*, *light*, and *happiness* are themselves compound (source: <http://zhongwen.com/>).

The borderline between molecules and thoughts is blurred in the practical work of a chemist who manipulates atoms and molecules on paper, in mind, or with a computer. In the mind of a chemist, ideas about molecules behave like the molecules in the test tube.

When Hamlet contemplates his actions in sequences of about 30 symbols of English alphabet and syntax, there is no direct conformity between the text and the action, and not much even between the text and the speech. Symbol **S** for entropy in physics looks more like a lithe snake than a state of flaccid disarray. The Gödel number is a far cry of a statement it enumerates.

The situation is different in chemistry where the chemical formula is still a clear pictograph. If it is converted, according to some rules, into a line of text from which the original structure can be reconstructed, it is no more a pictograph. The chemists do not think in the chemical names of substances, unless for a quick communication. They discuss pictographs of molecules. Thus, the idea of water in the head of a chemist, not a layman, is isomorphic to the actual molecule of water. Thinking about water, a chemist imagines its three constituting atoms, bonds between them, and sometimes even the angular shape of the molecule (\wedge or \sphericalangle). The chemist is used to think in images of molecules and their transformations, letting them play according to the rules of the chemical game. To compare, a musician may think about music and remember it in finger and hand movements, in addition to sounds.

The chemist deals with ideas of atoms **as if they were** labels pasted on real atoms. In imagination, helped with a sheet of paper or a computer simulation, the chemist lets the atoms and groups dance, bounce, and recombine. The imaginary balls and connecting sticks collide and adjust to each other in the mind of the chemist before the stage of the actual experiment, as well as *post factum*. Sometimes the chemist does it without any guiding idea, but more often, draws from known patterns. Then, after testing the idea in an experiment, the virtual play is resumed, and so on, until a satisfactory result is achieved.

Similar strategies appear to dominate other areas of creativity: writing poetry, doing science, and inventing. Thus, a poet starts with some word, line, or just an idea and grows this seed into a polymer of words, marking up its stressed areas, awkward interference of words, and mutual repelling of lines, changing the sequence until the stress is minimized (or enforced), and doing that in imagination or on paper.

The great Russian poet Anna Akhmatova: "If only you knew from what dirt the poems shamelessly grow."

Search and fitting for the right rhyme could be as painstaking as shopping by a movie star. The entire creative process, whether in science or, at least, in *pre-postmodern* humanities, falls into the same category of processes as protein folding, during which a line of a polymer through twisting, bending, and writhing, takes the most stress-free shape. The poet, however, invents his or her own thermodynamics.

Moreover, a large stretch of history can belong to this kind of processes, too. For example, the history of France, since the French Revolution up to our days, manifests a remarkable series of twists, turns, and contortions, through which the nation has been “stochastically relaxing” the contrast between the personal authority and the will of the people, see Part 5, *Stability in LMS*, Figures 5.3 and 5.4.

In the pattern model of the mind along Ulf Grenander [1], generators of the mind combine and recombine according to their affinity, which is a function of the previous state, random component, and stable constraints of the system, such as partitions of the generator space. Designing an artificial mind, one can take a different direction from this point, but the pattern-theoretical platform, covering a whole range of structures in the sense of Bourbaki with imposed constraints, will remain the same.

Chemical experience, in a way, is materialized PT.

5. Stability in LMS

It may seem at this point that we have departed from any artificial or natural intelligence, but in fact this brings us to the historical beginnings of AI.

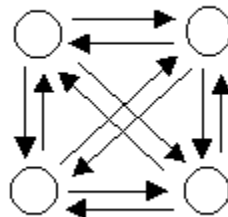


Fig. 5.1 Interactions in the homeostat

Concerning stability, it is appropriate to pay tribute to one of the almost forgotten ideas from the dawn of AI. In 1940, the homeostat of W. Ross Ashby (1903-1972) joined the class of systems consisting of particles interacting under constraints.

Ashby's *Design for a Brain* [12] and *An Introduction to Cybernetics* [13] are a fascinating reading. Ashby seems today, when the general ideas are buried under the sediment of narrow and technical papers, well ahead of his time because his model was, in essence, a

constrained by structure “condensed matter,” close to that of Ising, where topological neighbors influence each other. Figure 5.1 can be seen as an illustration to Ising model. Not only that, but the entire conceptual direction of Ashby presents, on the surface, an alternative to the celebrated Turing’s criterion of intelligence. Ashby’s refrain is **adaptation**. The criterion of intelligence, therefore, is adaptation to the intelligent environment.

Whether it is accidental that the adaptive AI was born in the native land of Darwin and not where Darwin has always been under siege—this is a good topic for a Turing test. An intelligent robot would start talking about the weather.

Extrapolating Ashby’s reasoning, since the environment, populated by humans and animals, from a pack of wolves to a scientific symposium, itself can possess intelligence at various degrees, the intelligence under consideration is measured, like physical temperature, as the intelligence of the environment with which the individual can stay in adaptive equilibrium at least for a day. According to the Turing test, the agent is either recognized as intelligent or not, while the Ashby test (not explicitly expressed by him) could give a measure of intelligence. We use this measure in everyday life. If we can match a person in a conversation, we have at least the same intelligence. The adaptive criterion echoes the Murphy’s law: everybody reaches his or her level of incompetence. As energy in chemistry, the IQ tests are nothing but the measure of the difference in intelligence of the test author and the object of testing.

Of course, an objection could follow that a buffalo has better chances of survival amidst a scientific symposium than facing a pack of wolves. The counterarguments are suggested as an exercise.

While the constraints in a spin glass are topological, the constraints in Ashby’s primitive system of four interacting “particles” are coming from the physical nature of the hardware, namely, from the mechanical inertia of its parts. Being disturbed, the homeostat, after a series of apparently random movements, comes to equilibrium. This system can be roughly compared

with four men (as the least reasonable gender) packed into a telephone booth: when one tries to turn, he disturbs the other three, until they all find the least uncomfortable new position. This kind of system has the topology of full graph, Figure 5.1, the same as for ideal gas where any particle can collide with any other. The connector, however, can be any. Ashby insisted that a large number of particles were needed for intelligence.

What is essential for us is the very type of behavior of Ashby's adaptive system. The homeostat reacts to a disturbance by entering a short **transitional** mode of intense movement and subsequent coming to a new equilibrium.

From the chemical point of view (which may be disputed by some chemists), reacting molecules in chemical environment behave as a homeostat. The action of a reagent knocks the molecule out of balance. A short-living transition state of the running reaction emerges that leads to a new equilibrium.

The mind, notwithstanding the inner mechanisms, behaves in the same way: a disturbance, whether external one or an inner fluctuation ("it struck me," "it just occurred to me") triggers a state of intense work and, therefore, an increased energy consumption until a new state of equilibrium, however temporary, is reached.

Evolution of society consists of periods of balance and stability interrupted by wars, revolutions, and drastic reforms. During the periods of unrest, the society is seeking ways to diminish the social stress, and if it is not achieved, the unrest can take a catastrophic form. A history of a nation consists of periods of relative calm interspaced with times of turbulence. The most spectacular example of the search for stability is history of France, Figures 5.3 and 5.4.

In social psychology, various *balance theories* emphasize the importance of an internal cognitive balance. If two opposite systems of belief violate the balance, the individual tends to adjust them in order to diminish the *cognitive dissonance* (Leon Festinger, [14]). A smoker trying to quit passes back and forth between smoking and non-smoking phases through a painful state of cognitive dissonance.

Ashby's ideas were more refined than it may seem: they included the concept of step function, which was close to the concept of mutation applied to behavior.

What is so unusual and pioneering about Ashby's model is its thermodynamics, which he noted only casually. It is an open system, maintained by an external source of electric current, without which it would come to a hold once and forever. The current brings into motion the cells and feeds the output. The system's behavior, Figure 5.2, consists of alternation of stable and unstable (i.e., probable and improbable) states.

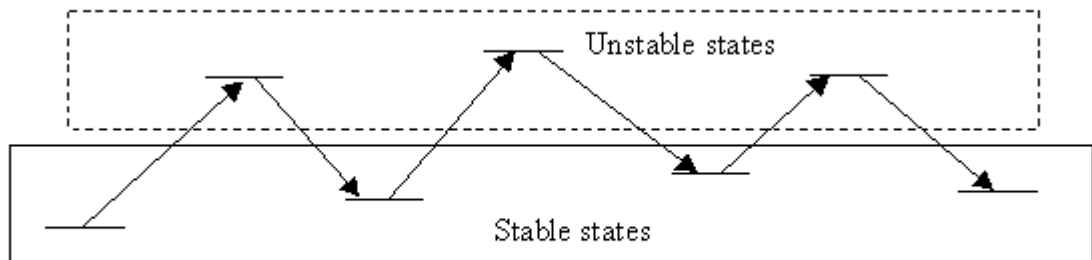


Figure 5.2 Alternation of stable and unstable states in Ashby's homeostat

LMS systems are usually characterized as adaptive. It means that they tend to achieve a state with an optimized parameter, let us call it stability, from which a spontaneous transition to another state is unlikely. If brought into a state far from optimum, they begin a search of a pathway toward stability. A war always ends with peace, but peace is punctuated with wars. The evolution of a stock market belongs to the same type of behavior.

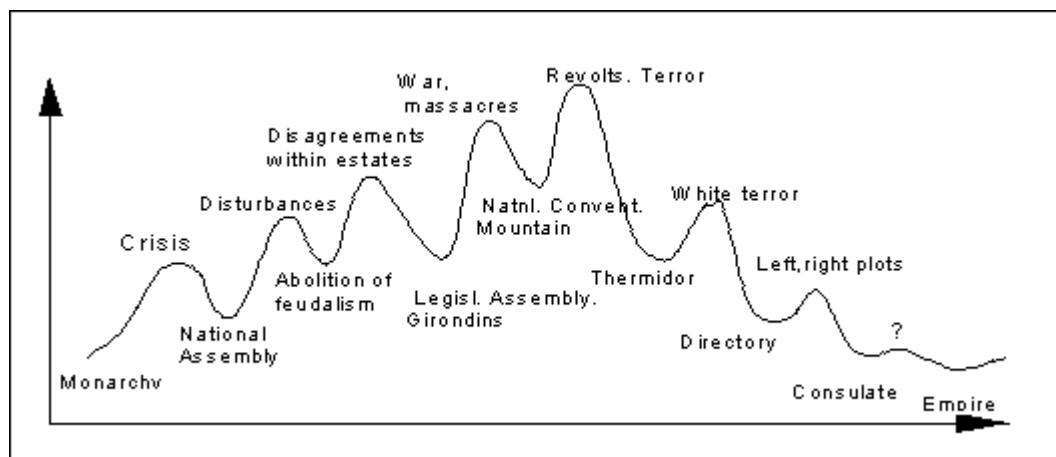


Figure 5.3 The energy profile of the French Revolution. Peaks mark instabilities.

For a physical system, the stable state is that of equilibrium and the measure of stability is energy. The stable state in an open system is not equilibrium but a steady state with a minimal production of entropy.

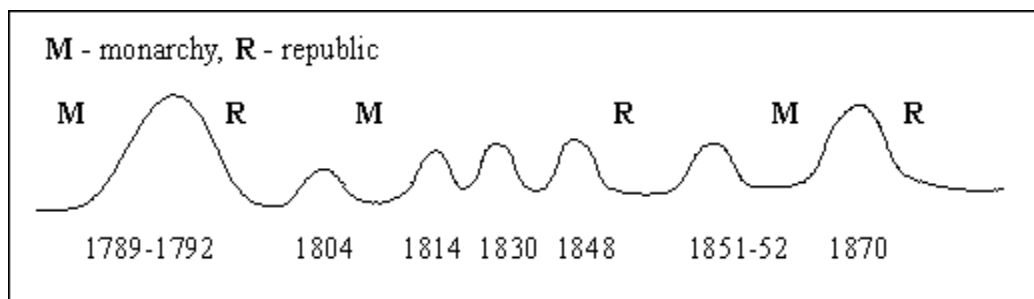


Figure 5.4 The historical roller coaster of France. Peaks mark instabilities.

A problem with open systems is that thermodynamics alone is not able to predict what kind of configuration will correspond to the stable state because thermodynamics has nothing to say about structure.. For example, the turbulent times of the 1960's changed American attitude toward war, but it is impossible to explain in which way by any general concept of homeostasis. Generally, we can expect a roller coaster after September 11, 2001, but of what kind? We need to enter the mind of the smoker as well as the mind of the nation and its enemies to **compare stabilities of different configurations.**

6. Patterns of Transformation.

Taxonomy of real-world chemical transformations is not different from the operations on configurations in *Patterns of Thought*. Chemical configurations are commonly disjoined because they correspond to mixtures of different substances.

The chemist starts with a set of configurations of all participating components and has to decide what is going to happen with it, if anything at all.

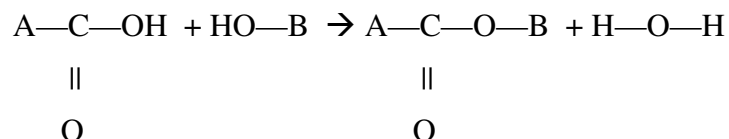
Patterns of chemical transformations usually consist of alternating steps of dissociation and locking of bond couples. In order for the initial and the final products to be regular, some bonds should be broken and other closed because loose bonds are an evidence of irregularity and such structures are unstable unless isolated or highly diluted.

Thus, the chemical reaction of substitution follows the pattern:

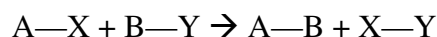


The difference in font symbolizes here the degree of our attention. In the neighborhood of **A**, **B** is changed for **C**. If we switch attention to **D**, **C** is changed for **B**.

Substitution is one of a few general patterns. The lower level includes various specific reactions involving particular functional groups. For example, *esterification*:



This reaction is an example of a more general pattern of *condensation*.



It looks no different than substitution, and in fact, it is not. The particularity of condensation is that X—Y is usually a very simple molecule, typically, water. This circumstance is crucial for biochemistry.

Although elementary steps are always simple, they can lead to a catastrophic change of a global connector.

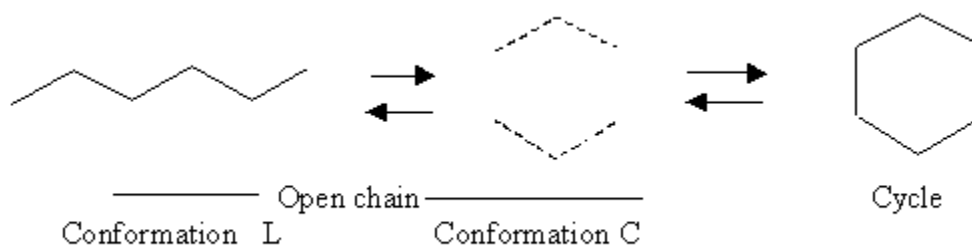


Figure 6.1 Cyclization of linear connector

Much more dramatic examples are known. Thus, the four cycles of steroids (Figure 2.1) can be closed *in vivo* from a linear molecule along a very short pathway.

To jump from a line to a circle, the configuration should take a certain position in the Euclidean background space, shown in the middle by broken lines, Figure 6.1. The ends of the chain must come into a close contact. The open chain and the chain in this pre-locked position are just different conformations, not different configurations.

In most chemical reactions, the events are strictly local in Euclidean background space. The local character of transformation in chemistry is a powerful means to manage complexity.

Such transformations as cycle closure, with the exception of some special cases, require additional energy to overcome the high entropy of distant ends of the forming cycle, which must be somehow compensated by forming additional bond couples.

7. Chemical kinetics and transition state

Chemical kinetics is concerned with the problem of the transformation speed. In pattern terms, it equals asking how fast the probabilities change toward the equilibrium. In the virtual world kinetics can impose limitations on the computation time, for example, the speed of convergence in stochastic relaxation, [2], p. 381.

In the chemical language, the transformation speed means the rate of concentration change.

Thus, for $A \rightarrow B$ (concentrations are in square brackets):

$$d[B]/dt = k [A] , \text{ where } k \text{ is } \textit{rate constant}, \text{ specific for each transformation,}$$

$$[A] + [B] = \text{Const.}$$

$$\text{For } A + B \rightarrow C : \quad d[C]/dt = k [A] [B], \quad [A] + [B] + [C] = \text{Const}$$

$$\text{For } A + B + C \rightarrow D: \quad d[D]/dt = k [A] [B] [C], \quad [A] + [B] + [C] + [D] = \text{Const}$$

$$\text{For } A + 2B \rightarrow C: \quad d[C]/dt = k [A] [B]^2, \quad [A] + [B] + [C] = \text{Const}$$

In other words, the rate of transformation depends on the probability of finding all participating components **in each other's neighborhoods** of Euclidean space. The collision of three and more particles is a rare event and complex transformations go through a sequence of simpler steps.

Note, that the total concentration of particles does not change, unless so intended. This is one of three major limitations of the real world vs. the virtual one:

1. Conservation of matter.
2. Conservation of energy.
3. Euclidean topology.

The meaning of the conservation of matter, in pattern terms, is that in configuration space \mathbf{C} , the probabilities $P(G_j^i)$ to find generator G^i in configuration C_j must be strictly normalized:

$$\sum_j P(G_j^i) = 1$$

The chemist does not deal with the unbearable He-complexity of the chemical configuration space, but cuts a small sector out of it, using various heuristics. No wonder, the chemist is often surprised and frustrated when a dark goo and other unanticipated impurities foul up the flask, which happens also with the best of minds.

Euclidean topology of the real world defines how entropy can be estimated. The transition configuration is possible only if all its generators occupy relative positions that make possible formation of new bonds without drastic displacement of atoms.

Considering the process of thinking, a chemist would say that most ideas do not occur to a mind simply because the rate of their formation is too low. This statement would extrapolate chemical experience that asserts that, while everything is possible, only a few transformations are fast enough to be realistically considered. The problem is that transformations go through unstable and evasive transition states. The intimate chemical process is predominantly a

redistribution of electron density, which is something chemistry cannot portray by classical chemical formulas.

The difference between the real dirty chemical world, the mind nested in the real brain of flesh and blood, and the mathematical abstractions should never be lost. Nevertheless, chemistry conforms to pattern theory pretty well. The main reason for that is that PT is as much a theory of regularity as of irregularity.

The tacitly accepted universal chemical principle (see Part 3, *Regularity and probability in chemistry*) that if we have a certain starting molecular configuration, then **anything we can imagine** can happen to it, presumes that generators, i.e., atoms, are neither created nor destroyed, and chemical regularity is preserved. The words “anything we can imagine” used here remind again about the more than metaphoric parallel between molecules and thoughts.

Putting side-by-side real molecules and thoughts may seem a mortal methodological sin. The definition of set given by Georg Cantor, “By a set we mean a grouping into one entity of distinct objects of our intuition or our thought” (quoted from [10], p.322), gives us a hope of absolution.

In a real chemical system, the factor of time can be more important than the position of equilibrium between the configurations involved. In real life, the absolute majority of possible outcomes are never realized for kinetic reasons: because of the conservation of generators, a few fastest transformations quickly **consume** the starting ones and the transformation rate drops. The slower transformations are, therefore, self-inhibiting. Note that the underlying reason is the limited resource of atoms. Different transformations **compete for a limited resource**.

Similarly, for a real mind in a real environment, there is hardly ever enough time for stochastic relaxation. The need to act interrupts the search for “the truth” or the optimum. The *competition for time* limits the relaxation even in the game of chess, not to mention real life because not all alternatives can be optimized and compared.

While the chemical system is always conservative, regarding the generators, it is not clear how this could be realized in the chemistry of thoughts. Intuitively, there could be only one generator “red” or “big” in the mind, but of course, scores of them in a text or speech. It is hard

to accept the idea that thoughts exist in duplicates, unless in different minds. It seems to violate Aristotle's law of identity. Copies are not identical in some aspect: location, storage, whatever. Something must be different, otherwise, two copies are just one.

Another reasonable question is: if most transformations are not realistic, why do they happen at all?

The crucial step to understanding why some chemical reactions happen, while most of them happen only in the mind, was made in 1889 by Svante Arrhenius (1859-1927), who, by the way, made other crucial steps in chemistry (electrolytic dissociation), as well as outside (ideas of panspermia and greenhouse effect).

The aside remarks of the last paragraph may seem a digression if we forget that we compare the thoughts and the molecules.

Svante Arrhenius had a clear idea that even if the transformation is feasible, only a part of all collisions between molecules result in a change, which, in real life, parallels the fact that only a part of all acquaintances result in friendship or marriage. He turned his attention to the rate constant K , which had been a strictly empiric number, and found that

$$K = A \exp(-\Delta G^* / RT) ,$$

where K is the rate constant of the reaction, ΔG^* is *energy of activation*, A is the fraction of "productive", i.e., consummate, collisions, and R is constant.

Universal gas constant R is a form of Boltzman constant k adjusted to the molecular mass: $R = N k$, where N is the number of particles in a mole of any pure substance (Avogadro's number).

Remarkably, ΔG^* is **always** larger than the energies of the initial and final states. It is the **difference** between the energies of the *transition state* and the initial and final states.

The form of this equation (same as for equilibrium) suggests that K reflects nothing but the probability of the initial configuration to reach energy G^* . It follows from statistical mechanics of J. Willard Gibbs (1839-1903), whose name was the source for *Gibbs energy* G that plays a crucial role in the real world because it accounts for its order, as well as chaos:

$$\Delta G = \Delta E - T\Delta S,$$

where S is entropy and E is the chaotic energy of heat (also notated as Q). Here $T\Delta S$ takes to account the degree of order that subtracts from the chaos. Note the deltas: chemists think only in differences.

Gibbs energy assumes that the pressure during the change is constant. There are other measures of the so-called *free energy*, i.e., energy capable of producing work. Gibbs energy is so popular because most chemists work at atmospheric pressure to avoid explosions, unless they use steel vessels.

Following Arrhenius, only the molecules that reach energy G^* (*activation energy*) are capable of transforming into products. A more metaphoric interpretation is that there is a barrier between the initial and final products that is necessary to overcome for the transformation and only a small part of molecules with the asymmetrical Maxwell-Boltzmann distribution have energy sufficient to overcome it.

Turning to real life, to win somebody's heart, you have to be not only insistent (E), but also liked in return (S), if odds (T) are against you.

The change of entropy in chemistry comes from the change in degrees of freedom in 3D space during the transformation. For example, the closure of a large ring from a linear chain is accompanied by a significant loss of entropy, the longer the chain the larger, because the ends have to find each other in ever larger space. As the chemists say, "it is difficult." To continue the

molecule-thought parallel, creativity means connecting distant ideas, because what is close on hand is obvious.

The entire picture of chemical equilibrium, therefore, looks like in Figure 7.1.

Between the **stable** initial state **A** and the **stable** final state **B** (the initial and final states can be reversed) lies an **unstable/improbable/irregular** transition state \mathbf{AB}^* . It is the equilibrium between the stable states and the unstable transition state that determines the rate of transformation.

The position of equilibrium between stable states does not depend on the energy of the unstable state because its concentration is negligible.

It is presumed that the equilibrium between \mathbf{AB}^* and both **A** and **B** establishes much faster than the equilibrium between **A** and **B**, and only because the probability/concentration of \mathbf{AB}^* is low, it becomes the true bottleneck of the transformation.

Rigorous logic may find obvious gaps in this reasoning. We still remain within the equilibrium paradigm and do not introduce any new and radical ideas about the kinetics itself. It is not clear how time can enter the picture.

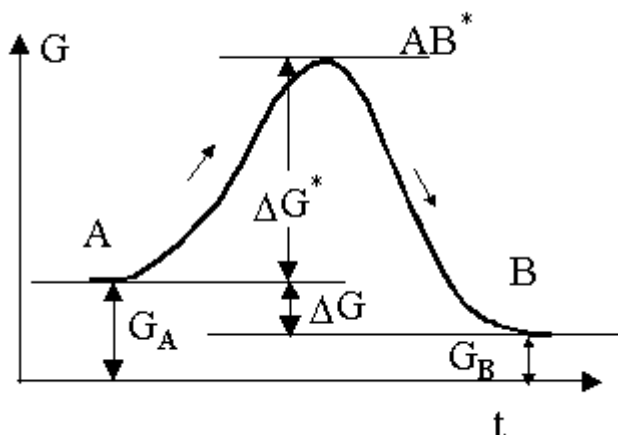


Fig. 7.1 Transformation of A into B

The study of absolute reaction rate and all details of the transition process is a separate area of theoretical chemistry of a strong quantum-mechanical flavor. It is beyond the scope of this paper. It must be noted, however, that the transition state is not a stable substance that could be kept in a jar overnight, but the entire *process* of transformation from **A** to **B**. A possible basis for our kinetic assumptions is that what happens in the transition state usually does not involve any radical displacement of the atomic nuclei and is limited to the redistribution of electron density, which in fact happens, by the human time standards of day and night, practically instantaneously. Anyway, in spite of its logical incompleteness, the concepts of transition state and activation energy serve chemistry very well because chemists, as intuitive Bayesians, operate with differences and not the absolute values. They are not interested in the absolute probability of a structure, which not only can be attained in an infinite time but also depends on what other structures are involved. It will suffice that the structure is stable.

Chemists are trying to figure out the most probable configuration on the condition that the known (sometimes, partially) initial configuration takes place at time t_0 , and the next measurement is taken at time t_n , i.e., for $A \rightarrow B$, they have to calculate $P(B_{t=n}|A_{t=0})$. To remind, the probabilities are expressed as concentrations. A chemist, however, practically never has a complete set of alternatives, which is exactly why chemical experience might present interest for pattern chemistry of the mind. Moreover, the chemist is usually interested in achieving a certain stable state with maximal probability, which is what an average mind carrier pursues, too.

Whether animals think or not is open to questioning, but they certainly pursue goals. What we call *goal* is the imaginary final state separated from the real initial state by a transition state, which is not quite clear in all detail. While pursuing goals, humans and animals alike, or, rather, their minds, work as typical chemists, optimizing the sequence of mental configurations ending with the goal. The usual problem is that another overlooked final state is quite possible. As the story of king Croesus and the oracle of Delphi tells us, final states could be well beyond our imagination even if we have reliable cues.

Along Herodotus, the oracle predicted that Croesus would destroy a great empire. The destroyed empire turned out to be his own.

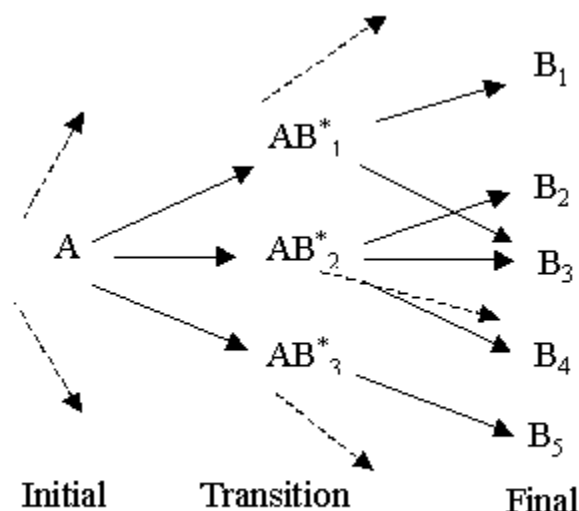


Figure 7.2 An incomplete transformation space. Broken lines symbolize other alternatives, not even imaginable.

The typically chemical situation looks like in Figure 7.2. There are a few possible transition states, each leading to one or a few final states, sometimes, overlapping. The chemical tree of choices is usually incomplete and most of the alternatives are discarded due to prior knowledge (the chemical “system of beliefs”) as well as because of clear cut principles. It is natural to assume that a similar tree of choices, in the form of regular and irregular configurations, should be optimized equally by a wolf or a businessman planning to make a kill, while the deer and the competitor have their own trees.

Bayesian inference has been a subject of numerous arguments and the opinion of a chemist weighs little, but a chemist would suspect that few arguments could arise over a well-defined system. Neither in chemistry, not in intelligence, however, nor, for that matter, anywhere in the world, except in the speeches of political leaders, do we have well-defined systems—a suspicion first expressed by Heraclitus. Thus, an escape from a prison or a catastrophe on the September 11 scale are possible only because neither the prison security nor national security are well-defined systems and some transition barriers happen to be invitingly low when the temperature is high enough.

The idea of transition state comes from the mere observation that nothing happens at once and there must be a reason why events happen at all. If not for the barrier of the transition states, all the molecules on earth would react and fall into equilibrium and all “life’s persistent questions” could be solved in an instant. In fact, nothing is instantaneous.

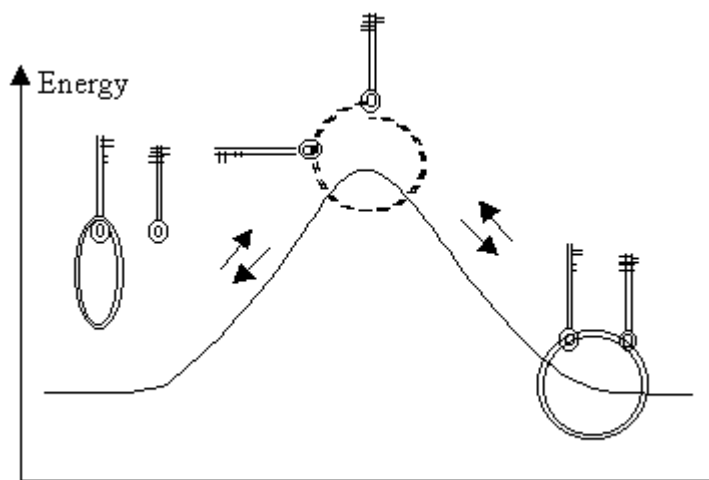


Figure 7.3 Metaphor of bonding

Figure 7.3 metaphorically illustrates the concept of transition state on the process of adding a key to a key ring. In the transition state, the ring is deformed and brought into an unstable shape, which alleviates the attachment of the second key.

Transition state as process is very well known in technology and meteorology. Everyday human activity also consists of stable periods punctuated by short-living transition states, among them, transitions between sleep and alertness. In Asby’s homeostat, all steps of the transition state are observable and recordable.

The following is an illustrations how the same chemical transformation can go through different transition states.

There are two possible mechanisms of recombination $A-B + C-D \rightarrow A-C + B-D$, which the chemists call *substitution*.

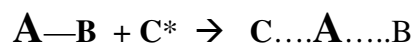
Generator space: A, B, C, D.

Mechanism 1.

Stage 1: Dissociation of a bond



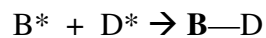
Stage 2: Formation of a triple transition complex and the new bond



Stage 3. Formation of a new bond

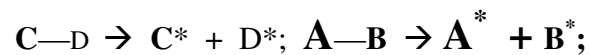


Stage 4: Recombination of fragments

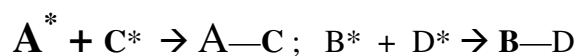


Mechanism 2.

Stage 1. Dissociation of a bond



Stage 2. Recombination of fragments



The arrow \rightarrow means everywhere the reversible transformation \leftrightarrow .

In Ulf Grenander's chemistry of thoughts, a configuration with incomplete bond couples is considered irregular, [1], (2.4), which is consistent with how the chemists see it. Irregular extra bonds, exceeding the regular arity, could also be added to that.

The transition state is always an irregular configuration, usually, with the rule of octet violated. Since transition states cannot be portrayed by common chemical formulas, new symbols were invented for them after their nature had become clear, and of course, by definition, they cannot be stored in a jar. It does not mean that they cannot be studied. Chemistry itself is in a perpetual transition state, few things are static, and we can expect in the future much more detailed knowledge of the intimate mechanisms of chemical transformations. The same can be stated about the science of the mind.

8. Catalysis

The question arises: how could transformations be made simple, selective, and fast if typical reactions in organic chemistry are notoriously slow and tend to run in many directions simultaneously, generating mixtures of products?

The most powerful tool in the chemical time managing is catalysis. Catalysis is a cardinal chemical concept that opens a passage from the classical equilibrium chemistry to the non-equilibrium phenomena of LMS. It prevents chemical chaos inside the living cell. It is easily rationalized in pattern terms. Naturally, some subtleties, meaningful for a chemist but nonessential for the pattern picture, will be sacrificed.

The closest pattern relative of catalysis is signal or message in information theory. While information changes the probability distribution of outcomes toward lower entropy, the catalyst does the same with transition states.

Catalysis has no influence on the position of equilibrium, but, like an earthquake, dramatically warps the kinetic landscape. Similarly to signal and earthquake, it makes a notch on the time axis. It starts at the moment of introducing the catalyst into the system, but in due time, as any information, becomes an old hat. Let us note this property of *novelty*, typical for LMS, because we shall return to it later. The catalytic effect dissipates with time in the same way every news becomes an old hat next day. In the long run, the effect of the disturbance created by the

catalyst is erased by equilibrium. The catalyst itself returns chemically unchanged, as an arrest warrant, after it has been read and produced the desired dramatic effect in a detective story.

In pattern terms, catalysis is based on the interplay between regular (solid lines) and irregular (broken lines) bonds, Figure 8.1. The irregular bonds in question are perfectly regular from the point of view of physics, but not from the pattern-chemical one. They are weak, labile, and often multiple.

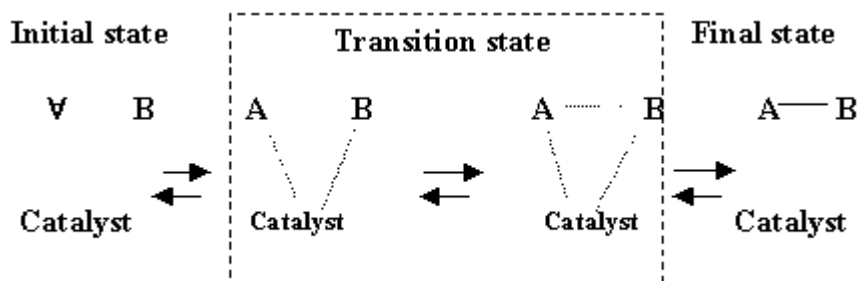


Figure 8.1 Pattern catalysis. Note that **A** is in a wrong initial position for binding

The transformation involves three initially disjoint configurations: **A**, **B**, and **Catalyst**. Configurations **A** and **B** could be subconfigurations of the same configuration, as, for example, the ends of a linear chain.

The entire initial configuration can have high entropy in the Euclidean space where the particles form bonds only in particular spatial orientations and at a close distance. To bring them into the bonding position, with much lower entropy, the energy is borrowed from “irregular” weak chemical bonds shown by broken lines. The transition state undergoes a transformation, coupling the provisional and irregular bond **A---B**, which becomes regular after the catalyst splits off the transformed substrate. This happens sooner or later because of the reversibility of all stages of the process.

The temporary bonds are “irregular” only against a certain definition or standard of regularity in a certain way. As we saw, the intuitive and fuzzy understanding of chemical regularity amounts to the question of stability of a chemical substance. In fact, it is not the walls of the glass jar on the lab shelf that prevent the transformation but the invisible walls of kinetic

barriers. It is appropriate here to compare the kinetic barriers to the barriers of understanding erected by ignorance, prejudice, bias, and habit.

There are different types of chemical catalysis. They all work in three basic steps. The catalyst

- (1) binds to a specific substrate (Gibbs energy decreases),
- (2) forms a new transition state (Gibbs energy increases but stays lower than for the non-catalytic transition state), thereby strongly increasing the speed of the transformation, and
- (3) separates from the changed substrate after the transformation is complete (Gibbs energy decreases and can be either higher or lower than in the initial state).

By catalysis we mean here only the so-called heterogeneous and template catalysis, omitting the homogenous type, which is somewhat subtler.

The distinction between the strong and weak bonds is crucial for catalysis, as well as for all living systems. The weak bonds are very labile, which means that they close and break up in the temperature range where the strong bonds cannot dissociate into highly irregular loose atoms. The weak bonds could be compared with joined magnets or pieces of modeling clay, while the strong bonds are, so to say, locked by bolts and nuts and can be taken apart only with a tool or an explosive. At a very high temperature, of course, all bonds are weak and chemical complexity disintegrates. Properties of various bonds is illustrated in Figure 8.2.

Catalysis simply restructures the energy balance sheet of the system, without changing the bottom line. This is why it has no effect on the position of equilibrium and equally enhances the direct and the reverse transformations. The systems like life, mind, and society exist because the initial intake of free energy and its dissipation into heat and simple metabolites prevent the equilibrium.

If the three initially disjoint configurations—two components of the substrate and the catalyst—lose their independence, it means a significant drop of entropy, which requires energy

to compensate for. If the ΔS contribution to $\Delta G = \Delta Q - T\Delta S$ decreases, ΔG increases, and the reaction slows down. The source of this energy is formation of weak and labile bonds that are outside the area of "regular" strong chemical bonds that are difficult to break (hydrogen bonds, Van der Waals bonds, electrostatic interaction, interaction with the solvent, etc.). The disconnected irregular fragments of regular bonds have high energy and low probability. The fragments of weak irregular bonds, for example, the bonds between molecules of water, are individual and stable regular molecules.

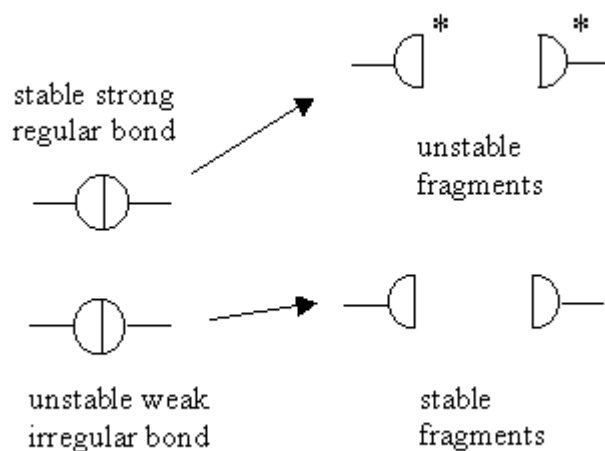


Figure 8.2 Properties of regular and irregular bonds

The most interesting case is when the substrate and the catalyst conform to each other like lock and key. To continue the analogy, some important catalysts work rather like the safe deposit box and two keys to it. Figure 8.3 illustrates this case by the joining of the two keys with a single ring, this time aided by fixing the positions of the keys, which simplifies the operation and eliminates unnecessary fumbling with the objects in the transition state.

It is important to emphasize that the catalyst works in both directions and does not change the position of the equilibrium, which does not depend on the transition state. The remarkable effect of catalysis can be seen only at non-equilibrium conditions, which is exactly what life, mind, technology, and society require for functioning. In the long run, the

thermodynamics overrides kinetics, and the catalytic effect is completely erased. In a non-equilibrium open system, however, nothing is “long-run”.

Transformations of relatively small compounds—small in comparison with polymers—may go in just a few directions because of large differences in ΔG^* between different transition states. If we deal with gigantic polymers, like proteins and nucleic acids, where the configuration space produced by combinatorial explosion, all the polymers have close energies. In such a degenerated system, an ultimate chemical mess would be expected if not for the catalysis. The catalyst brings order into a highly chaotic system and, therefore, works no different of any package of information.

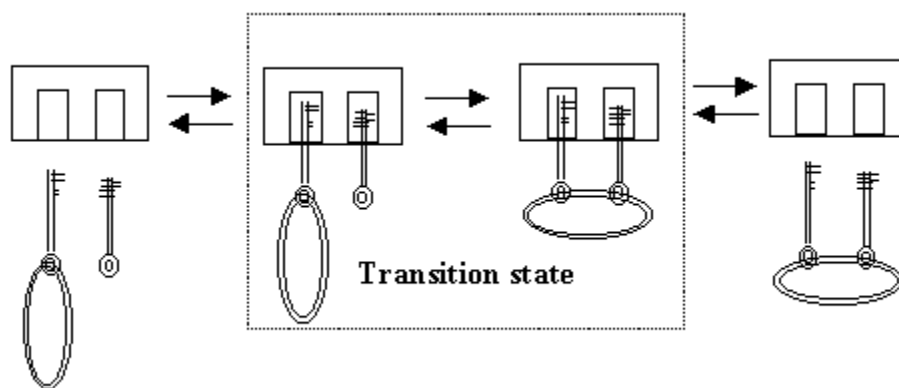


Figure 8.3 A metaphor of catalytic transformation: the joining of two keys by a ring is made easier by the fixed positions of the keys, of course, not by two locks.

A degeneration of configuration space parallels the situation in a computer where any sequence of symbols of the same length requires the same time—and energy—to transfer and process. Classical thermodynamics in both systems does not depend on the content of a configuration, which is always a linear sequence of a limited number of symbols. Unlike the chemical system, the computer is, ideally, completely frozen and nothing happens in it unless on command, while life and society have a significant degree of spontaneity and can extract information from the world

Finally, we shall formulate what catalysis means in pattern terms, without any recurrence to chemistry:

Two generators in the neighborhood of the third are in the neighborhoods of each other.

Or:

Coupling of two generators with the third strongly increases the probability of their coupling.

Or:

The probability/affinity of a bond between two topologically closest generators sharply increases if they are bonded to the same third generator.

The concept of catalysis presents a curious problem related to the lack of the concept of history in physics, where anything that happens for the first time has to be pre-existing. In information theory, the events display between the input and the output and they are of repetitive and reproducible nature. If a pinch of the catalyst is dropped into a flask, however, this may never happen again in the same system with the same result.

W.Ross Ashby noted that circumstance while observing his homeostat. He suggested (in an exaggerated interpretation) that the unique event would simply mean that, for example, the input voltage has been zero for half eternity and then changed to 1 and, maybe, back to zero, where it could remain for the second half of eternity.

An alternative point of view is the fundamental for LMS concept of evolution consisting of a chain of unique events, with the current result explainable only in terms of historical record. The concept of **pattern evolution** means that the generator space and the configuration space, as well as regularity, cannot be formulated axiomatically once and forever. The *historical* (or Heraclitean) systems are characterized by a complete absence of ergodicity: the representative point never passes the same cell twice. Paraphrasing Heraclitus, one cannot step into the same

phase space twice. It expands, contracts, and warps as in the most audacious sci-fi movies. What is remarkable, however, **the same patterns can be traversed repeatedly**. He-systems can be ergodic at the pattern level. There are no principal obstacles for accommodating this view by PT, which could open a case on **patterns of history**, where transition state would take the central place and patterns can be revisited in the pattern space. Nevertheless, the parameter of novelty precludes the ergodicity of classical statistical ensembles.

In the 1950's and 60's, when physicists turned their attention to life, an apparent impossibility to assemble a large molecule from atoms without pre-existing information had been the greatest mystery. From the point of view of physics, origin of life was impossible, although life itself was thermodynamically understandable as a non-equilibrium open system. From the point of view of chemistry, there was no problem at all: in a very large He-complex configuration space, complexity can develop from a very simple combinatorial base set in a long sequence of simple steps.

Looking back, the conundrum was a natural consequence of the inherent reluctance of the pre-computer physics to deal with irreducible complexity, i.e. objects represented by lists that cannot be compressed into formulas. Chemistry, on the contrary, developed as an art of navigating through the irreducible complexity of millions of individual compounds and their transformations. Although chemistry has arrived at a set of general concepts, similar to a well-balanced literary analysis of Shakespeare, the true joy of chemistry can be found in the lab, which is a perennial Wild West.

The basics of the chemical art of navigating in large configuration space include the principle that the change in a large system is sequential and local. Similarly, the marine navigation is based on assumption that the ship does not hop all over the world ocean, from one hemisphere to the other, but moves through a sequence of close positions on a 2D surface.

On the contrary, abstract statistical ensemble of independent particles has no such limitation: under the principle of ergodicity, a sequence of states may be arbitrary, as for the gas-like ensemble of colliding particles. The main property of the virtual world is, probably, that any state of the computer monitor can be followed by any else, even though the sequence of intermediate stages can greatly vary. In the real chemical world, the jumps of the phase trajectory are rare and short. At the same time, jumps in the mind are quite natural.

9. Competition and Selection of Configurations

If cybernetics was the alchemy of the mid-20th century, then Walter, Ashby, Beer and Pask were the Magi. (Andy Pickering, [15]).

Artificial Life (often abbreviated as Alife or A-life) is a small universe existing parallel to the much larger Artificial Intelligence. The origins of both areas were different. Alife arose as an abstract mathematical study of generalized life **after** the molecular biology had taken its modern shape and the molecular mechanisms of life had become transparent. On the contrary, AI, as if anticipating a slow progress of the study of the intimate mechanisms of Natural intelligence (NI), took up the mind as a black box and focused on imitating and amplifying its functions.

While AI is a huge area of research involving many people who pursue practical goals, Alife, though ambitious, remains a kind of an intellectual game. Having come from chemistry, it presents interest as generalization of non-equilibrium and non-linear **chemical** experience.

The full story of AL, with purely chemical roots going back to Svante Arrhenius, is beyond the scope of this paper. Its modern chapter starts with chemist Manfred Eigen (Nobel Laureate in chemistry, 1967). People in AI are aware of his works, mostly from the point of view of game theory, while Alife is well aware of the Ising model. Ilya Prigogine and Manfred Eigen inspired the modern science of complexity, which today is best of all represented by the Santa Fe Institute

(Stuart Kauffman, John Holland, Christopher Langdon, Peter Schuster, and many others). It studies the theoretical aspects of LMS, excluding the US Tax Code, the most complex creation of all.

Ross Ashby captured the state of evolutionary divergence of the emergent AI into computer and life sciences in his *An Introduction to Cybernetics* [13]. In spite of Alan Turing's own biological interests, the Turing Machine gave a great impetus to AI toward computer science rather than life science. Nevertheless, the anthropomorphic Turing test was based on live human intelligence as the reference point and was, in essence, a test for adaptability of AI in the environment of NI. It seems that the advent of computers greatly favored the formal AI in competition with adaptive AI. Today, however, when the exchange of ideas is as common as the exchange of flu viruses, AI, Alife, and science of complexity look like a single continent in the shape of the Americas with Alife as the Panama Isthmus between the science of complexity and AI.

What is abstract life without trees, elephants, and humans who try to destroy and save them all and each other? Alife tries to answer the question "what is life" by modeling the major properties of life at the basic molecular level, but, in the pattern spirit, not being overly obsessed with chemical formulas. Alife accepts the Darwinian paradigm that life is competition of species, such as trees, elephants, and humans, for limited resources in an evolving system. The term **evolving system** means not only that the system is thermodynamically open and far from equilibrium, but, more important for us, is a system of chemical type, i.e., evolving in a complex and rich configuration space. It is a system of competing configurations and patterns that reproduce themselves.

It is a matter of convention whether generators and configurations exist in multiple copies in both structural chemistry and PT. In Alife, as in the material world, generators exist in copies and configurations can multiply. In AI, as in mathematics, two identical ideas are just one idea.

The multiple generators of whatever kind do not contradict the general framework of PT if we assume similarity transformation COPY.

The phenomenon of reproduction has been long known in chemistry as autocatalysis without any biological connotations: the catalyst catalyses its own formation. Figure 9.1 shows how it works in an abstract form.

Configuration **D** (disjoined, as it is common in chemistry), consists of four generators **A** and four generators **B** existing in four copies of each. Two generators are coupled. The multiplicity of free generators simulates the availability of building blocks in the environment.

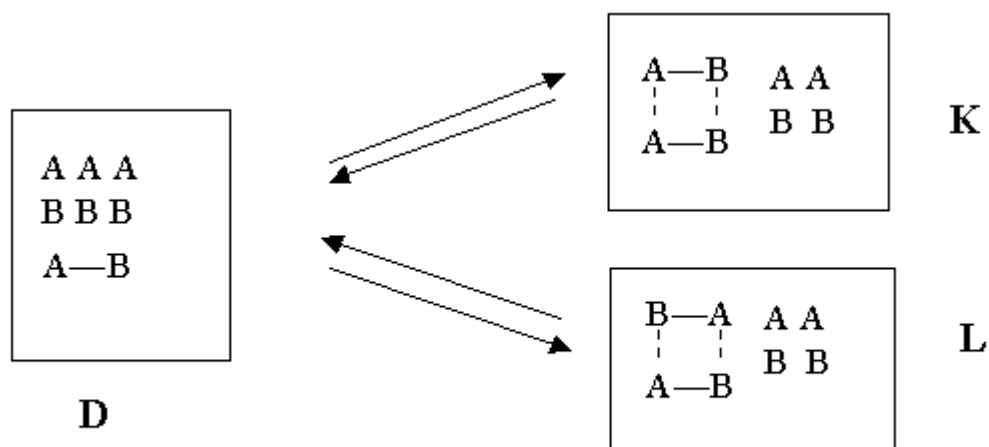


Figure 9.1 Template catalysis in replication

$P(A-A) > P(A-B)$ leads to **K**, $P(A-A) < P(A-B)$ leads to **L**

Suppose, generators can form regular and irregular bonds. There are two cases: identical generators form a stronger (more probable) irregular bond, shown by broken lines, than the different generators:

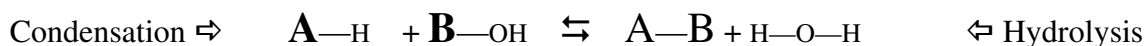
$$P(A-A) > P(A-B) \text{ or } G(A-A) < G(A-B)$$

Then **A—B**, as in Figure 9.1, or **A—A** and **B—B** otherwise, will catalyze their own replication. One dimer works as a template for another.

In the opposite case, when the greatest affinity is between different generators, the replication will be complementary, as in natural life. Note, that the errors are inherent in this

kind of probabilistic reproduction, depending on difference/ratio of energies/probabilities of the two irregular bonds.

The question arises, if free uncoupled generators are irregular, how can they be loose and lonely, as in Figure 9.1? They cannot. In biochemical systems, the **strong** bonding between generators is, at mild temperature, practically always not a coupling but a **recombination**, with the participation of water and its fragments. It is called *condensation*; the reverse transformation is *hydrolysis*.



For biopolymers to be formed, a supply of Gibbs energy is required because the equilibrium involving water is shifted toward hydrolysis. This energy comes from ATP, the universal energy carrier of life. The biochemical details are not essential for us, however. What is essential, biopolymers can form only in a system with consumption of Gibbs energy and its dissipation into heat.

We do not talk about “supply” of thermal energy when considering a system at a certain temperature. We need, however, a supply of Gibbs energy because it is a perishable commodity, turning into heat if not used for work.

As soon as we postulate replication in a chemical system, it becomes a model, although very much incomplete, of life. The pioneering work of Manfred Eigen [16, 17], who investigated the kinetics of this type of systems, gave an impetus to the whole new area

Manfred Eigen was concerned mainly with linear sequences for two reasons: the linear model is the simplest for simulation and it is the closest to natural linear chains such as proteins, DNA, and texts.

Manfred Eigen’s main question was: what can happen in this kind of a system from the point of view of chemical kinetics, provided the configurations act as self-replicators, i.e., each

polymer enhances the formation of its copy from monomers. To ensure replication, a supply of generators (monomers) and Gibbs energy to link them were postulated. The linear polymers multiplied like the hare and lynx in Lotka-Volterra's famous model. The total number and length of generators existing in multiple copies in the basic model were kept constant, although that was not a necessary condition.

The replication is prone to errors and the most probable one is a mutation in a single generator. Hammett distance defines the metrics in the *sequence space*, Figure 9.2. The sequences longer than trimers occupy the vertices of hypercubes with most probable mutations along the edges.

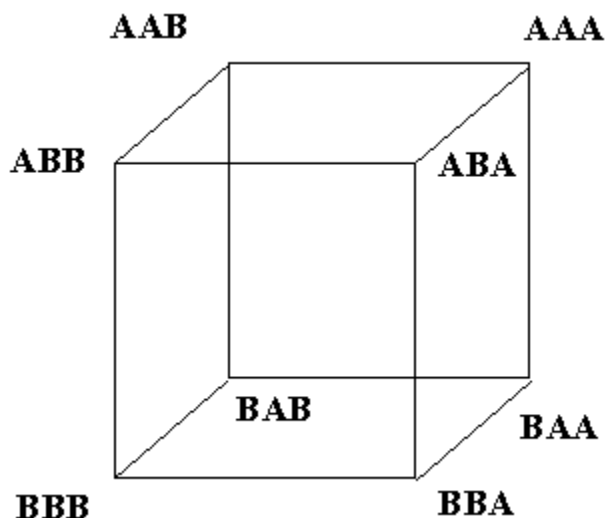


Figure 9.2 The sequence space for trimers

The realism of Eigen's model was not in detail but in the type of kinetics that it employed. It was a starting theme for a multitude of subsequent variations in *Alife*.

In the simplest case, the imaginary system under consideration comprises n species (linear configurations) with x_1, x_2, \dots, x_n individuals in each.

In Eigen's model, the simplest system is described by the following kinetic equation:

$$dx_i/dt = A_i Q_i x_i - D_i x_i + \sum_{j \neq i} w_{ij} x_j \quad (9.1)$$

$$d \sum_i x_i / dt = 0$$

where $A_i X_i > 0$ is the component of self-reproduction (birth), diminished by $Q_i < 0$ as quality parameter, i. e., the measure of errors during reproduction,

$D_i X_i$ stands for spontaneous decomposition (death), and

$\sum_{j \neq i} W_{ij} X_j$ is the production of species X_i through mutations from all the other species.

It is the canonical form of kinetic equation for a system with gain, loss, and interaction. The first term is growth, not necessarily through replication, and the second term is decay. The third term represents influence of topological neighbors. Replication is the only way a population can grow, but the equation is not limited to discrete metrics: X_i can be, for example, probability. The presence of neighbors assumes a topology.

Eigen's simple system possesses Ar-complexity: all generators are listed in advance. The configurations are combinations of symbols of a certain length. Neither the symbols nor the length enter the equations. As Eigen noted, for combinatorial reasons, the number of all possible sequences can easily exceed the number of available monomers. The term evolution can be applied here in its narrow physical sense, as the movement of the representative point over the phase space of a however large but constant volume.

The third term of the equation is similar to the term of the exchange with the neighbors in Ising model. The connector, however, is not a 2D lattice but the sequence space.

The mathematical picture of competition, based on replication with errors, is very general. It seems that various biological and physical models belong to the same general class of processes. The class is described by the differential equations that in the most general case contain the following terms:

1. Birth (or remembering, multiplication, growth, formation, self-perpetuation, success)

2. Death (or forgetting, extinction, decline, dissipation, decomposition, failure)
3. Interaction with topological neighbors in terms of probability of birth and death (in a relaxed version, success and failure).

The phenomena of birth and death demarcate the border between “plain chemistry” and biochemistry, or, to put it differently, between meta-chemistry and LMS.

The possibility of birth and death in an open chemical system needs explanation. It is appropriate to distinguish between two types of bonds, positive and negative, see Figure 9.3.

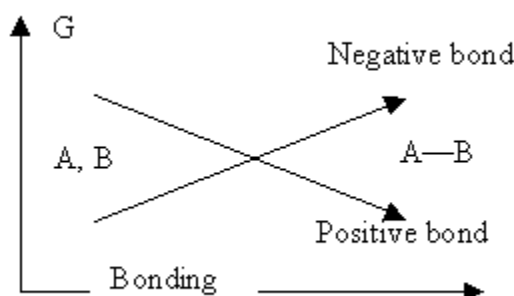


Figure 9.3 Positive and negative bonds

The positive chemical bonds require energy to break them and the negative bonds require energy to form and maintain them. All chemical bonds, whether strong or weak, are positive: the stable bond forms with the release of energy. This is why catalysis is possible: the initial bonding with the substrate is spontaneous.

The quantum-mechanical picture of chemical bond includes the negative and neutral versions as anti-bonding and non-bonding molecular orbitals, along with the regular bonding orbital. They are solutions of Schrödinger equation.

In biochemistry, where the bonds are formed by condensation, with the evolution of water, the equilibrium is thermodynamically shifted toward hydrolysis (breakup) of the

sequence. Therefore, a bond couple between monomeric generators can form only on the condition that energy is delivered selectively to the site of bonding, which is done through ATP (Adenosine Triphosphate) in the presence of an enzyme.

This is not possible in spin models, where the energy may come only from a field. Thus,

the Ising model has the Hamiltonian $H = \sum_{\langle ij \rangle} -J\sigma_i\sigma_j - h \sum_i \sigma_i$ where h is a uniform

applied field. This illustrates the dramatic difference between physical and LMS models.

Thermodynamically, life is a *dissipative structure*, like the eddies in the turbulent flow, Bénard structures in water in a container on a hot plate, tornadoes, and other phenomena existing only due to the supply of energy. The physics of dissipative processes in connection with life was explored in-depth by Ilya Prigogine, the founder of non-equilibrium thermodynamics, and his school [Prigogine is author of numerous books on the subject]. As Eigen formulated, “Systems of matter, in order to be eligible for selective self-organization, have to inherit physical properties which allow for metabolism, i.e., the turnover of energy-rich reactants to energy-deficient products, and for (‘noisy’) self-reproduction. These prerequisites are indispensable.” [16].

The mind, located in the brain, 2% of the body by weight, consumes 20% of energy. We do not know how this energy is used, but it is obvious that only a small part of all daily content of the brain leaves any trace in it, while a part of the earlier stored material disappears. Two hypotheses on thought dynamics can be inferred from this fact.

The first hypothesis of cardinal importance is that the **thoughts**, or whatever configurations in the brain are behind them, **must compete for the energy supply** in order to come to existence, albeit for a short time. Like the polymers in biochemistry, they need Gibbs energy, and, probably, they are polymers of a kind, in the pattern sense.

The second hypothesis is that the conscious thoughts are just the top of the iceberg, like the most active molecules in Maxwell-Boltzmann distribution. They reach the high energy level

of consciousness. Below them are scores of other—subconscious—configurations that fall into the medium part of the distribution.

The remarkable consequence of competition for a limited resource is that it displays in time because of the form of the canonical equations. The goal of the “survival” is to “multiply existence” toward the next moment. This is how time enters the picture.

The complexity of life appears to be a consequence of an extremely large size of biosphere, while the complexities of modern society come from the limited size of the globe. As far as mind is concerned, the interesting question is the relation between the size of the real world and the upper and lower limits of the size of the mind that can adapt to it. Obviously, the size of the world of a squirrel is not only small but also fluctuating within a limited range. The size of the human world, however, is that of an expanding He-system. Probably, it was the use of tools and language that launched the expansion. It can be classified, in Eigen’s terms, as a hypercycle: each segment of the closed cycle catalyzes the next. Without the scale-of-sets mechanism, however, it is difficult to understand why life has been growing more complex throughout history. The population dynamics alone does not explain it.

The mathematical analysis of Eigen’s system showed a complex behavior depending on the ratios of the coefficients in the equations. The selected configuration is a **population**, not a single species, with a probability distribution of configurations around a certain average. The population may either drift through a sequence space or come to a dominating population, or experience a collapse of information content. Populations are characterized by their *fitness*, which is a value similar to energy (but is maximized instead of minimized in spontaneous processes). The populations have certain positions on a fitness landscape, where those with high fitness (high stability) reside on peaks, while the unstable ones take up valleys ([5], p. 199).

It is the concept of a landscape that unites all LMS systems because it introduces a universal function similar to Hamiltonian in an abstract metric, but generally non-Euclidean, space. Within the framework of Alife, it is the sequence space. Ulf Grenander calls its intellectual version *mindscape* ([1], 2.9). As it can be seen from figure 7.2, a chemical system of a sufficient complexity is also a peculiar collection of points on an energy landscape (*chemscape*) consisting of

peaks of the transition states and valleys of stable states. The positions of the points are neither independent nor static.

The concept of fitness landscape is appealing as a metaphor, but highly controversial. Thus, according to the concept, on a smooth landscape, two close sequences may have close fitness, while on a rugged landscape, a step aside may have dramatic consequences. But why? The concept does not provide any causality. Moreover, it does not take to account the kinetics that may drastically disrupt the bliss of classical statistical mechanics. Besides, as Alife realizes, the landscape changes right under the feet of populations. The LMS science of the future can draw realism from chemistry in its generalized form of PT, however complex it may seem.

Next, some general principles of evolving He-systems will be illustrated by computer models.

10. The Competitive Mind

Birds do it, bees do it
Even educated fleas do it
Cole Porter [18]

If molecules, species, things, and humans compete, then thoughts—their shadows in the mind—must do it, too.

Henri Poincaré (1854-1912) seems to be the first to express, around 1901, the concept of thoughts competing in the mind for a limited place in consciousness [19]. His reasoning had the same starting point as, much later, Manfred Eigen's. As Poincaré put it, it would take a whole lifetime to examine all thoughts and facts in human head one after another, although the absolute majority would be absolutely useless for thinking in a certain direction. Poincaré was puzzled by the observation that the irrelevant thoughts were unable to step over “the threshold of consciousness” and ever come to the mind of the thinker.

What is the cause that, among thousands products of our unconscious activity, some are called to pass the threshold while others remain below? Is it a simple chance which confers this privilege? [19]

Antonio Damasio, who works in the area of neurobiology of the mind but has a bird's eye view of the entire area of mind research, used a similar language in 1999.

...I sense that stepping into the light is also a powerful metaphor for consciousness, for the birth of the knowing mind, for the simple and yet momentous coming of the sense of self into the world of the mental, [20], p.3.

Manfred Eigen noted that out of about 10^{100} proteins of moderate length (more than the whole universe can comprise) the absolute majority is quite useless for living organisms and does not exist. Both Poincaré and Eigen pointed to the process of selection, which in the cloudless times of Poincaré meant only Darwinian selection. Eigen specifically mentioned Darwin.

We have to derive Darwin's principle from known properties of matter, [16], p.469.

The only difference between the terms *competition* and *selection* appears to be that selection is the result of competition. Formally, however, selection, meaning narrowing (mapping a set onto its subset), can be done without competition. Biology makes distinction between natural and artificial selections. We will understand selection as natural, i.e., stochastic. In the adaptive systems of AI, based on learning, the creation of information is the result of teaching, while in natural selection the human teacher is nowhere to be found and the set narrows because of the competition for a limited resource.

The central question for us is how to apply the kinetics of selective systems, developed by Eigen, to the mind where configurations do not form multiple copies and there are no populations of chemical or biological type. A tentative answer is that instead of concentrations, typical for chemistry, we have to come back to PT probability. In order to do that, we need a well-defined system with a finite set of possibilities, which seems impossible for a He-system by definition. As we shall see, we will still be able to have populations of a kind: in time, not in space.

The problem, therefore, splits into two sub-problems: competition on He-structures and building up a He-structure that could code the history of the system. The first problem amounts to a change of connector from hypercube to tree or an irregular Bethe-type lattice. A model for a He-configuration space will be considered in Part 11, *SCALE*.

10.1 BIRDS

To illustrate the principles of simulation, we start with an Ising-type square lattice as connector.

The model is called BIRDS because its behavior is reminiscent of a flock of birds that sometimes change the direction of flight in a coordinated way, but with a certain degree of dissent. It does not aim at simulating birds' behavior, for which there are plenty of much better models.

The description of the algorithm follows.

The program calculates directions of birds in a flock.

There are 36 birds B_m ($m=1,2,\dots,36$) in a flock.

The topology of the flock is a rectangular 6 x 6 grid.

The birds are numbered:

1	2	3	4	5	6
20	21	22	23	24	7
19	32	33	34	25	8
18	31	36	35	26	9
17	30	29	28	27	10
16	15	14	13	12	11

Each bird has 8 close neighbors. For example, #29 has # 13, 14, 15, 30, 31, 36, 35, and 28 as its neighbors.

The order of numbering is chosen to differentiate between inward and outward bias for some experiments. The program compensates for the lower arity on the fringe of the flock.

Each bird can move in 32 discrete directions α_i ($i=1, 2 \dots 32$).

The probability that bird B_m moves next moment in direction α_i is ${}^*P_{m,i}$.

The next state of the system is determined by the 36×32 matrix of probabilities ${}^*P_{m,i}$.

BIRDS calculates the probability distribution *P over all directions for bird B_m as:

$${}^*P_{m,i} = P_{m,i} + M_{m,i} F + \sum_{k,i} (g_{k,i} P_{k,i}), \quad k \neq m,$$

where $P_{m,i}$ is probability in the previous distribution, $M_{m,i}$ is memory about previous distribution, $F < 1$ is parameter of forgetting, $g_{k,i}$ is parameter of influence, $k \neq m$, and k marks all neighboring birds.

The new distribution is stored in memory. $M_{m,i} = P_{m,i}$ for all birds and directions, except for the previously selected direction. To make room for experiments, each bird remembers its last selected direction I as $P_{m,I} = H$, but the neighbors remember it as $P_{k,I} = C$. It is not reflected in the above equation.

It means that each selected direction stores H for this direction in the memory of the bird, but reports C for this direction to the neighbor who witnessed the turn. The higher H , the higher individual conservatism. The higher C , the higher global coherence.

Interpretation: each bird tends to move in the **same** direction, but it also tends to **forget** this direction. It is also **influenced** by its perception of the movement of several close birds in the flock.

Anthropomorphic interpretation: the bird “thinks” about choosing a direction, taking to account its neighbors, and 32 thoughts compete in its brain. There is one winner.

Parameter **C** reflects how a bird, that suddenly changes its direction, is perceived by its neighbors: do they take it seriously? **C** is the measure of “seriousness.” **H** is parameter of conservatism, **F** is parameter of flexibility.

The program has two kinds of output. One is the grid with the numbers of directions, Figure 10.1.1.

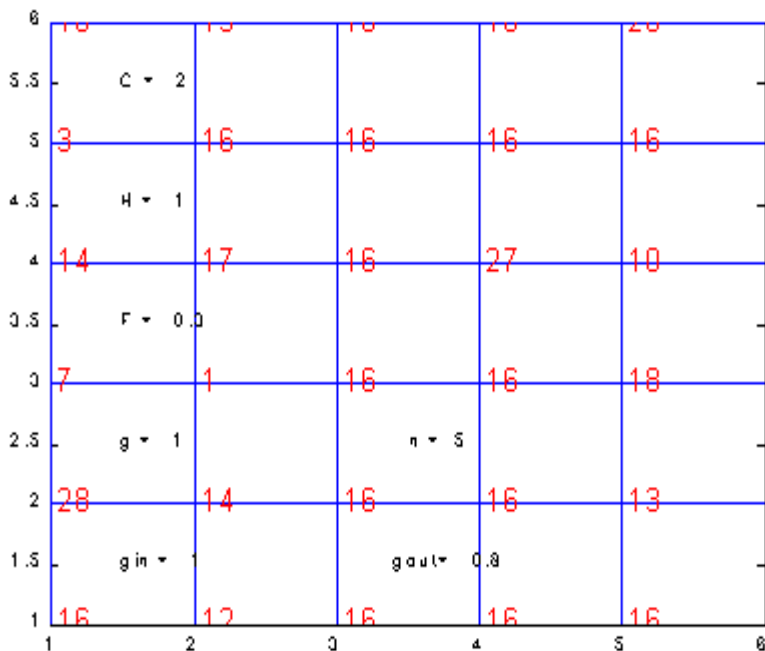


Figure 10.1.1 Example of grid output; directions are at the nodes

The other is quiver diagram, Figure 10.1.2.

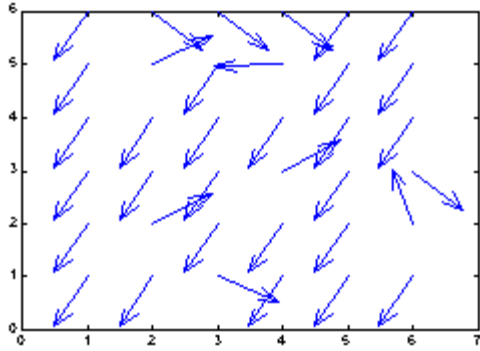


Figure 10.1.2 Example of quiver output

The quiver output is generated by script **bq**. It is the very last line of the program. If it is removed from the code, the grid output will be seen.

Script **bf** is used to start the simulation. It erases the previous information. After that, script **bf2** is recommended to change one or a few parameters with the arrays intact.

Additional parameters:

n: number of program cycles .

d: initial direction, one of 32 around full circle. It is not present in script **bf2**.

g: influence of the last direction **d** on the probabilities of directions

d+1 and **d-1**, i.e., “circular neighbors” on the dial of directions. Instead of this “stiff” distribution, normal distribution for directions could be used, but not in this program.

gin: influence by a neighbor with a higher number (inward).

gr: bias toward the center of the flock or outward; $gout = gin * gr$

gout: influence by a neighbor with a lower number (outward).

To use BIRDS, copy the workspace BIRDS.mat , copy scripts bf.m , bf2.m, and bq.m.

Start by entering bf. After that, use bf2. Script bf2 already has settings necessary to observe a coherent behavior. They are: $F=0.3$; $C=2$; $H=1$; $gin=1$; $gr=0.8$; $g=1$; $gout=gin*gr$;

However, only after a certain number of cycles (50-100), the system enters the collective mode. In terms of physics, it reaches a steady state far from equilibrium.

For **bf2**, $n=1$ to 10 is recommended. In this mode, drastic changes of direction can be observed even after one cycle.

Here is the beginning of BIRDS:

```
%SCRIPT bf

%INITIAL PARAMETERS.

nf=0; b=0; q=0; gg=0; gin=0; gout=0;g=0;q=0; w=0;

SUM=0; s=0; ss=0; S=0; nf=0; gr=0;

%INPUT; CAN BE CHANGED MANUALLY IN THE SCRIPT,

% BUT IT IS BETTER TO USE SCRIPT bf2 FOR THAT.

n=5; d=16; F=0.3; C=2;H=1; gin=1; gr=0.8; g=1;gout=gin*gr;

etc. ....
```

Script **bf2** is the part of **bf** that starts with the line:

```
%START. SCRIPT bf2 STARTS FROM HERE.
```

An example of several consecutive outputs is shown in Figure 10.1.3.

In terms of Ising model, BIRDS is a lattice with 32 values of “spin” number. The nodes tend to coordinate their “spins,” preserve the previous position, but lose its memory due to thermal relaxation. Competition takes place between the values of “spin,” the selection ratio is 32:1.

In terms of collective human behavior, the model approximately corresponds to a group of students in an auditorium choosing among a set of actions and trying to accommodate the actions of neighbors. There are many other similar interpretations in the area of collective behavior.

The social topology in the Internet Age is an intriguing topic. The connector is by no means a full graph, as enthusiasts of Internet expected. Its typical subgraph is, probably, a star with many rays.

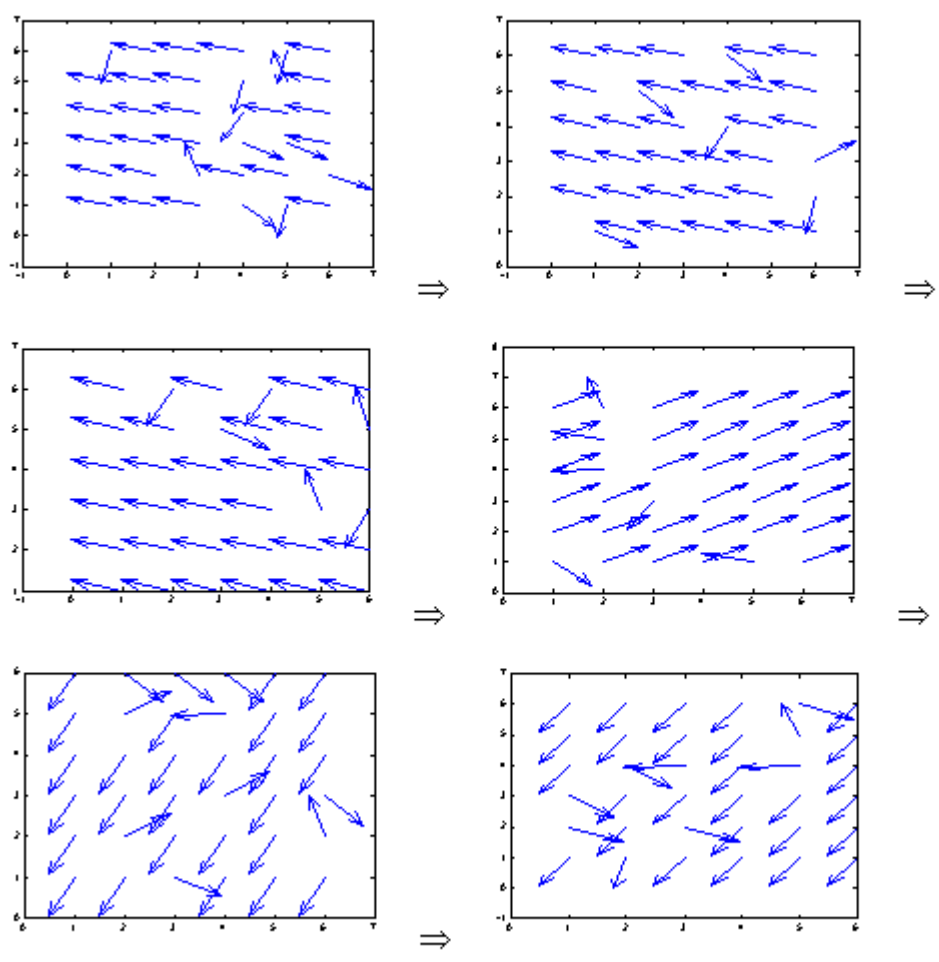


Figure 10.1.3 Examples of output of BIRDS

The program size does not depend on the size of configuration space. The model consists of two layers of different complexity. One has the local complexity of arrays and the other has the global complexity of the parameters. The devil here is not in the details of the arrays, which are updated by the program, but in global parameters, which require input and can be numerous, generating a combinatorial complexity of their own. Nevertheless, their number never comes even close to the size of the generator space.

10.2 PROTO

Let us try to apply the idea of BIRDS to the competition of mental patterns (“thoughts”) for an unspecified limited resource, which we call, following Poincaré and Damasio, **the spotlight of consciousness**. It is just a name of a model that, as any model, should not be understood too literally unless it looks persuasive to a specialist closely familiar with the real world.

The following simple but scalable system, called PROTO, simulates some aspects of selection on a connector representing an area of knowledge.

PROTO calculates the probability of a generator to win the competition for the next selection. This time, unlike BIRDS, we have only one winner for the entire generator space.

To remind, in a scale of sets, each configuration or pattern is represented by a single generator. This is why the difference in terminology between generators and configurations does not really matter. At the same time, the difference between the up or down direction of bonds, important in [1], is important in PROTO.

The connector here mimics a radial lattice of Bethe type, also known as Cayley tree, Figure 10.2.1.

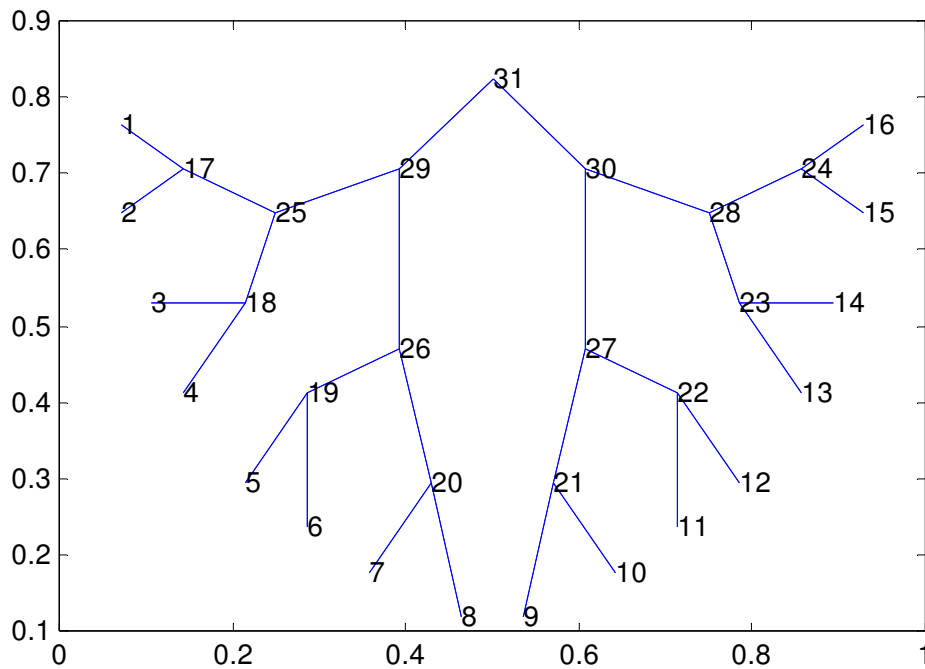


Figure 10.2.1 Connector of PROTO

The topology of the connector graph with 31 nodes can be seen as a subscale of sets built on the base of 16 elements. It can be partially interpreted, for example, as:

1. Cat	4. Tiger	25. Animal
2. Dog	17. Pet	29. Living form
3. Lion	18. Wild feline	31. Material object

The connector can be made much more complicated, for example, nodes 1, 3, 4, and 18 can all be connected to an additional node **feline** (25A), connected also to node 25, Figure 10.2.2. The connector does not need to be regular and the Cayley tree can be somewhat disheveled.

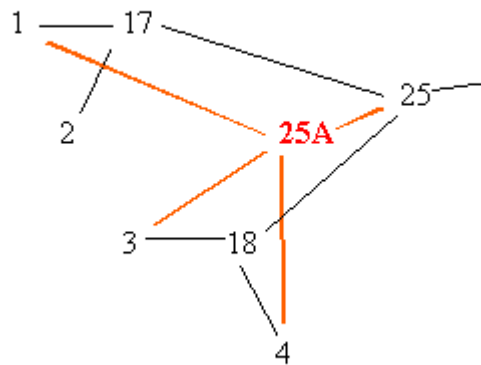


Figure 10.2.2 Node 25A, **feline** is added to the connector in Figure 11.2.1

PROTO calculates probability P_i of selecting generator G_i ($i = 1, 2, \dots, 31$) at time $t+1$. The generators are selected at random, according to their probability distribution.

We attribute the following properties to the generators in PROTO:

1. The longer the generator is in the spotlight of consciousness, the longer it will stay there, by making, so to say, its own copies in time.
2. The longer the generator stays in the spotlight, the shorter time it will stay there because of forgetting.
3. The neighbors in the connector graph positively influence the generator.

The question how a generator can sense the probability of a neighbor will be left here without an answer, but with mentioning the wave function in quantum physics as a very distant metaphor.

Calculation starts with the distribution of probabilities at time t . PROTO remembers only the previous probability distribution and is a typical Markov process in an Ar-system. .

The following equation describes the behavior of PROTO:

$$P_i^{t+1} = A P_i^t - F M_i + \sum_{i \neq j} P_j^t g_{ij} \quad (10.2.1)$$

$M_i = P_i^t$, except for the generator selected at time t , for which $P_i^t = C$, but $P_i^{t+1} = 0$.

This is not a necessary modification of the basic Eigen's equation. It is done in order to exclude the earlier selected generator (*acton*) from the next selection and prevent the stagnant repetitive selection. It simulates the phase of rest after the excitation of the neuron and keeps the ball of excitation in the air. Another complication, for the sake of experiment, is that the neighboring generators accept acton's probability as $C \cdot H$, but in acton's own memory, the past probability is written as C , similarly to how it was done in BIRDS. To simplify the picture, $A=1$ everywhere.

On this basis, the probability distribution for the next selection is calculated. The absolute values of parameters do not matter because the distribution is always normalized.

The model uses parameters:

F, forgetting; **C**, memory of an acton right after selection; **H**, factor of perception of acton's probability by neighbors, and **g**, factor of influence, which for the tree connector can be split into **gup** and **gdown**, depending on the direction on the tree.

Parameters **gup** and **gdown** are designed in such a way that the arity of the node is taken to account. The experimenter can play with them, too.

At a certain combination of parameters, the system can freeze around some nodes, slowly drift over its phase space, retaining its compactness, scatter over large areas, or it can jump between distant areas, imitating a spontaneous hypothesis about some new properties of the world. This link between distant nodes is a precondition of creativity.

PROTO spontaneously scans not just generators, but also their bond couples. The phase trajectory of the system, i.e., the sequence of actons, can be obtained as output.

Simply speaking, the more we think about the subject, the more we tend to think about it next moment, but the more we think about it, the more we get tired of it and tend to jump to something else (and this is exactly what various asides in this paper illustrate). These simple principles, as well as the influence of close neighbors, as Manfred Eigen demonstrated, describe “natural” selection of structures built of atom-like objects.

It is important to bear in mind that we do not use here any knowledge about the nature of neural processes in the brain. A neuro-physiologist would say “firing” instead of selection, but we carefully avoid any physiological interpretation. Nevertheless, neurophysiology in an oblique way influences some aspects of the model. The “naturalness” of the model lies in the most general principles of competition and selection in living systems, but not in its details.

The same principles define the Lotka-Volterra systems. The more hares today, the more tomorrow. The more hares today, the less tomorrow because the lynx will multiply. Such “games of life” over many millennia shaped new species, creating new genetic knowledge.

The MATLAB program PROTO requires workspace PROTO.mat, is stored as scripts proto (main), proto1, and proto2, and generates a figure of the tree with red asterisks meaning acts of selection (actons).

The output of the system, depending on the number of iterations n , is a **population** of actons of size n over a segment of time $t=n$. To visualize the population, the positions of the asterisks symbolizing consecutive actons are slightly randomized. The green asterisk indicates the starting node. The starting node can be externally enforced in the beginning or at any moment during an experiment. In principle, two or more actons could be enforced, in a Pavlovian mode.

To activate the program, save workspace (matrices P, T, and GXY) and the scripts. The main program offers a choice of starting from equal probability distribution (proto1) or continuing

from the previous workspace, parameters, and probability distribution (proto2). The starting program can prompt for:

n, number of steps (selections),

a, initial acton, from 1 to 31,

C, memory of previous selection as acton; stored in the memory of the acton,

H, factor for probability of the acton, as neighbors see it: $P_a = C * H$.

F, factor of forgetting; if set to a value >1 , it corresponds to Eigen's $A > 1$.

The following parameters are preset, but can be changed:

gup=0.5, parameter of influence upon neighbors (toward the root of the tree), and

w=2, **gdown**=w*gup.

Prompts can be blocked or activated in the PARAMETERS SECTION of the script.

The parameters can be changed by entering at any point between the executions. The initial settings are:

$H=0.7$; $F=0.9$; $C=1$; $gup=0.5$; $w=2$; $a=2$; $t=0.1$

Entering `tra`, after the program stops, gives the sequence of actons. Matrix PP (31,2) is the probability distribution, normally not displayed.

To test the program, load the workspace, type `proto` and set the rest of parameters equal to one (which is not quite realistic).

The program includes pause **t** after each selection, in the end of the code. Parameter **t** is set to 0.1 sec.

Large **C** and **F** make the walk conservative and restricted to small areas. High **H**, **gup**, and **gdown** increase ergodicity.

If some parameters should be kept constant in order to minimize input, the necessary modification can be easily entered into the code.

The basic matrix P (32 x 11) in the code has a spare column 10 for modified experiments. It has a spare row 32 with zeros. The connector graph is coded with matrix T (31 x 31). The coordinates

of the nodes are stored in matrix GXY. Number 32 is used instead of 0 to signify the absence of a neighbor, in order to avoid a problem with zero coordinate of a matrix element. Row 32 stores zeros.

A hypothesis silently incorporated in this model draws a parallel between the action of a catalyst in chemistry and the match-making properties of nodes. It states that two generators that are close to a third one are close to each other even if they are not coupled. For example, if in a certain knowledge representation CAT is close to PET, and DOG is close to PET, CAT and DOG are closer to each other than if there was no such triangulation. On the contrary, CAT and GRASS are not in the same neighborhood. Yet, if in our representation MOUSE is in the GRASS and CAT is in the GRASS, we expect a HUNT, i.e., a link between CAT and MOUSE. Regardless of that, MOUSE, CAT, and HUNT form a stable cluster in yet another or the same representation.

The following examples illustrate the behavior of PROTO.

PROTO was run at: $a=2$, $n=50$, $F=0.8$, $H=0.2$, $C=2$, $gup=0.5$, $w=2$ (therefore, $gdown=2*0.5=1$). The results are shown in Figure 10.2.3, where two populations of “thoughts” can be seen.

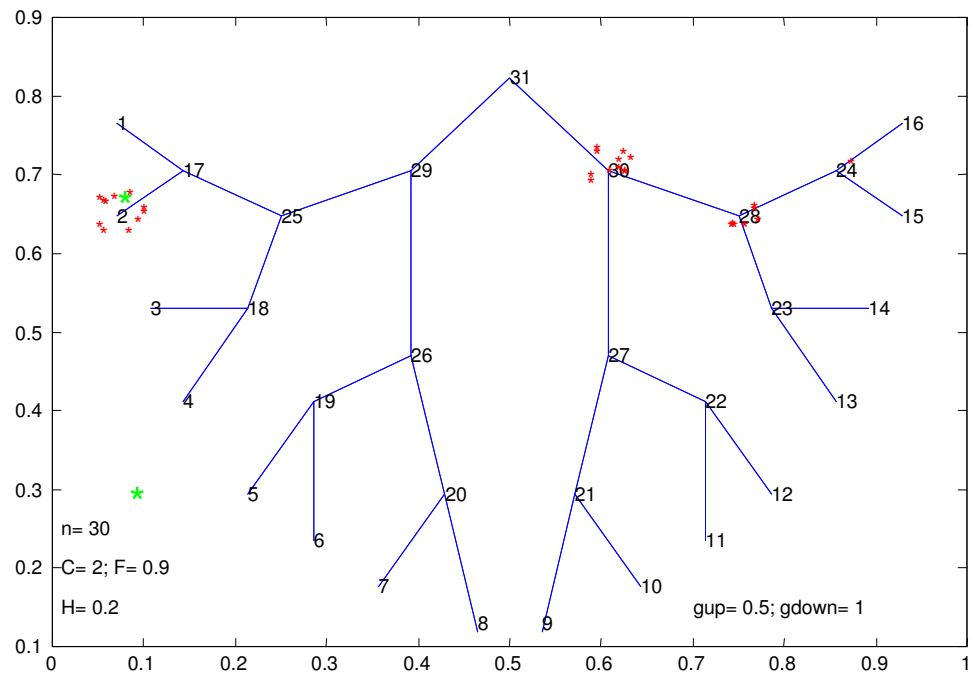


Figure 10.2.3 Two populations of “thoughts’ in PROTO , 30 cycles

The trajectory of the system was (after initial acton 2):

tra = 30 → 28 2 30 2 30 28 2 28 2 30 2 30 28 30 →
 28 30 2 30 2 28 30 2 30 2 28 24 2 30 → 2

After adding 60 more cycles (total of 90), no new populations appeared, Figure 10.2.4 .
 The system was too conservative because of high C and low H.

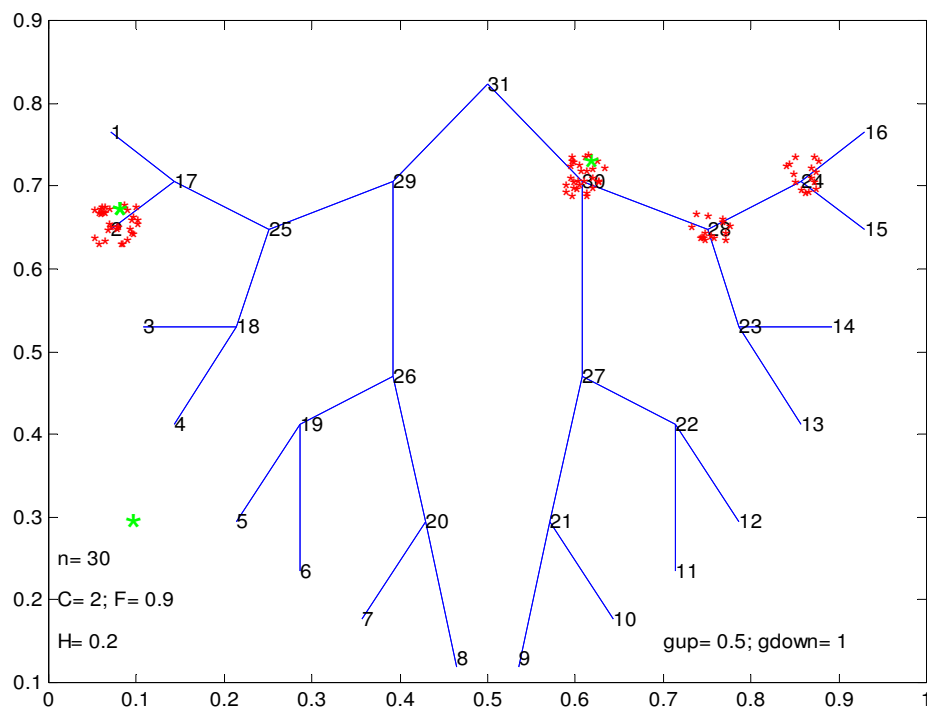


Figure 10.2.4 Two populations of “thoughts” in PROTO; 90 cycles

Next, in the CONTINUE mode, the parameters were changed to: $C = 0.5$, $H = 0.5$, $F = 0.5$. Figure 10.2.5 shows the immediate scattering of one of the populations. After 120 cycles, however, PROTO still remembers its original acton 2, but keeps exploring its second area of the connector.

Trajectory: tra = 30 → 2 28 24 2 28 2 21 23 2 21 2 27 22 27 →
 21 22 27 2 22 2 27 2 21 22 24 23 22 2 → 21

Finally, Figure 10.2.6 illustrates two populations formed at a different, less relaxed set of parameters: $n=30$, $a=2$, $F=0.8$, $C=1$, $H=0.5$.

Trajectory: tra = 8 2 18 27 2 27 2 27 2 27 2 27 2 27 18 2
 22 2 22 18 22 2 22 18 2 22 2 18 22 18

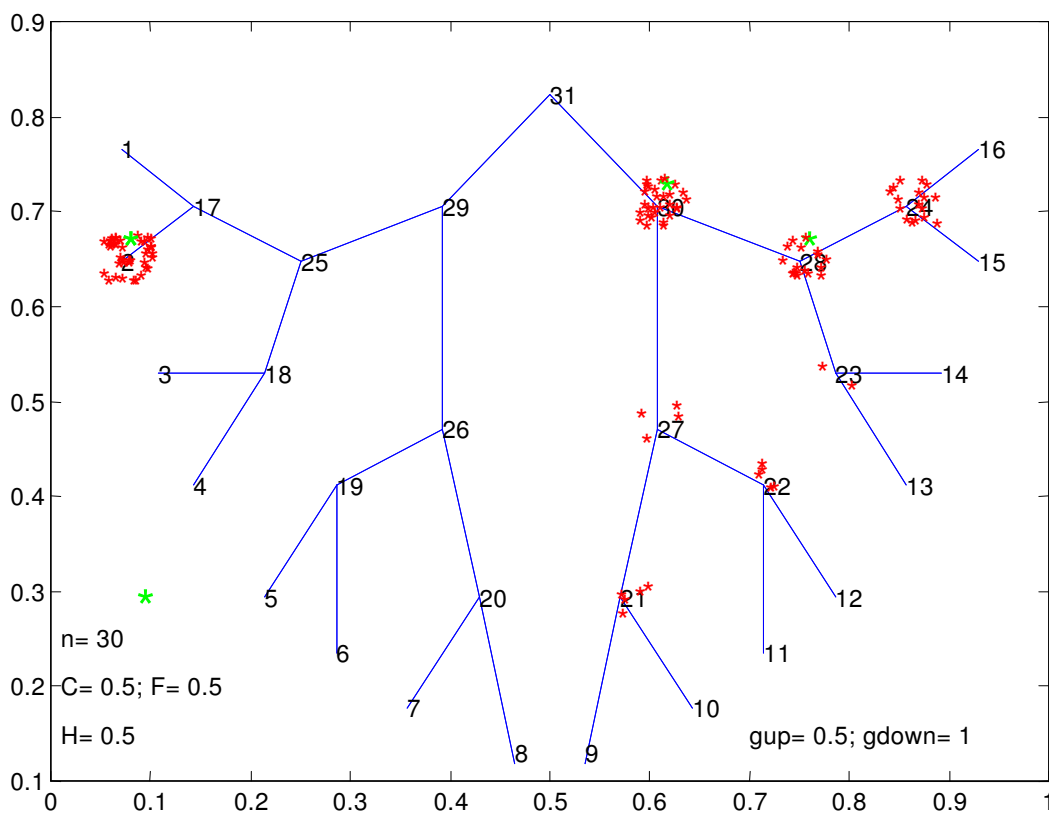


Figure 10.2.5 Two populations of “thoughts” in PROTO; relaxed parameters, 30 new cycles

In this series, node 8 was the initial acton (after 2), but the populations there did not put roots. The bridge 17—25 between nodes 2 and 18 remains, so to speak, subconscious.

The absence of limits imposed by percolation, i.e., possibility of jumps over the connector, seems to be the most striking property of the model. The jumps between distant nodes can be regarded as an evidence of dynamic memory or, in terms of the science of complexity, emergent behavior. **PROTO remembers its initial acton for a long time, although it is not stored anywhere explicitly.**

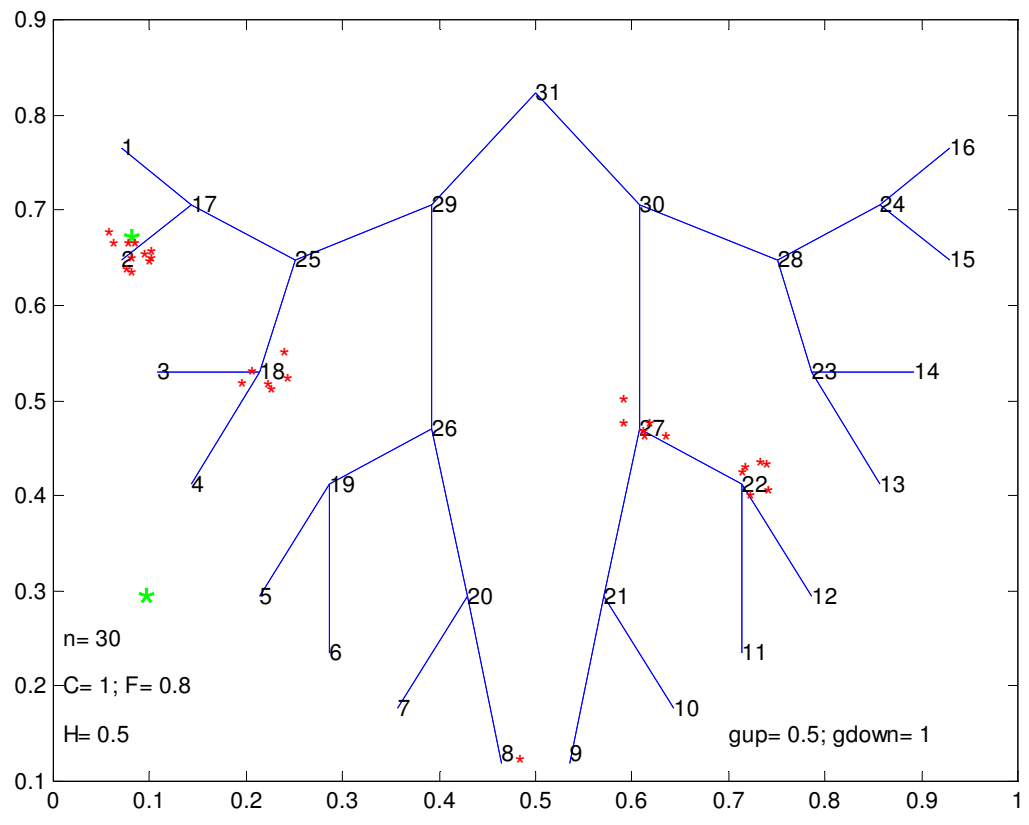


Figure 10.2.6 Three populations of “thoughts” after 30 cycles

There is the famous problem of the origin of elephant's trunk: when it is small, it is of no use, when it is large, it cannot be explained by small mutations. Of course, there is Rudyard Kipling's explanation, but it is quite a stretch. The jumps in PROTO suggest that if the genome is organized as the scale of sets, then mutations can happen in such a way that the whole block of phenotype changes.

Discussion

After many experiments, which would take too much space to report here, a conclusion could be drawn that the system manifests a rather rich behavior, depending on parameters. Even though the experimental generator space was small, the continuous multidimensional **parameter** space was large. An unexpected problem (probably, common for all virtual models) was the temptation to explore this primitive model and to play with it, instead of building a more complex and realistic one. Before the expansion could be done, some preliminary observations may be of interest.

Even if we do not know what exactly consciousness is, we can tentatively answer what the subconscious is. We select in PROTO only the most probable candidate for the focus of consciousness, but we can compile a list of runner-ups, as in a beauty contest, with decreasing probability. Technically, we can do it by casting a random number over the distribution of probability remaining after the previous selection, collapsing the winning probability segment to zero and starting a new selection. Those subconscious levels of thinking form the subconscious bulk of the mental iceberg. They may or may not influence our thinking, which normally is mostly conscious, but not quite, and we do not even know to what extent because, by definition, we cannot see beyond the focus of consciousness.

We shall also attempt to answer the question why we need consciousness at all and what its biological role is.

In short, why are we able to describe something observable (a grazing horse) and convey it? We are able—involuntarily, because of the design of our mind where only one or two thoughts can come to consciousness at a time—to separate the thoughts *horse* and *graze* as consecutive thoughts and, therefore, separate and express as consecutive terms of the sentence. The same is even more true about describing complex and extended in time events. Since the content of consciousness is ordered in time, it is ordered in speech. Consciousness makes the parsing of reality possible. It is a condition for an analytical mind.

One could see a deep analogy with the mechanism of ribosomal synthesis of a peptide over the RNA script. The ribosome selects one nucleotide triplet at a time, being “unconscious” about the rest. Of course, there is not much entropy in following the 1D Ariadne’s thread.

Language is a social phenomenon, understanding of an utterance is expected, and wherever we have communication between two animals or people about an external object, we may suspect a form of consciousness. A bird’s song or a lion’s roar communicate, probably, only the internal states of the animals, as a cell phone communicates a low battery or end of charging, but a warning shriek of a monkey seeing a predator seems to indicate consciousness and language.

Consciousness spontaneously scans the content of the mind, converting it into a linear sequence of states. As we suggested earlier, the fact of understanding is confirmed by the act of the communication of the result of understanding to somebody else. **Consciousness, therefore, is a more technical than mystical term.** The geese that saved Rome manifested their patriotic consciousness in their warning cries.

Spontaneous thinking, in chemical terms, is an autocatalytic process, like life itself. The mathematics and physics of such processes were explored in detail by Ilya Prigogine, Manfred Eigen, and others, especially, around the Santa Fe Institute of Complexity. Order (new knowledge) is created in such systems because of the inflow of Gibbs energy and dissipation of most of it as heat. The difference is retained as order. In our model, the forgetting embodies the loss in the form of dissipation, and novelty creates new order. The conflict between the old and the new creates information.

The next step of development of this model should be formation and extinction of bonds and nodes as result of **spontaneous** activity, in other words, generation of new knowledge by pure invention and mental game—not acquisition, because there would be no external source. It could go through stressed transition states created by an imposed problem.

Our modest model alone does not justify the above far-reaching conclusions, hypotheses, and mere fantasies, but it may point to a rewarding direction of “artificial natural” intelligence. Following this idea, we may stumble at a definition of consciousness, for example, but we are

not forbidden to look for its abstract foundations even without knowing what exactly it means as a chemical and physical phenomenon.

In our model, no homunculus is required. The algorithm of natural selection is all we need. The system behaves as a non-linear cellular automaton. It is not a learning neural network because it gives no functional output. To see how a useful function could be built on the platform of spontaneous activity is our future task.

Even if we design a humanoid utterly clever, we may confront unforeseen consequences that would conflict with our design. We must part with our creation, giving it the last touch, as in the fresco by Michelangelo. Moreover, we should expect it to discover forbidden knowledge and to revolt against its creator, as the image of Golem suggests.

11. SCALE

Both BIRDS and PROTO are Ar-systems because their generator space and connector remain fixed. The purpose of SCALE is to simulate evolution of a He-system from zero, exploiting the property of *novelty*.

The MATLAB program SCALE builds a record of its inputs (*history*) in the form of matrix WORLD, which is a sub-scale of sets, partially ordered along time axis. Time here is the discrete Leibniz time, i.e., the ordered set of events (“... time is an order of successions,” [21], p.25). Time does not move if nothing happens.

Recall again that in the scale of sets, each configuration is also a generator. WORLD is the connector graph, the nodes of which are generators. Therefore, WORLD is a configuration. Each generator has a unique *name*, which can be a word or a number. The name is just a symbol and is extralinguistic: it is not necessarily a word or symbol of an existing language. SCALE stores the sequence of names in the order of their issue.

In the beginning of the *history* of WORLD, the generator space contains a single “empty” generator with the name ‘!’.

SCALE works in the following sequence of stages (examples of inputs are in square brackets).

1. SCALE displays:

1 to start, 2 to continue [1]

Once started by typing 1, it can be continued with the same WORLD by typing 2. Typing 1 erases the previous WORLD.

2. It asks for the number of cycles in the session by prompting:

nn [16]

3. It prompts:

enter components ['1 8 7'] or ['cat dog']

Components must be entered interspaced and as a single character string.

4. If the input cannot be found in WORLD:

This is new. Name it ['['] or ['pet']

5. If the input is a single generator and can be found in WORLD as single generator, the output is:

This is old

If the input is a set of generators, for example, 'l e o n' (spaced) the program asks:

Looks like W32: Leon

Is it new? 1/0

[0 (i.e., no)]

Output **Looks like** means that WORLD contains a permutation of the input, for example N o e l. SCALE distinguishes between 'a b c d', 'c a d b', and 'abcd'. The first two are sets of four signs, while the third is a single name, for example, the name for the first.

Suppose, we enter 'N o e l' and get the same response:

Looks like W32: Leon

Is it new? 1/0

[1 (i.e., yes)]

If so, SCALE will ask for a name, which can be entered as 'Noel.'

This feature is intended to simulate, in a simplified form, the coding of configurations, with similarity transformation PERMUTATION, as a model of more complex transformations, for example, SIZE.

When a new generator enters WORLD, it is always either new single or a new combination of old ones. The connections between members of the combination and the name are stored in the WORLD matrix, expanding the connector. Therefore, throughout the *history* of WORLD, both generator space and connector change.

The following example of a gradually created small world illustrates the variety of possible WORLDS. The WORLD (fragmentary) contains the words in English, Swedish, Russian, and Latin, Figure 11.1. The top line is the base of the scale of sets.

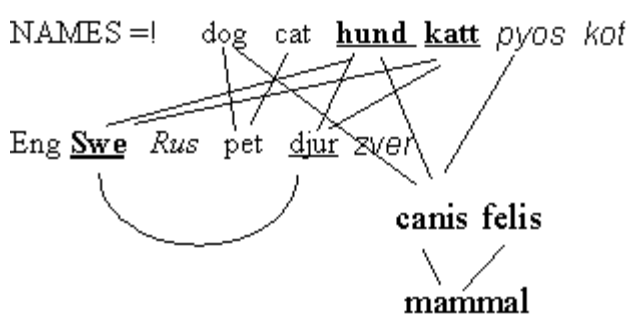


Figure 11.1 Example of a polylingual WORLD with five sub-WORLDS: four languages and biotaxonomy (incomplete).

Figure 11.2 presents a WORLD in 3D. It portrays some relationships between characters of TV sitcom *Providence*. The model was suggested by Ulf Grenander.

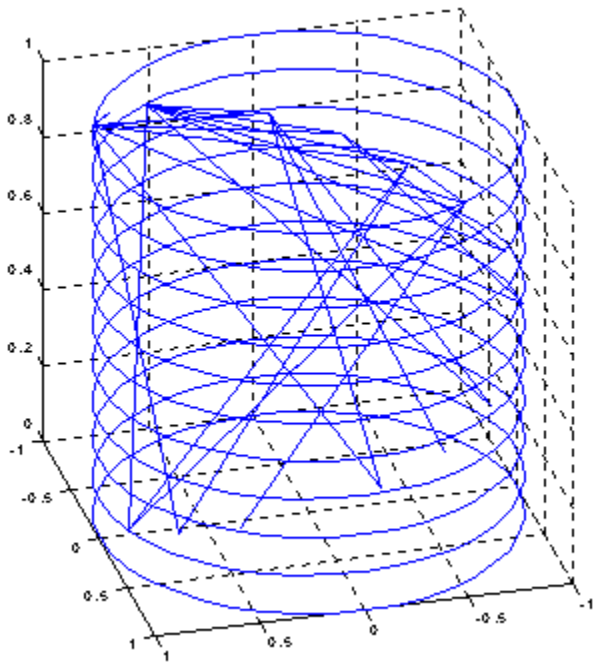


Figure 11.2 The WORLD of a TV sitcom in 3D. History runs along Z axis.

Axis Z is the *historical time*, i.e. the sequence of building the WORLD.

In figure 11.3 the same WORLD is projected on the plane of the base set.

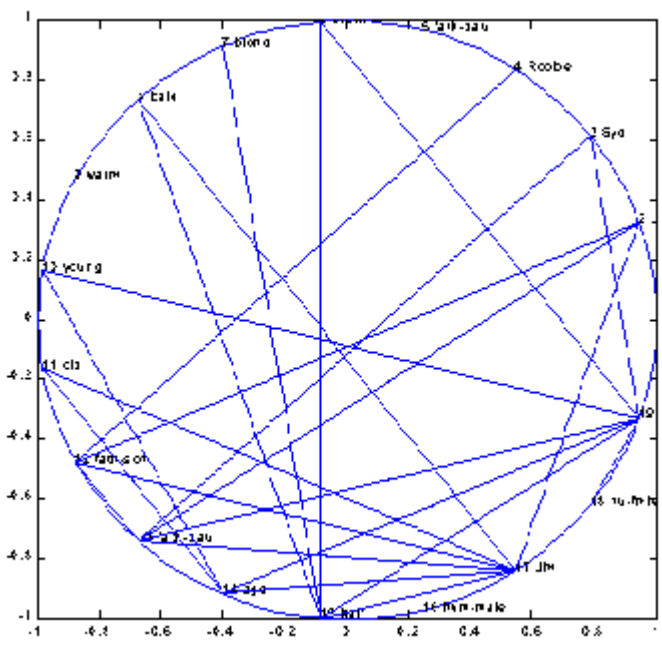


Figure 11.3 The WORLD of Figure 11.2 in 2D

SCALE does not need a teacher or instructor because the names are not essential. The main property to be recognized for the evolution of the WORLD is novelty. WORLD, therefore, reflects not only a certain artificial or natural world, but also the history of the presence of the internal WORLD in the external world. The old is recognized, while the new is remembered.

The WORLD “LINES” is built in the following way.

Nine cells of a mini-retina are numbered as in Figure 11.4. Cell 9 is the empty generator.

1	2	3
8	9	4
7	6	5

Figure 11.4 Numeration of cells in a mini-retina

The WORLD fills up first with individual cells from 1 to 9 , named from '1' to '9' and then their combinations. For example, X is a combination of / and \. The following is a slightly re-formatted actual output.

```

enter components      '1 8 7'
This is new. Name it '['
enter components      '3 4 5'
This is new. Name it ']'
enter components      '1 2 3'
This is new. Name it '~'
enter components      '7 6 5'
This is new. Name it ' _ '
enter components      '1 9 5'
This is new. Name it '\ '
etc.

```

In Figure 11.4, letters are formed out of simpler subsets of the retina.

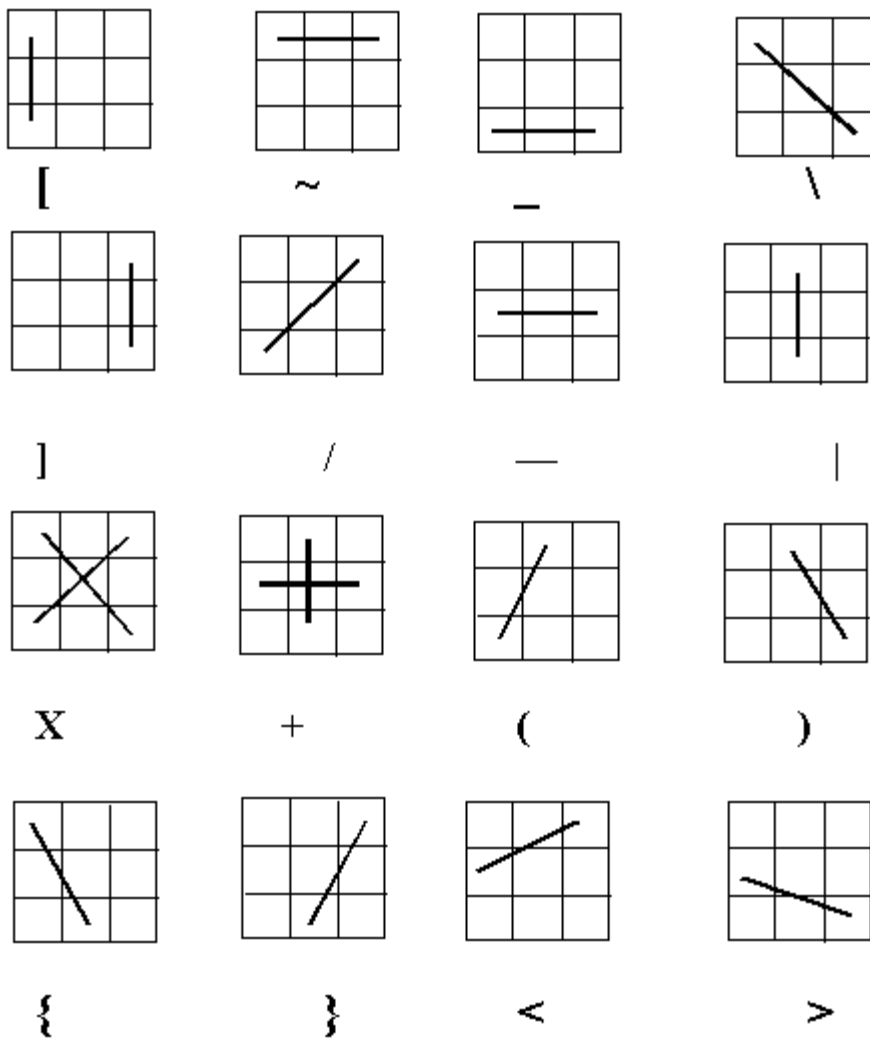


Figure 11.4 Formation and naming of retina subsets

Next, the triplets of the cells and larger retina subsets are combined and named, see Figure 11.5.

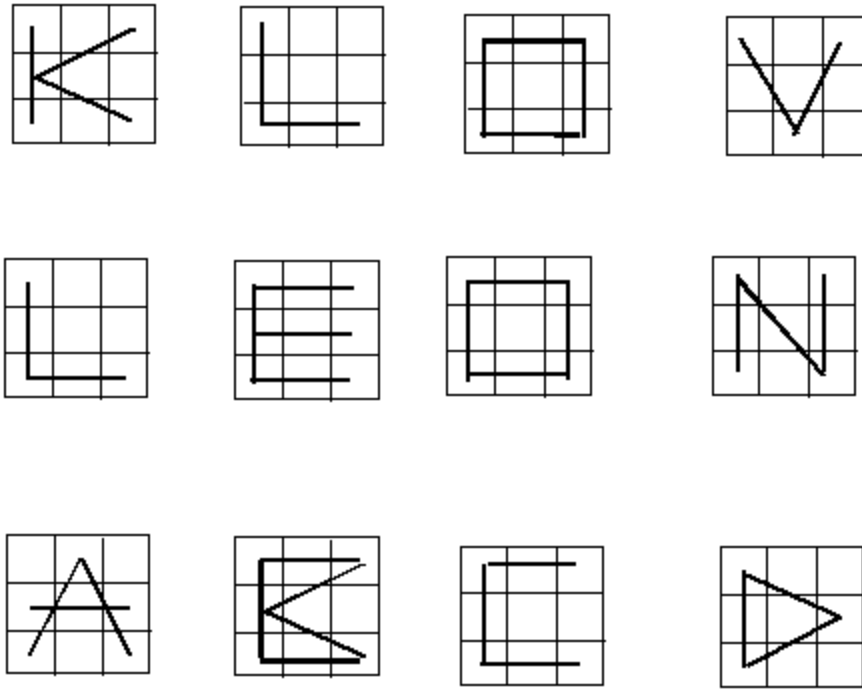


Figure 11.5 Letters formed from lines

Figure 11.6 presents two projections of the WORLD “LINES” built on the base set of nine pixels.

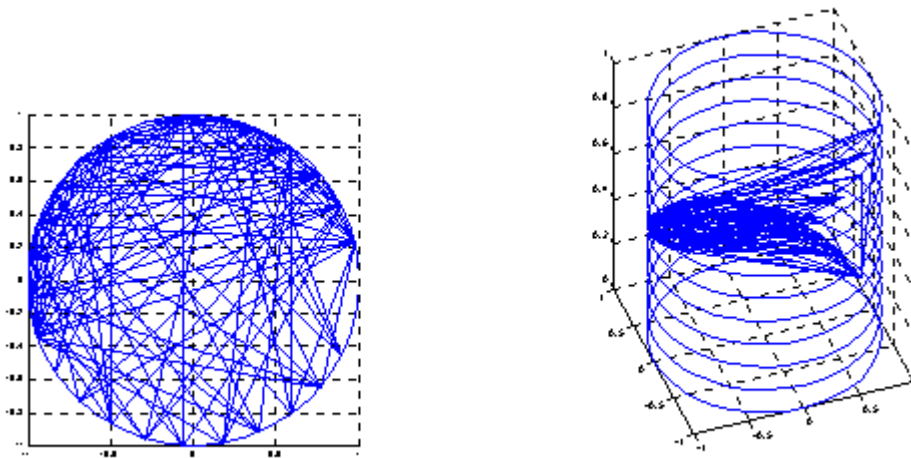


Figure 11.6 Projections of the WORLD of LINES

Figure 11.7 presents the flat and 3D projections of the WORLD of PROTO, built with SCALE, node by node from 1 to 31.

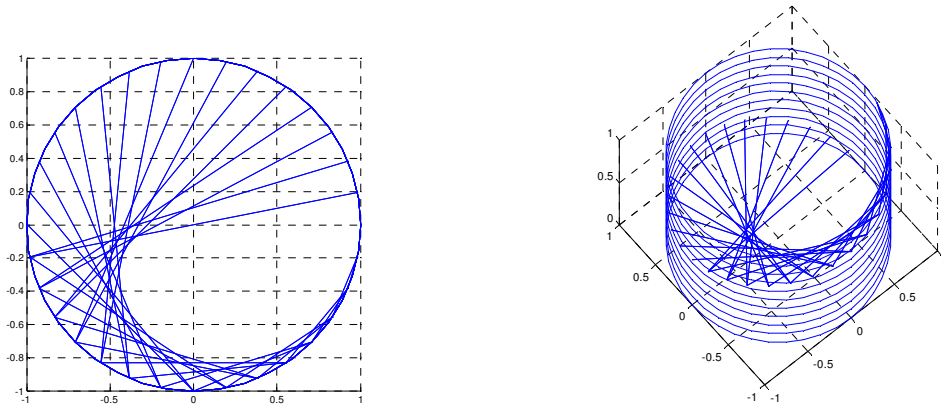


Figure 11.7 Projections of the WORLD of PROTO

SCALE has some mini-utilities:

1. If you want to check WORLD for a name, type: link
2. To see NAMES, type: NAMES (or NM)
3. To display the 3D world, type plotW

Of course, the WORLD matrix (WW) can be displayed, too, for example, as sparse matrix `sparse(WW)`.

Program LINK gives the complete *spectrum* of an old generator, listing its name and all its entries in the WORLD, i.e., downward and upward connected generators, for example:

» link

NAME to check 'x'

/ \

Also, for more complex combinations:

```

» link
NAME to check      'K'
/ E L O X [ \

```

```

» link
NAME to check      '/'
! - 3 7 < > K X [ \ ] _ | ~

```

```

» link
NAME to check      '~'
/ 1 2 3 < > E O T [ \ ] |

```

The generator space for the WORLD in figure 11.6 is

```
NAMES = ! 1 2 3 4 5 6 7 8 | - \ / [ ] ~ _ X T + E L O K < > (size 28)
```

If desired, the spectrum can be split into up and down entries, the entries of new samples of an old type can be made, but not in this program.

Evolution of a MIND where a WORLD is being built is a separate subject. In short, with time, most of the WORLD is forgotten, but part of it turns into KNOWLEDGE, i.e., a flat WORLD, as in Figure 11.6 (left), is stored in the long-term memory. Probably, the entries compete for the place in KNOWLEDGE, too. Even the bees do it.

Conclusion

The following propositions have been combined in this paper:

1. **Ulf Grenander:** Objects in the mind (“thoughts”) are configurations within the framework of Pattern Theory. This thesis, for the first time, was used by Ulf Grenander for the groundwork in building a model of the mind that does not ignore its complexity. The model demonstrates meta-chemical properties.
2. **Henri Poincare:** Objects in the mind (“thoughts”) compete for the place in consciousness.
3. **Manfred Eigen:** Darwinian competition of linear sequences in the sequence space follows formal chemical kinetics. This proposition can be generalized to configurations in the sense of PT.
4. **Chemical kinetics** is based on the concept of transition state. This proposition can be generalized to irregular configurations in the sense of PT, which closes the cycle of the four propositions at a different level and returns us to Proposition 1.
5. **Bourbaki:** A simple system can expand as the scale of sets toward unlimited complexity. From the concept of the scale of sets, the distinction between Ar- and He-complexity was suggested.

The described models are just some toys to play with while designing a mind that would connect AI with NI. Some of their meaningful properties, however, can be seen even at their embryonic stage. Thus, they do not require any sweep strategy: they are self-sweeping (or self-scanning). If realized as parallel systems of cellular automaton type, they do not require any numbering of their generators. Neither do they need to store any large arrays. In other words, they are homunculus-free. It is the same as to say that they belong to NI as much as to AI.

Further, the models can have a limited number of global parameters and an unlimited number of simple local nodes. Notably, the size of SCALE, as the size of human brain, does not depend on the size of the world it stores, perceives, and processes, while the world expands. This means, most important, that they are contractible in the sense of homotopy theory: the large system can be reduced to zero volume without any change in the algorithm. Conversely, a small system can be expanded as a homotopy. Even more important, the expansion due to the interaction with environment can occur, up to a point, in an autonomous way, as self-learning based on the distinction between the old and the new.

Homunculus wears two hats in AI: as internal operator and external teacher. The models in this paper avoid homunculus by making the core of the program so simple that it can be entrusted for execution to a single cell in a cellular automaton in the most general sense.

This treatise, inclusive of such subjects as AI and chemistry, as well as vacuum cleaners and bees, seems to deal with different worlds. World is a useful axiomatic concept that cannot be defined. A tentative classification of worlds can be suggested:

<u>Real</u>	<u>RW</u>
natural	RNW
artificial	RAW

<u>Virtual</u>	<u>VW</u>
real	VRW
unreal	UVW

The virtual real world is a simulation based on observable principles, for example, for scientific purposes, while the virtual unreal world, for example, a simulated transformation of a man into a vampire, is based on arbitrary or highly hypothetical principles.

Stephen Spielberg's film *Artificial Intelligence*, unlike such films as *Lord of the Ring*, tries to preserve realism of the laws of nature, given the basic premise of the plot. Both brilliantly told tales, regardless of their message, illustrate the difference between real and unreal virtual worlds. At the same time, both preserve realistic patterns of human behavior and attitudes.

The borderlines between the worlds are not strictly defined and a theory of worlds regarding the above distinctions could be an independent subject. The imaginary world of sci fi and political prophesies, as, for example, those concerning the gloom future of earth environment and Nazism before it came to power, and are often self-fulfilling. Of course, for each such prophesy there is the opposite, later forgotten.

Human beings have been constantly pushed by modern medicine into RAW, which long ago was populated only by stone tools and pottery.

The balance between the global loss and growth of the real world, quickly shrinking in its biological and ethnographic sectors while growing in the technological ones, as well as of the virtual variety of ideas and attitudes, can be an intriguing subject of applied mathematics. Eigen's kinetics might well be applicable to the real world in its entirety. Rivers struggle for existence, too.

The next steps in moving along the pathways sparsely marked in this paper could be:

1. The WORLD where generators compete for presence, while fading due to forgetting boosted by the lack of retrieval, and being revitalized due to subsequent referrals. This presumes a contact with environment. The process of the transformation of the world as history (Figure 12.2) into the world as knowledge (Figure 11.3) is of particular interest.

2. Simulation of the environment that imposes its own order on the spontaneous activity of the mind. This was attempted with PROTO by forced activation of generators and, of course, had the expected effect.

3. Creation of autonomic agents that may have a preset perception systems (vision, hearing), but are self-learning in the sense that they build their internal WORLDS without a teacher, through distinction between new and old. For example, a baby Roomba can be created, which explores the environment and creates its WORLD before going into the stage of maturity where success and failure are reinforced and discouraged, accordingly, by “good girl!” and “stop it!”

A preset (inborn) system of perception for vision, for example, could use various similarity transformations on two-dimensional lattices. PT provides an ideal theoretic apparatus for that. This could generate extralingual **pattern** outputs, such as, for example, named for convenience in English “line,” “L-shape,” “human face,” “grass,” etc., ready for entering the WORLD where PERMUTATION is, most probably, the only feasible transformation. There is no physical movement in the brain comparable with the powerful transformations of the eye movements.

4. Transition from extralingual WORLD to language, which is, probably, just a reversed SCALE: not from inputs to the world but from WORLD to linguistic outputs. Ulf Grenander’s model offers well-tilled soil for that.

5. Fine chemistry of thoughts that follows the mechanism of transition from regular thoughts to new regular thoughts through an irregular transition state.

Pattern kinetics and **pattern history** seem to be other directions worth exploring. Author and Ulf Grenander have made some steps toward pattern theory of history in their unpublished

manuscript *History as Points and Lines*, from which Figures 5.3 and 5.4 were reproduced. Some rich food for pattern thought can be found in the new book by Bertrand Roehner and Tony Syme *Pattern and Repertoire in History* [22]. *The Sociology of Philosophies: A Global Theory of Intellectual Change* by Randall Collins [23] is a striking intellectual adventure in the pattern spirit where the competition of ideas is in the focus. Even the title of the first chapter, “*Coalitions in the Mind*,” gives the taste of the whole, the chapter starting with:

Intellectuals are people who produce decontextualized ideas. These ideas are meant to be true or significant apart from any locality, and apart from anyone concretely putting them into practice. A mathematical formula claims to be true in and of itself, whether or not it is useful, and apart from whoever believes it.

Randall Collins [23], p.20

Another proposition, expressed by the author and Ulf Grenander in *History as Points and Lines* states that the apparatus of the Internet, for the first time in history, opens the possibility to actually measure the state of the real world close to the real time, its position on the “globescape,” and to follow its transition states. Similar idea was expressed in another highly relevant and fundamental book by Bertrand Roehner, *Patterns of Speculation*, [24], p. xv. Of course, the same can be done on any sub-world, such as economics or even arts. The latter offers a rich array of irregularities and transient modes.

Relatively recently, a large number of spectacular computer-generated images ranging from configurations reflecting the Internet topology and traffic [25] to the configurations of gift exchange among the !Khung San tribes in Botswana and Namibia [26] have been posted on the Web. The accumulation of such images with quantitative measures of generators and bond couples can be regarded as a beginning of visualization of global and local states of large systems. From a different perspective, it is a visualization of “global thoughts.” The measures are expressed simply by the thickness of the bond couples and the size of generator symbols, as the importance of an event has been always expressed by the size of the headlines in the newspapers and the time given to coverage on TV.

Chemical knowledge at any particular moment is an Ar-system, for which history is irrelevant. It represents part of the real world of molecular structures known today. As a creation in human mind, however, chemistry has a history coded by references in chemical literature, as well as in CAS registry. No philosophic position is required to appreciate this fact because both chemistry and its history are **observable** objects. The collective human mind builds both systems, day by day. Chemistry here is just an example, and AI or football can be substituted for it.

Much later than her other big sister sciences, chemistry has come to self-awareness as an intellectual undertaking with a paradigm of its own, irreducible to physics. An evidence of that can be found in [27], where many aspects of the chemical vision of the world, including the autonomous character of chemical thinking, “iconic” (pictorial) nature of chemical language, similarity, and complexity are discussed by eminent chemists. Some even half-rhetorically suggest that modern science would look differently if chemistry, instead of physics, attempted to create a general picture of the world.

Traveling back to the small but dense world of ancient AI, we may discover there a richness of vision lost today among the vast expanses.

ACKNOWLEDGEMENT: Author is deeply indebted to Ulf Grenander for generous support, encouragement, and criticism, as well as for great lessons of pattern thinking, MATLAB virtuosity, and intellectual independence.

The short MATLAB codes are available from the author at yuri@ids.net.

REFERENCES

1. Source: Ulf Grenander, <http://www.dam.brown.edu/ptg/REPORTS/mind.pdf>
2. Ulf Grenander, *General Pattern Theory: a Mathematical Study of Regular Structures*. Oxford: Clarendon Press, 1993
3. Ulf Grenander, *Elements of Pattern Theory*. Baltimore: Johns Hopkins University Press, 1996.
4. Ulf Grenander, *Lectures in Pattern Theory*. Vols 1-3. Berlin: Springer-Verlag, 1976-1981.
5. Christoph Adami, *Introduction to Artificial Life*, Berlin: Springer-Verlag, 1988.

Some Alife web sites:

<http://www.alcyone.com/max/links/alife.html>

<http://www.lalena.com/ai/>

<http://www.alife.org>

6. Source on Roomba: <http://www.hammacher.com/publish/66632.asp>
7. Sources on Grey Walter: www.csulb.edu/~wmartinz/rssc/newsletters/may99.pdf
www.soc.uiuc.edu/faculty/pickerin/tortoises.pdf.
8. Carl G. Looney , *Pattern Recognition Using Neural Networks*, New York: Oxford University Press, 1997, p.221.
9. CAS substance counter: <http://www.cas.org/cgi-bin/regreport.pl>

CAS site: <http://www.cas.org/substance.html>.

10. Nicolas Bourbaki, *Elements of Mathematics: Theory of Sets*, Addison-Wesley, originally published by Hermann (Paris), 1968.
11. John C. Kotz, and Paul Treichel, Jr., *Chemistry and Chemical Reactivity*, Saunders College Publishing, 1999, p. 396
12. W. Ross Ashby, *Design for a Brain: The Origin of Adaptive Behavior*, 2nd Ed., New York: Wiley, 1960 (originally, 1952).
13. W. Ross Ashby, *An Introduction to Cybernetics*, London: Chapman & Hall, 1956/1964.

(A short gracious bio: <http://www.issis.org/lumashby.htm>)
14. Leon Festinger, *A Theory of Cognitive Dissonance*, Stanford: Stanford University Press, 1962.
15. Source: <http://www.soc.uiuc.edu/faculty/pickerin/tortoises.pdf>
16. Eigen M. Eigen, Selforganization of Matter and the Evolution of Biological Macromolecules, *Die Naturwissenschaften*, **58**, 465-522 (1971).
17. M. Eigen, The Hypercycle, *ibid*, 64, 541-565 (1977), 65, 7-1 (1987).

Also published as separate book: Manfred Eigen and Peter Schuster, *The Hypercycle - A Principle of Natural Self-Organization*, Berlin: Springer-Verlag, 1979.
18. Source: http://www.kaytat.com/lyrics/lets_do_it.html
19. H. Poincare, *The Foundations of Science*, Lancaster, PA: The Science Press, 1946, p. 393.
20. Antonio Damasio, *The Feeling of What Happens: Body and Emotions in the Making of Consciousness*, NY, San Diego, London: Harcourt, Brace, & Company, 1999.

21. H. D. Alexander, Ed., *Leibniz-Clarke Correspondence*, Manchester University Press, 1956, p.25. Last reprinted in 1998.
 22. Bertrand M. Roehner, Tony Syme, *Patterns and Repertoire in History*, Cambridge, MA, London, England: Harvard University Press, 2002.
 23. Randall Collins, *The Sociology of Philosophies: A Global Theory of Intellectual Change*. Cambridge, Mass.: Belknap Press, 1998.
 24. Bertrand Roehner, *Patterns of Speculation*, Cambridge: Cambridge University Press, 2002.
 25. Martin Dodge, *CyberGeography site*: <http://www.cybergeography.org/atlas/topology.html>
 26. Lothar Krempel, *Gallery of Social Structures*: <http://www.mpi-fg-koeln.mpg.de/~lk/netvis/>
 27. *Of Minds and Molecules: New Philosophical Perspectives on Chemistry*, Nalini Bhushan and Stuart Rosenfeld, Editors, Oxford, NY, etc.: Oxford University Press, 2000.
-